

Full wwPDB X-ray Structure Validation Report (i)

Feb 19, 2024 – 06:38 PM EST

PDB ID : 4KTQ Title : BINARY COMPLEX OF THE LARGE FRAGMENT OF DNA POLY-MERASE I FROM T. AQUATICUS BOUND TO A PRIMER/TEMPLATE DNA Authors : Li, Y.; Waksman, G. Deposited on : 1998-09-09

Resolution : 2.50 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 (i)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.50 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	$\begin{array}{c} {\rm Whole \ archive} \\ (\#{\rm Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	$5231 \ (2.50-2.50)$
Sidechain outliers	138945	5233 (2.50-2.50)

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%

Note EDS was not executed.

Mol	Chain	Length		Quality of chain		
1	В	12	33%	67%		_
2	С	13	38%	62%		
3	А	539	30%	56%	14%	•



$4 \mathrm{KTQ}$

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 4769 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 DNA (5'-D(*GP*AP*CP*CP*AP*CP*GP*GP*CP*GP*CP*GP*CP*GP))-3').

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace			
1	В	12	Total 240	C 114	N 48	O 67	Р 11	0	0	0

• Molecule 2 is a DNA chain called DNA (5'-D(*GP*GP*GP*CP*GP*CP*GP*TP*GP* GP*TP*C)-3').

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
2	С	13	Total 267	C 126	N 51	O 78	Р 12	0	0	0

• Molecule 3 is a protein called PROTEIN (LARGE FRAGMENT OF DNA POLYMERASE I).

Mol	Chain	Residues		Atoms			ZeroOcc	AltConf	Trace	
3	А	539	Total 4159	C 2652	N 740	0 754	S 13	0	0	0

• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	В	8	Total O 8 8	0	0
4	С	11	Total O 11 11	0	0
4	А	84	Total O 84 84	0	0



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. 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. 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.

Note EDS was not executed.

• Molecule 1: DNA (5'-D(*GP*AP*CP*CP*AP*CP*GP*GP*CP*GP*CP*(DOC))-3')

Chain B:		33%	67%	
G101 A102 C103 C104 A105 C106 G107	6108 C111 C112			
• Molecu	le 2: DNA	A (5'-D(*GP*GP*	GP*CP*GP*CP*CP	*GP*TP*GP*GP*TP*C)-3')
Chain C:		38%	62%	
G204 G205 G206 C210 G211 G211 T212	6213 6214 7215 C216			
• Molecu	le 3: PRC	DTEIN (LARGE F	FRAGMENT OF DN	A POLYMERASE I)
Chain A:	3	30%	56%	14% •
L294 A297 P298 W299 P300	F306 V307 G308 F309 V310 L311 S312	R313 R314 R314 R315 R315 R316 M316 M316 M316 M316 L322 L322 L322 L322 L322 L322	H333 H335 R336 R336 R336 R336 R336 R336 R336 R	1347 1347 1348 1349 1350 1350 1355 1355 1355 1355 1355 1355
L367 P368 D371 D371 P372 P373 M374	L375 L376 A377 A377 L379 L380 D381	P382 3383 3384 17386 73884 7388 8389 8389 8389 8389 8393 7393 7393	E397 W3998 W3998 E400 E401 E401 A405 A405 A406 A406 E412 E412 F412	L416 L416 W417 E418 E421 E420 E423 E423 E423 E425 L426 L426 L426 L426 L426 L426 L428 L428 L428 E431 Y430 E433
V433 E434 R435 P436 L437 S438 S438	L441 M444 T447 G448 V449	R450 [451 [451 [452 [453 [455 [455 [455 [461 [461 [461 [461	E465 E466 E466 1467 A468 E473 F474 F475 R476 A477 A477 A477 A479 G479 F480 F481	N483 1.484 N485 8485 8486 8486 8486 8486 8486 8486 8486 8487 8486 8486 8487 9489 1499 8491 8492 1493 1494 8496
K505 T506 E507 K508 (510 K511	R512 S513 S513 S515 S515 V518 L519	E520 A521 L522 R523 E524 A525 H525 H527 1528 V531 K531	L533 Q554 Y555 F535 F535 F535 T539 T539 K540 L541 L541 L549 F550 P551	L552 L553 H554 H565 H567 G568 R565 R565 R565 R565 R563 R563 R563 R563
G572 R573 L574 S575 S576 S576 S577 D578	P579 N580 L581 Q582 N583 I584 P585	V586 T588 T588 T588 T589 L590 G591 G591 G591 R593 R595 R595 R595 R597	1599 A600 E601 E602 G603 G603 U605 L605 L606 L606 L609 D610 D610 B612 S612 G613	1614 1615 1615 1615 1616 1617 1619 1624 1623 1623 1628 1628 1628 1628 1628 1628 1628 1628
F632 (1533 E634 (1535 (1535 R636 R635 D637 D637 T638	H639 T640 E641 T642 W645 M646	F647 F647 F647 F650 F655 F655 L657 K659 K659	T664 1665 N666 F667 F667 F667 V669 V669 V670 Y671 K677 L678 K677 L678 S674 S673	q680 B681 L683 A683 A683 P685 F684 F686 E684 E688 E694 F695 F695 F695 F695 F695 F695 F695



K831 M765 F7 00 K765 V766 M704 F769 K704 F700 F776 K771 K704 F776 K774 K704 F776 K774 K704 F776 K774 K704 F776 K774 K704 K774 K774 K704 K779 K774 K716 K779 K774 K714 K779 K714 K714 K779 K714 K714 K779 K714 K714 K785 K794 K714 K786 K794 K726 K794 K726 K726 K794 K726 K744 K794 K726 K746 K794 K746 K746 K804 K746 K746 K804 K746 K746 K804 K746 K746 K804 K746 K746



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants	110.84Å 110.84 Å 90.84 Å	Deperitor
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 - 2.50	Depositor
% Data completeness	91.8 (30.00-2.50)	Depositor
(in resolution range)	51.8 (50.00-2.50)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.227 , 0.298	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4769	wwPDB-VP
Average B, all atoms $(Å^2)$	51.0	wwPDB-VP



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: DOC

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	Mol Chain		lengths	Bond angles		
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	В	0.47	0/249	0.73	0/382	
2	С	0.53	0/299	0.83	0/461	
3	А	0.36	0/4249	0.58	0/5776	
All	All	0.38	0/4797	0.61	0/6619	

There are no bond length outliers.

