Full wwPDB X-ray Structure Validation Report (i)

Feb 26, 2014 – 07:59 PM GMT

PDB ID	:	4KTQ
Title	:	BINARY COMPLEX OF THE LARGE FRAGMENT OF DNA POLYMERASE 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 validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at http://wwpdb.org/ValidationPDFNotes.html

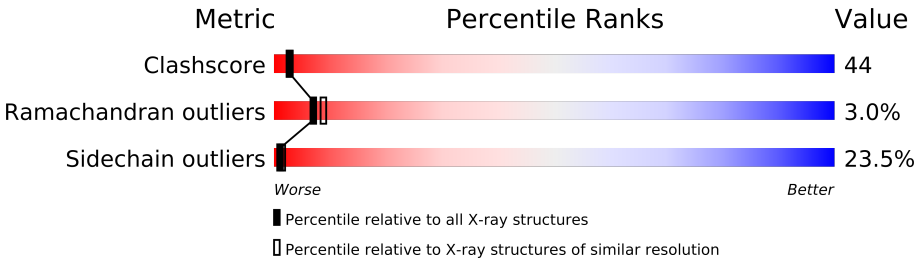
The following versions of software and data (see references) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	21963
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	B	12	
2	C	13	
3	A	539	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4769 atoms, of which 0 are hydrogen and 0 are deuterium.

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*(DOC))-3').

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

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

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

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

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	84	Total	O	0	0
			84	84		
4	B	8	Total	O	0	0
			8	8		
4	C	11	Total	O	0	0
			11	11		

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 (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.

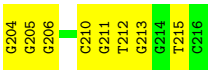
Note EDS was not executed.

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

Chain B:

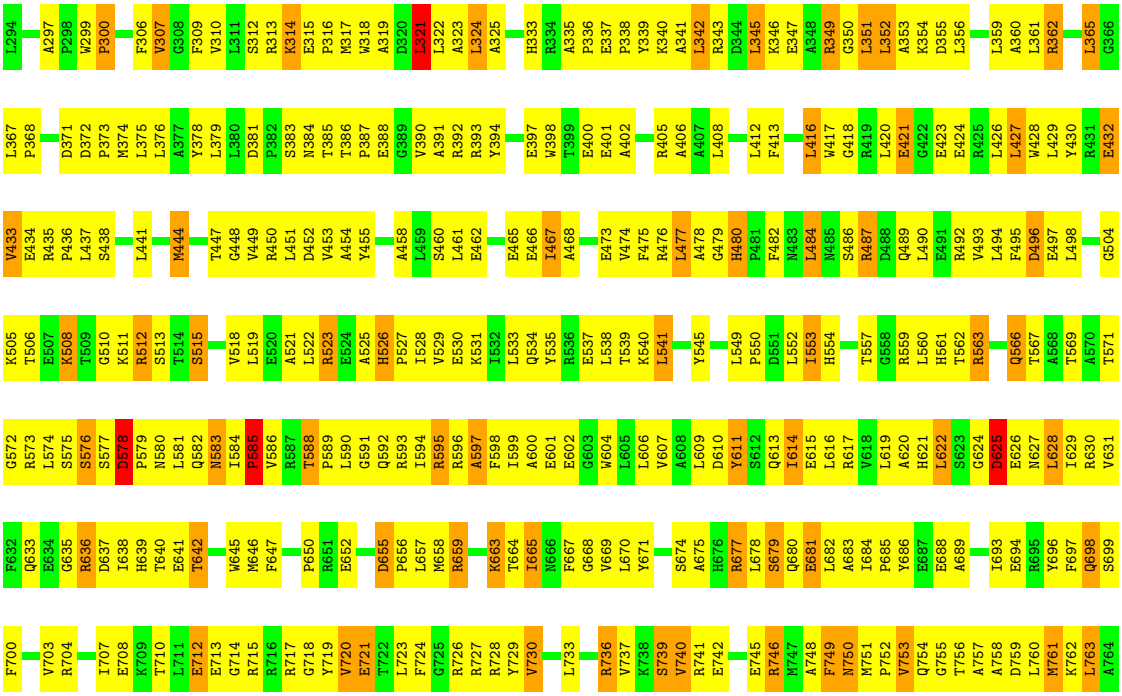
• Molecule 2: DNA (5'-D(*GP*GP*GP*CP*GP*CP*CP*GP*TP*GP*GP*TP*C)-3')