There are no bond angle outliers.

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	В	240	0	134	12	0
2	С	267	0	147	17	0
3	А	4159	0	4117	385	0
4	А	84	0	0	8	0
4	В	8	0	0	1	0
4	С	11	0	0	1	0
All	All	4769	0	4398	397	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 44.



• · · · ·		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
3:A:351:LEU:HD23	3:A:374:MET:HG2	1.34	1.06
3:A:780:LEU:HD11	3:A:790:GLU:HG3	1.40	1.02
3:A:614:ILE:HD11	3:A:760:LEU:HD12	1.49	0.95
3:A:779:MET:HA	3:A:789:LEU:HD12	1.50	0.93
3:A:677:ARG:HH12	3:A:746:ARG:HH12	1.17	0.91
2:C:212:DT:H2"	2:C:213:DG:H5'	1.54	0.87
3:A:769:PHE:O	3:A:772:LEU:HB2	1.77	0.85
2:C:204:DG:H2"	2:C:205:DG:OP2	1.76	0.85
3:A:569:THR:HG22	3:A:572:GLY:H	1.41	0.84
3:A:574:LEU:HD12	3:A:782:GLN:NE2	1.92	0.84
3:A:713:GLU:CB	3:A:717:ARG:HH21	1.93	0.81
3:A:730:VAL:HG11	3:A:748:ALA:HB2	1.61	0.80
1:B:106:DC:OP1	3:A:508:LYS:HG2	1.83	0.79
3:A:639:HIS:ND1	3:A:663:LYS:HE3	1.98	0.77
3:A:569:THR:HG21	3:A:573:ARG:H	1.49	0.77
3:A:351:LEU:HG	3:A:373:PRO:HG2	1.66	0.76
3:A:562:THR:HG23	3:A:579:PRO:O	1.86	0.76
3:A:768:LEU:HD11	3:A:803:ALA:HA	1.68	0.76
3:A:677:ARG:HH12	3:A:746:ARG:NH1	1.83	0.76
3:A:669:VAL:HG21	3:A:696:TYR:CE2	2.19	0.76
3:A:526:HIS:ND1	3:A:527:PRO:HD2	2.02	0.75
3:A:474:VAL:HG21	3:A:484:LEU:HD11	1.67	0.75
3:A:576:SER:HG	3:A:580:ASN:HA	1.53	0.74
3:A:737:VAL:HB	3:A:740:VAL:HG13	1.69	0.73
3:A:315:GLU:HB3	4:A:3047:HOH:O	1.88	0.73
3:A:655:ASP:HB3	3:A:658:MET:SD	2.29	0.73
3:A:562:THR:HG22	3:A:563:ARG:N	2.05	0.72
3:A:576:SER:OG	3:A:580:ASN:HA	1.90	0.71
3:A:769:PHE:HD1	3:A:772:LEU:HD12	1.55	0.71
3:A:698:GLN:HG2	4:A:3060:HOH:O	1.89	0.71
3:A:584:ILE:HB	3:A:595:ARG:HH21	1.55	0.71
3:A:682:LEU:HD22	3:A:683:ALA:H	1.56	0.70
3:A:299:TRP:CZ2	3:A:341:ALA:HB1	2.27	0.69
3:A:523:ARG:HG3	3:A:523:ARG:HH11	1.57	0.69
3:A:809:GLY:O	3:A:812:PRO:HD3	1.93	0.69
3:A:621:HIS:ND1	3:A:813:LEU:HB3	2.08	0.68
3:A:779:MET:HG3	3:A:789:LEU:HD11	1.74	0.68
2:C:204:DG:H5"	3:A:677:ARG:NE	2.09	0.68
3:A:813:LEU:C	3:A:815:VAL:H	1.97	0.67
3:A:482:PHE:HE2	3:A:490:LEU:HD12	1.58	0.67

All (397) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.



Interatomic Clash					
Atom-1	Atom-2	distance (Å)	overlap (Å)		
3:A:557:THR:OG1	3:A:561:HIS:HE1	1.75	0.67		
3:A:549:LEU:HD22	3:A:560:LEU:HD11	1.75	0.67		
3:A:569:THR:HG21	3:A:573:ARG:N	2.10	0.67		
3:A:629:ILE:HG13	3:A:630:ARG:N	2.10	0.66		
3:A:569:THR:HG21	3:A:573:ARG:HB2	1.76	0.66		
3:A:682:LEU:HD22	3:A:683:ALA:N	2.11	0.66		
3:A:489:GLN:O	3:A:493:VAL:HG23	1.96	0.66		
3:A:408:LEU:O	3:A:412:LEU:HG	1.96	0.66		
3:A:309:PHE:CD2	3:A:356:LEU:HD13	2.32	0.65		
3:A:684:ILE:HD12	3:A:689:ALA:HB2	1.79	0.65		
3:A:383:SER:O	3:A:385:THR:HG23	1.95	0.65		
3:A:562:THR:HG22	3:A:563:ARG:H	1.59	0.65		
3:A:773:GLU:C	3:A:775:MET:H	2.00	0.65		
3:A:591:GLY:HA2	3:A:594:ILE:HD12	1.79	0.65		
3:A:780:LEU:HD11	3:A:790:GLU:CG	2.23	0.64		
3:A:807:MET:O	3:A:810:VAL:HG12	1.97	0.64		
3:A:756:THR:HA	3:A:759:ASP:OD2	1.97	0.64		
3:A:359:LEU:HA	3:A:362:ARG:HG2	1.80	0.64		
3:A:575:SER:HA	3:A:582:GLN:HE22	1.63	0.64		
3:A:493:VAL:O	3:A:498:LEU:HG	1.97	0.64		
3:A:314:LYS:HG3	3:A:315:GLU:OE1	1.98	0.63		
3:A:490:LEU:HD23	3:A:494:LEU:HD11	1.81	0.63		
3:A:337:GLU:HB3	4:A:3001:HOH:O	1.98	0.63		
3:A:822:GLY:HA3	3:A:830:ALA:O	1.99	0.63		
3:A:306:PHE:O	3:A:406:ALA:HB1	1.99	0.63		
3:A:647:PHE:CZ	3:A:658:MET:HG2	2.33	0.63		
3:A:762:LYS:O	3:A:766:VAL:HG23	1.98	0.62		
3:A:386:THR:HB	3:A:387:PRO:HD2	1.82	0.62		
3:A:490:LEU:CD2	3:A:494:LEU:HD11	2.30	0.62		
3:A:682:LEU:CD1	3:A:684:ILE:HG12	2.30	0.61		
3:A:655:ASP:HB3	3:A:658:MET:HB2	1.83	0.61		
3:A:449:VAL:HG12	3:A:560:LEU:HB2	1.81	0.61		
3:A:375:LEU:HD23	3:A:430:TYR:CE1	2.36	0.61		
3:A:523:ARG:HG3	3:A:523:ARG:NH1	2.15	0.61		
3:A:506:THR:O	3:A:510:GLY:HA2	2.00	0.61		
3:A:588:THR:O	3:A:592:GLN:HG3	2.00	0.61		
3:A:450:ARG:HG2	3:A:599:ILE:HG13	1.83	0.60		
3:A:787:LEU:HD12	3:A:807:MET:HE3	1.83	0.60		
3:A:665:ILE:HG21	3:A:696:TYR:CD1	2.36	0.60		
3:A:829:SER:C	3:A:831:LYS:H	2.04	0.60		
3:A:418:GLY:O	3:A:421:GLU:HG3	2.02	0.60		



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
3:A:602:GLU:HA	4:A:3066:HOH:O	2.00	0.60
3:A:310:VAL:HA	3:A:405:ARG:NH1	2.17	0.60
3:A:342:LEU:HA	3:A:345:LEU:HD11	1.84	0.59
3:A:423:GLU:C	3:A:427:LEU:HD12	2.22	0.59
3:A:665:ILE:O	3:A:669:VAL:HG23	2.02	0.59
3:A:451:LEU:HD12	3:A:597:ALA:O	2.01	0.59
3:A:309:PHE:CZ	3:A:356:LEU:HB2	2.37	0.59
3:A:450:ARG:HD3	3:A:601:GLU:HA	1.84	0.59
3:A:607:VAL:HG12	3:A:609:LEU:HD11	1.85	0.59
3:A:627:ASN:O	3:A:631:VAL:HG23	2.04	0.58
3:A:375:LEU:HD21	3:A:434:GLU:HB3	1.85	0.58
3:A:386:THR:HB	3:A:388:GLU:OE1	2.04	0.58
3:A:679:SER:HA	3:A:684:ILE:HG13	1.84	0.58
3:A:779:MET:HG3	3:A:789:LEU:CD1	2.33	0.58
3:A:583:ASN:C	3:A:583:ASN:HD22	2.05	0.58
3:A:388:GLU:HG3	3:A:398:TRP:HD1	1.69	0.58
3:A:721:GLU:HA	3:A:726:ARG:O	2.04	0.58
3:A:315:GLU:HA	3:A:563:ARG:HD2	1.86	0.58
3:A:398:TRP:CZ3	3:A:405:ARG:HG2	2.39	0.57
3:A:429:LEU:HD21	3:A:724:PHE:CB	2.34	0.57
3:A:310:VAL:HA	3:A:405:ARG:HH12	1.68	0.57
3:A:714:GLY:O	3:A:718:GLY:N	2.34	0.57
3:A:697:PHE:HE1	3:A:703:VAL:HG12	1.69	0.56
3:A:482:PHE:CE2	3:A:490:LEU:HD12	2.39	0.56
3:A:574:LEU:HD12	3:A:782:GLN:HE22	1.71	0.56
3:A:765:MET:SD	3:A:782:GLN:HG3	2.45	0.56
2:C:204:DG:H5"	3:A:677:ARG:HE	1.70	0.56
3:A:393:ARG:HG2	3:A:394:TYR:CE2	2.41	0.56
3:A:601:GLU:O	3:A:604:TRP:HB2	2.04	0.56
1:B:112:DOC:O2	3:A:573:ARG:NH2	2.39	0.56
3:A:346:LYS:O	3:A:368:PRO:HD2	2.06	0.56
3:A:677:ARG:O	3:A:681:GLU:HB2	2.05	0.56
3:A:636:ARG:HB3	3:A:641:GLU:CD	2.26	0.55
3:A:518:VAL:O	3:A:521:ALA:HB3	2.06	0.55
3:A:580:ASN:OD1	3:A:582:GLN:HB2	2.06	0.55
3:A:563:ARG:O	3:A:576:SER:HA	2.06	0.55
3:A:435:ARG:N	3:A:436:PRO:HD2	2.22	0.55
3:A:453:VAL:HG12	3:A:454:ALA:N	2.21	0.54
3:A:473:GLU:O	3:A:477:LEU:HD12	2.08	0.54
3:A:595:ARG:HH11	3:A:832:GLU:HG3	1.72	0.54
3:A:390:VAL:O	3:A:394:TYR:HD2	1.89	0.54



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
3:A:391:ALA:C	3:A:393:ARG:H	2.11	0.54
3:A:768:LEU:HD23	3:A:779:MET:CE	2.38	0.54
3:A:742:GLU:HA	3:A:745:GLU:HG3	1.89	0.54
3:A:449:VAL:CG1	3:A:560:LEU:HB2	2.38	0.54
3:A:361:LEU:HA	3:A:365:LEU:O	2.07	0.54
3:A:417:TRP:HB3	4:A:3088:HOH:O	2.07	0.54
3:A:562:THR:HA	3:A:579:PRO:HD2	1.89	0.54
3:A:613:GLN:O	3:A:617:ARG:HG3	2.08	0.54
3:A:813:LEU:O	3:A:815:VAL:N	2.41	0.54
3:A:474:VAL:HG23	3:A:475:PHE:N	2.23	0.54
3:A:461:LEU:O	3:A:465:GLU:HG3	2.08	0.53
3:A:492:ARG:O	3:A:496:ASP:HB2	2.08	0.53
3:A:813:LEU:C	3:A:815:VAL:N	2.61	0.53
3:A:505:LYS:HA	3:A:511:LYS:O	2.09	0.53
3:A:318:TRP:CH2	3:A:554:HIS:HA	2.43	0.53
1:B:104:DC:H42	2:C:213:DG:H1	1.56	0.53
3:A:569:THR:HB	3:A:573:ARG:O	2.08	0.53
3:A:646:MET:SD	3:A:696:TYR:HB2	2.48	0.53
3:A:675:ALA:HB1	3:A:689:ALA:CB	2.38	0.53
3:A:324:LEU:HB2	3:A:338:PRO:HB3	1.90	0.53
3:A:349:ARG:HG2	3:A:371:ASP:HB2	1.91	0.53
3:A:761:MET:HE3	3:A:761:MET:HA	1.90	0.53
3:A:682:LEU:HD13	3:A:684:ILE:HG12	1.90	0.53
3:A:343:ARG:HE	3:A:365:LEU:HD21	1.74	0.53
3:A:494:LEU:O	3:A:498:LEU:HB2	2.09	0.53
3:A:562:THR:OG1	3:A:581:LEU:HG	2.08	0.53
3:A:323:ALA:HA	3:A:338:PRO:HG3	1.90	0.52
3:A:339:TYR:O	3:A:343:ARG:NH1	2.42	0.52
3:A:589:PRO:O	3:A:593:ARG:HG3	2.09	0.52
3:A:423:GLU:O	3:A:427:LEU:HD12	2.09	0.52
3:A:610:ASP:OD1	3:A:786:GLU:HB2	2.09	0.52
3:A:429:LEU:HD21	3:A:724:PHE:HB3	1.90	0.52
3:A:549:LEU:HD22	3:A:560:LEU:CD1	2.39	0.52
3:A:324:LEU:HG	3:A:342:LEU:HD23	1.91	0.52
3:A:313:ARG:HG3	3:A:315:GLU:OE1	2.10	0.51
3:A:321:LEU:HD11	3:A:342:LEU:HD21	1.92	0.51
3:A:450:ARG:HB3	3:A:599:ILE:O	2.10	0.51
3:A:679:SER:HB3	3:A:684:ILE:O	2.11	0.51
3:A:802:LEU:O	3:A:806:VAL:HG23	2.10	0.51
3:A:340:LYS:O	3:A:343:ARG:HB2	2.10	0.51
3:A:576:SER:H	3:A:582:GLN:NE2	2.08	0.51



	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)
3:A:360:ALA:HB2	3:A:367:LEU:HD23	1.93	0.51
3:A:371:ASP:OD2	3:A:413:PHE:CZ	2.64	0.51
3:A:616:LEU:O	3:A:619:LEU:HB3	2.11	0.51
2:C:204:DG:C5'	3:A:677:ARG:NE	2.73	0.51
3:A:428:TRP:O	3:A:432:GLU:HB2	2.11	0.51
3:A:678:LEU:HD23	3:A:684:ILE:HD11	1.91	0.51
3:A:763:LEU:HB3	3:A:810:VAL:HG21	1.93	0.51
1:B:102:DA:H5"	4:B:3079:HOH:O	2.10	0.51
3:A:299:TRP:CE2	3:A:341:ALA:HB1	2.46	0.51
3:A:768:LEU:CD1	3:A:803:ALA:HA	2.38	0.51
3:A:683:ALA:O	3:A:684:ILE:HG23	2.11	0.51
3:A:720:VAL:O	3:A:727:ARG:HA	2.11	0.51
3:A:751:MET:SD	3:A:751:MET:C	2.89	0.51
3:A:350:GLY:O	3:A:353:ALA:HB2	2.11	0.51
3:A:664:THR:O	3:A:668:GLY:N 2.44		0.51
3:A:375:LEU:HD21	3:A:434:GLU:C	2.31	0.50
2:C:212:DT:H2"	2:C:213:DG:C5'	2.32	0.50
3:A:335:ALA:HB1	3:A:341:ALA:HB2	1.92	0.50
3:A:606:LEU:O	3:A:823:ILE:HA	2.12	0.50
1:B:107:DG:OP2	3:A:508:LYS:HB2	2.12	0.50
3:A:309:PHE:HA	3:A:402:ALA:HB1	1.93	0.50
3:A:373:PRO:O	3:A:376:LEU:N	2.44	0.50
3:A:633:GLN:C	3:A:635:GLY:H	2.13	0.50
3:A:682:LEU:HD12	3:A:684:ILE:HG12	1.93	0.50
3:A:351:LEU:HA	3:A:372:ASP:OD2	2.12	0.50
3:A:466:GLU:HG3	3:A:538:LEU:HD21	1.92	0.50
1:B:107:DG:P	3:A:508:LYS:HB2	2.51	0.50
3:A:593:ARG:O	3:A:596:ARG:HB2	2.11	0.50
3:A:625:ASP:OD1	3:A:700:PHE:HA	2.12	0.50
3:A:312:SER:HA	3:A:322:LEU:HD11	1.93	0.50
3:A:530:GLU:O	3:A:533:LEU:HB2	2.12	0.49
3:A:773:GLU:C	3:A:775:MET:N	2.66	0.49
3:A:342:LEU:HA	3:A:345:LEU:CD1	2.43	0.49
3:A:562:THR:CG2	3:A:563:ARG:H	2.25	0.49
3:A:310:VAL:HG21	3:A:400:GLU:O	2.12	0.49
3:A:339:TYR:O	3:A:342:LEU:HB2	2.13	0.49
3:A:360:ALA:CB	3:A:367:LEU:HD23	2.42	0.49
3:A:317:MET:HE1	3:A:362:ARG:HB3	1.94	0.49
3:A:739:SER:HB3	4:A:3006:HOH:O	2.11	0.49
3:A:804:LYS:O	3:A:808:GLU:HG3	2.12	0.49
3:A:340:LYS:O	3:A:343:ARG:HD2	2.13	0.49



	A L C	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
3:A:626:GLU:HA	3:A:629:ILE:HG12	1.93	0.49
3:A:309:PHE:N	3:A:309:PHE:CD1	2.81	0.49
3:A:487:ARG:NH2	3:A:512:ARG:O	2.44	0.49
2:C:212:DT:C4	2:C:213:DG:C6	3.01	0.48
4:C:3012:HOH:O	3:A:677:ARG:NH1	2.46	0.48
3:A:317:MET:HG3	3:A:561:HIS:HB3	1.95	0.48
3:A:386:THR:O	3:A:390:VAL:HG23	2.12	0.48
3:A:829:SER:C	3:A:831:LYS:N	2.65	0.48
3:A:375:LEU:CG	3:A:434:GLU:HB3	2.42	0.48
3:A:448:GLY:O	3:A:559:ARG:NH1	2.46	0.48
3:A:436:PRO:HB2	3:A:766:VAL:CG1	2.44	0.48
3:A:467:ILE:HG22	3:A:468:ALA:N	2.26	0.48
3:A:615:GLU:HG2	3:A:753:VAL:O	2.13	0.48
3:A:563:ARG:HD3	3:A:578:ASP:OD1	2.14	0.48
3:A:768:LEU:C	3:A:770:PRO:HD2	2.34	0.48
3:A:495:PHE:O	3:A:498:LEU:O	2.32	0.48
3:A:609:LEU:HG	3:A:821:VAL:HG13	1.96	0.48
3:A:309:PHE:CE2	3:A:356:LEU:HB2	2.49	0.48
3:A:343:ARG:HH21	3:A:365:LEU:HD21	1.78	0.48
3:A:600:ALA:HB2	3:A:606:LEU:HG	1.95	0.48
3:A:576:SER:N	3:A:582:GLN:NE2	2.62	0.47
2:C:212:DT:H4'	3:A:486:SER:HA	1.97	0.47
2:C:215:DT:H6	2:C:215:DT:H5'	1.79	0.47
3:A:375:LEU:CD2	3:A:434:GLU:HB3	2.43	0.47
3:A:552:LEU:HD13	3:A:579:PRO:HB3	1.96	0.47
3:A:513:SER:OG	3:A:515:SER:HB3	2.14	0.47
3:A:636:ARG:NH1	3:A:636:ARG:HA	2.29	0.47
3:A:768:LEU:HD23	3:A:779:MET:HE2	1.95	0.47
2:C:211:DG:H2'	2:C:212:DT:H72	1.96	0.47
3:A:535:TYR:CE2	3:A:539:THR:HG21	2.49	0.47
1:B:111:DC:O4'	3:A:583:ASN:HA	2.15	0.47
3:A:647:PHE:CE1	3:A:658:MET:HG2	2.50	0.47
3:A:778:ARG:HD2	3:A:790:GLU:OE1	2.15	0.47
3:A:412:LEU:O	3:A:416:LEU:HB2	2.15	0.47
3:A:436:PRO:HB2	3:A:766:VAL:HG13	1.97	0.47
2:C:204:DG:H5"	3:A:677:ARG:CZ	2.44	0.47
3:A:636:ARG:HA	3:A:636:ARG:CZ	2.45	0.47
2:C:206:DG:OP1	3:A:728:ARG:NH2	2.43	0.46
3:A:541:LEU:HD23	3:A:590:LEU:HG	1.97	0.46
3:A:769:PHE:HA	3:A:772:LEU:HB2	1.97	0.46
3:A:352:LEU:O	3:A:355:ASP:HB2	2.15	0.46



Interatomic Clash					
Atom-1	Atom-2	distance (Å)	overlap (Å)		
3:A:646:MET:SD	3:A:696:TYR:HD1	2.38	0.46		
3:A:679:SER:O	3:A:682:LEU:O	2.32	0.46		
3:A:637:ASP:OD1	3:A:659:ARG:NH2	2.49	0.46		
3:A:466:GLU:OE2	3:A:466:GLU:HA	2.16	0.46		
3:A:477:LEU:HD22	3:A:528:ILE:HB	1.96	0.46		
3:A:624:GLY:O	3:A:626:GLU:N	2.49	0.46		
3:A:736:ARG:HG3	3:A:736:ARG:HH11	1.79	0.46		
3:A:325:ALA:HB3	3:A:402:ALA:O	2.16	0.46		
3:A:374:MET:SD	3:A:390:VAL:HG21	2.56	0.46		
3:A:518:VAL:O	3:A:522:LEU:HG	2.16	0.46		
3:A:665:ILE:CG2	3:A:696:TYR:CD1	2.99	0.46		
3:A:441:LEU:O	3:A:444:MET:HB2	2.15	0.46		
3:A:478:ALA:O	3:A:480:HIS:HD2	1.98	0.46		
3:A:595:ARG:HD3	3:A:832:GLU:OE2	2.15	0.46		
3:A:313:ARG:NH2	3:A:315:GLU:OE2	2.46	0.46		
3:A:388:GLU:HG3	3:A:398:TRP:CD1	2.48	0.46		
3:A:420:LEU:O	3:A:427:LEU:HD11	2.16	0.46		
3:A:455:TYR:O	3:A:458:ALA:N	2.50	0.46		
3:A:571:THR:HG21	3:A:754:GLN:NE2	2.31	0.46		
3:A:324:LEU:HD22	3:A:325:ALA:H	1.81	0.45		
3:A:512:ARG:HE	3:A:512:ARG:HB2	1.60	0.45		
3:A:378:TYR:HB2	3:A:567:THR:HB	1.97	0.45		
3:A:567:THR:O	3:A:567:THR:OG1	2.32	0.45		
3:A:753:VAL:O	3:A:753:VAL:HG23	2.15	0.45		
3:A:583:ASN:C	3:A:583:ASN:ND2	2.70	0.45		
3:A:826:ASP:OD2	3:A:829:SER:HB2	2.16	0.45		
3:A:596:ARG:HA	3:A:826:ASP:OD1	2.17	0.45		
3:A:750:ASN:OD1	3:A:750:ASN:C	2.54	0.45		
3:A:299:TRP:O	3:A:300:PRO:C	2.54	0.45		
3:A:585:PRO:HB2	3:A:591:GLY:CA	2.47	0.45		
3:A:637:ASP:CG	3:A:659:ARG:HH21	2.19	0.45		
3:A:756:THR:HG22	3:A:757:ALA:N	2.31	0.45		
3:A:438:SER:HB3	3:A:566:GLN:HE22	1.81	0.45		
3:A:569:THR:HG22	3:A:572:GLY:N	2.20	0.45		
3:A:655:ASP:HA	3:A:658:MET:CE	2.47	0.45		
3:A:667:PHE:HA	3:A:670:LEU:HD12	1.98	0.45		
3:A:808:GLU:HG2	3:A:819:VAL:CG2	2.46	0.45		
3:A:808:GLU:HG2	3:A:819:VAL:HG23	1.97	0.45		
3:A:569:THR:CG2	3:A:571:THR:H	2.30	0.45		
3:A:704:ARG:O	3:A:707:ILE:HB	2.17	0.45		
3:A:749:PHE:O	3:A:752:PRO:HD2	2.17	0.45		



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
3:A:391:ALA:C	3:A:393:ARG:N	2.70	0.45
3:A:379:LEU:HB3	3:A:426:LEU:HD22	1.98	0.44
3:A:562:THR:CG2	3:A:576:SER:OG	2.66	0.44
3:A:637:ASP:HB3	3:A:640:THR:HB	1.99	0.44
3:A:447:THR:CG2	3:A:778:ARG:HD3	2.47	0.44
3:A:788:VAL:C	3:A:789:LEU:HD13	2.38	0.44
3:A:317:MET:CE	3:A:362:ARG:HB3	2.48	0.44
3:A:633:GLN:C	3:A:635:GLY:N	2.70	0.44
3:A:719:TYR:HB3	3:A:729:TYR:CD2	2.53	0.44
3:A:312:SER:O	3:A:313:ARG:HB3	2.16	0.44
3:A:703:VAL:HG12	3:A:704:ARG:N	2.32	0.44
3:A:617:ARG:O	3:A:620:ALA:HB3	2.18	0.44
3:A:740:VAL:CG2	3:A:741:ARG:N	2.80	0.44
3:A:450:ARG:HD3	3:A:601:GLU:CA	2.48	0.44
3:A:783:VAL:O	3:A:783:VAL:HG12	2.18	0.43
3:A:393:ARG:HG2	3:A:394:TYR:CD2	2.53	0.43
3:A:429:LEU:HD21	3:A:724:PHE:HB2	1.99	0.43
3:A:578:ASP:HA	3:A:579:PRO:HA	1.86	0.43
1:B:112:DOC:O5'	1:B:112:DOC:H6	2.19	0.43
3:A:526:HIS:CG	3:A:527:PRO:HD2	2.53	0.43
3:A:638:ILE:O	3:A:642:THR:HB	2.17	0.43
3:A:763:LEU:HB3	3:A:810:VAL:CG2	2.48	0.43
3:A:307:VAL:CG2	3:A:349:ARG:H	2.32	0.43
3:A:755:GLY:O	3:A:758:ALA:HB3	2.19	0.43
3:A:309:PHE:HA	3:A:402:ALA:CB	2.49	0.43
3:A:310:VAL:HG22	3:A:405:ARG:NH1	2.34	0.43
3:A:341:ALA:C	3:A:343:ARG:N	2.71	0.43
3:A:349:ARG:HE	3:A:371:ASP:HB2	1.84	0.43
3:A:324:LEU:HG	3:A:342:LEU:CD2	2.48	0.43
3:A:437:LEU:HD22	3:A:762:LYS:HD3	2.00	0.43
3:A:685:PRO:HD2	3:A:688:GLU:CB	2.49	0.43
3:A:299:TRP:HB2	3:A:336:PRO:HD3	2.01	0.43
3:A:341:ALA:C	3:A:343:ARG:H	2.21	0.43
3:A:375:LEU:HG	3:A:434:GLU:HB3	2.01	0.43
3:A:504:GLY:HA2	4:A:3018:HOH:O	2.18	0.43
3:A:637:ASP:O	3:A:640:THR:HB	2.19	0.43
3:A:313:ARG:HG2	3:A:319:ALA:HB2	2.01	0.43
3:A:323:ALA:HA	3:A:338:PRO:CG	2.49	0.42
3:A:391:ALA:O	3:A:393:ARG:N	2.52	0.42
3:A:553:ILE:O	3:A:553:ILE:HG22	2.18	0.42
3:A:595:ARG:HG2	3:A:832:GLU:OE2	2.19	0.42



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:106:DC:P	3:A:508:LYS:HG2	2.59	0.42
3:A:317:MET:CE	3:A:317:MET:HA	2.48	0.42
3:A:417:TRP:O	3:A:420:LEU:HB2	2.19	0.42
3:A:426:LEU:HD23	3:A:426:LEU:HA	1.88	0.42
3:A:519:LEU:O	3:A:522:LEU:N	2.38	0.42
3:A:611:TYR:CD1	3:A:819:VAL:HG22	2.54	0.42
3:A:622:LEU:HD12	3:A:622:LEU:HA	1.88	0.42
3:A:736:ARG:HG3	3:A:736:ARG:NH1	2.34	0.42
3:A:476:ARG:C	3:A:478:ALA:H	2.23	0.42
3:A:593:ARG:HE	3:A:593:ARG:HB3	1.58	0.42
3:A:482:PHE:HA	4:A:3055:HOH:O	2.18	0.42
3:A:746:ARG:HA	3:A:749:PHE:CE2	2.54	0.42
2:C:210:DC:H2"	2:C:211:DG:C8	2.55	0.42
3:A:324:LEU:HD22	3:A:325:ALA:N	2.35	0.42
3:A:569:THR:CG2	3:A:573:ARG:H	3:A:573:ARG:H 2.26	
3:A:381:ASP:HB3	3:A:384:ASN:ND2	2.34	0.42
3:A:441:LEU:CD1	3:A:566:GLN:HG3	2.49	0.42
3:A:541:LEU:HA	3:A:545:TYR:HD1	1.85	0.42
2:C:204:DG:C2'	2:C:205:DG:OP2	2.58	0.42
3:A:297:ALA:HB3	3:A:333:HIS:CD2	2.55	0.42
3:A:763:LEU:HD23	3:A:763:LEU:HA	1.72	0.42
3:A:549:LEU:HB2	3:A:550:PRO:HD3	2.01	0.42
3:A:569:THR:HG23	3:A:571:THR:H	1.85	0.42
3:A:637:ASP:O	3:A:640:THR:N	2.46	0.42
3:A:717:ARG:NH1	3:A:719:TYR:CE1	2.82	0.42
2:C:204:DG:C5'	3:A:677:ARG:CZ	2.98	0.42
3:A:314:LYS:O	3:A:316:PRO:HD3	2.20	0.42
3:A:450:ARG:NH1	3:A:599:ILE:CD1	2.83	0.42
3:A:493:VAL:O	3:A:497:GLU:HB2	2.20	0.42
3:A:596:ARG:HG3	3:A:828:LEU:HD23	2.02	0.42
3:A:675:ALA:HB1	3:A:689:ALA:HB1	2.01	0.41
3:A:739:SER:OG	3:A:740:VAL:N	2.51	0.41
1:B:108:DG:N2	3:A:540:LYS:NZ	2.68	0.41
3:A:433:VAL:O	3:A:436:PRO:HG2	2.20	0.41
3:A:601:GLU:OE2	3:A:604:TRP:NE1	2.53	0.41
3:A:599:ILE:HA	3:A:826:ASP:HA	2.03	0.41
3:A:631:VAL:HG13	3:A:641:GLU:HG3	2.03	0.41
3:A:674:SER:HB2	3:A:677:ARG:HG3	2.02	0.41
1:B:102:DA:H2"	1:B:103:DC:O5'	2.20	0.41
3:A:309:PHE:O	3:A:405:ARG:NH1	2.52	0.41
3:A:712:GLU:O	3:A:713:GLU:C	2.58	0.41



A + 1	A + 2	Interatomic Clash			
Atom-1	Atom-2	distance (\AA)	overlap (Å)		
3:A:479:GLY:O	3:A:480:HIS:HB3	2.19	0.41		
3:A:534:GLN:O	3:A:537:GLU:HB3	2.20	0.41		
3:A:719:TYR:HD2	3:A:729:TYR:CE2	2.39	0.41		
3:A:584:ILE:HA	3:A:585:PRO:HD2	1.83	0.41		
3:A:596:ARG:O	3:A:598:PHE:N	2.54	0.41		
3:A:678:LEU:HD23	3:A:684:ILE:CD1	2.50	0.41		
3:A:697:PHE:CD1	3:A:704:ARG:HB2	2.56	0.41		
2:C:205:DG:H22	3:A:573:ARG:HH22	1.67	0.41		
3:A:321:LEU:HD13	3:A:338:PRO:CB	2.51	0.41		
3:A:452:ASP:O	3:A:455:TYR:HB3	2.21	0.41		
3:A:604:TRP:HA	3:A:792:PRO:HA	2.02	0.41		
3:A:693:ILE:HG22	3:A:694:GLU:OE2	2.20	0.41		
3:A:636:ARG:HB2	3:A:641:GLU:HG3	2.01	0.41		
3:A:768:LEU:HD12	3:A:806:VAL:HG11	2.03	0.41		
3:A:769:PHE:C	3:A:772:LEU:HB2	2.38	0.41		
1:B:108:DG:H21	3:A:540:LYS:NZ	2.19	0.40		
3:A:822:GLY:C	3:A:823:ILE:HG13	2.41	0.40		
3:A:800:ALA:HB1	3:A:821:VAL:HG11	2.03	0.40		
3:A:474:VAL:CG2	3:A:475:PHE:N	2.83	0.40		
3:A:625:ASP:O	3:A:628:LEU:N	2.51	0.40		
3:A:655:ASP:N	3:A:656:PRO:HD3	2.36	0.40		
3:A:441:LEU:HD11	3:A:566:GLN:HG3	2.02	0.40		
3:A:455:TYR:CD2	3:A:597:ALA:HB2	2.57	0.40		
3:A:522:LEU:O	3:A:529:VAL:HG21	2.22	0.40		
3:A:828:LEU:HA	3:A:832:GLU:OE1	2.21	0.40		
3:A:430:TYR:HA	3:A:434:GLU:HB2	2.03	0.40		
3:A:585:PRO:HB2	3:A:591:GLY:HA3	2.02	0.40		
3:A:752:PRO:O	3:A:756:THR:HB	2.21	0.40		
3:A:783:VAL:O	3:A:784:HIS:HB2	2.21	0.40		

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	А	537/539~(100%)	419 (78%)	102 (19%)	16 (3%)	4 6

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	А	525	ALA
3	А	625	ASP
3	А	681	GLU
3	А	586	VAL
3	А	597	ALA
3	А	814	ALA
3	А	392	ARG
3	А	496	ASP
3	А	321	LEU
3	А	424	GLU
3	А	300	PRO
3	А	578	ASP
3	А	774	GLU
3	А	585	PRO
3	А	433	VAL
3	А	650	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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	А	412/441 (93%)	315~(76%)	97~(24%)	1 1

All (97) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	А	307	VAL
3	А	314	LYS
3	А	321	LEU
3	А	324	LEU
3	А	342	LEU



Mol	Chain	Res	Type
3	А	345	LEU
3	А	347	GLU
3	А	349	ARG
3	А	351	LEU
3	А	352	LEU
3	А	354	LYS
3	А	362	ARG
3	А	365	LEU
3	А	397	GLU
3	А	401	GLU
3	А	416	LEU
3	А	421	GLU
3	А	427	LEU
3	А	432	GLU
3	А	444	MET
3	А	460	SER
3	А	462	GLU
3	А	467	ILE
3	А	477	LEU
3	А	480	HIS
3	А	484	LEU
3	А	487	ARG
3	А	508	LYS
3	А	512	ARG
3	А	515	SER
3	А	523	ARG
3	А	526	HIS
3	А	531	LYS
3	А	541	LEU
3	А	553	ILE
3	А	563	ARG
3	A	566	GLN
3	А	576	SER
3	A	577	SER
3	А	578	ASP
3	А	583	ASN
3	А	585	PRO
3	А	588	THR
3	А	595	ARG
3	А	611	TYR
3	А	614	ILE
3	А	622	LEU



Mol	Chain Re		Type		
3	А	625	ASP		
3	А	628	LEU		
3	А	636	ARG		
3	А	642	THR		
3	А	645	TRP		
3	А	652	GLU		
3	А	655	ASP		
3	А	657	LEU		
3	А	659	ARG		
3	А	663	LYS		
3	А	665	ILE		
3	А	671	TYR		
3	А	677	ARG		
3	A	679	SER		
3	A	680	GLN		
3	А	686	TYR		
3	А	698	GLN		
3	А	699	SER		
3	А	708	GLU		
3	А	710	THR		
3	А	712	GLU		
3	А	715	ARG		
3	А	720	VAL		
3	А	721	GLU		
3	А	723	LEU		
3	А	730	VAL		
3	А	733	LEU		
3	А	736	ARG		
3	А	739	SER		
3	А	740	VAL		
3	А	746	ARG		
3	А	749	PHE		
3	А	750	ASN		
3	А	753	VAL		
3	A	761	MET		
3	A	763	LEU		
3	A	771	ARG		
3	A	773	GLU		
3	А	775	MET		
3	A	778	ARG		
3	А	781	LEU		
3	А	782	GLN		



COULL	Continueu from previous page									
Mol	Chain	Res	Type							
3	А	789	LEU							
3	А	797	GLU							
3	А	802	LEU							
3	А	815	VAL							
3	А	817	LEU							
3	А	818	GLU							
3	А	831	LYS							
3	А	832	GLU							

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Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
3	A 415		ASN
3	А	443	HIS
3	А	480	HIS
3	А	534	GLN
3	А	561	HIS
3	А	566	GLN
3	А	582	GLN
3	А	583	ASN
3	А	627	ASN
3	А	754	GLN

5.3.3RNA (i)

There are no RNA molecules in this entry.

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

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).

Mal	Mol Tuno Chain		Pog Link		Bond lengths			Bond angles		
	туре	Chain	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
1	DOC	В	112	1,2	16,19,20	0.40	0	$20,\!26,\!29$	0.41	0



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	DOC	В	112	1,2	-	0/7/18/19	0/2/2/2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	В	112	DOC	2	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)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.