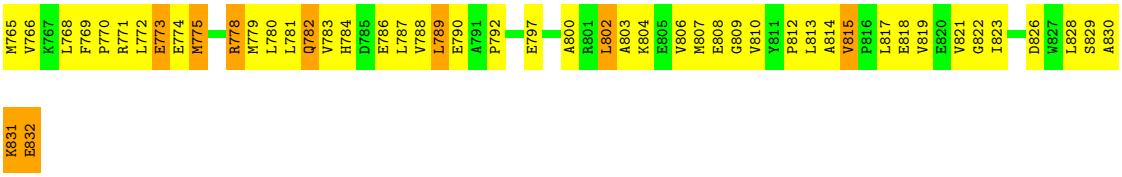
Chain C:



• Molecule 3: PROTEIN (LARGE FRAGMENT OF DNA POLYMERASE I)

Chain A:




M765
V766
K767
L768
F769
P770
R771
L772
E773
E774
M775
R778
M779
L780
L781
Q782
V783
H784
D785
E786
L787
V788
L789
E790
A791
P792
E797
A800
R801
L802
A803
K804
E805
V806
M807
E808
G809
V810
Y811
P812
L813
A814
V815
P816
L817
E818
V819
E820
V821
G822
I823
D826
W827
L828
S829
A830
K831
E832

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	110.84Å 110.84Å 90.84Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.50	Depositor
% Data completeness (in resolution range)	91.8 (30.00-2.50)	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

5.1 Standard geometry

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).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	B	0.47	0/249	0.73	0/382
2	C	0.53	0/299	0.83	0/461
3	A	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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	240	0	134	12	0
2	C	267	0	147	17	0
3	A	4159	0	4117	385	0
4	A	84	0	0	8	0
4	B	8	0	0	1	0
4	C	11	0	0	1	0
All	All	4769	0	4398	397	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including

hydrogens) of the entry. The overall clashscore for this entry is 44.

All (397) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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:768:LEU:HD11	3:A:803:ALA:HA	1.68	0.76
3:A:562:THR:HG23	3:A:579:PRO:O	1.86	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:769:PHE:HD1	3:A:772:LEU:HD12	1.55	0.71
3:A:576:SER:OG	3:A:580:ASN:HA	1.90	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:557:THR:OG1	3:A:561:HIS:HE1	1.75	0.67

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:A:482:PHE:HE2	3:A:490:LEU:HD12	1.58	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:575:SER:HA	3:A:582:GLN:HE22	1.63	0.64
3:A:359:LEU:HA	3:A:362:ARG:HG2	1.80	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:647:PHE:CZ	3:A:658:MET:HG2	2.33	0.63
3:A:306:PHE:O	3:A:406:ALA:HB1	1.99	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
3:A:602:GLU:HA	4:A:3066:HOH:O	2.00	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:665:ILE:O	3:A:669:VAL:HG23	2.02	0.59
3:A:423:GLU:C	3:A:427:LEU:HD12	2.22	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:386:THR:HB	3:A:388:GLU:OE1	2.04	0.58
3:A:779:MET:HG3	3:A:789:LEU:CD1	2.33	0.58
3:A:679:SER:HA	3:A:684:ILE:HG13	1.84	0.58
3:A:375:LEU:HD21	3:A:434:GLU:HB3	1.85	0.58
3:A:583:ASN:HD22	3:A:583:ASN:C	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: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
3:A:482:PHE:CE2	3:A:490:LEU:HD12	2.39	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:677:ARG:O	3:A:681:GLU:HB2	2.05	0.56
3:A:346:LYS:O	3:A:368:PRO:HD2	2.06	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:595:ARG:HH11	3:A:832:GLU:HG3	1.72	0.54
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:390:VAL:O	3:A:394:TYR:HD2	1.89	0.54
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:562:THR:HA	3:A:579:PRO:HD2	1.89	0.54
3:A:417:TRP:HB3	4:A:3088:HOH:O	2.07	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:813:LEU:C	3:A:815:VAL:N	2.61	0.53
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: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
3:A:569:THR:HB	3:A:573:ARG:O	2.08	0.53
1:B:104:DC:H42	2:C:213:DG:H1	1.56	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:761:MET:HA	3:A:761:MET:HE3	1.90	0.53
3:A:349:ARG:HG2	3:A:371:ASP:HB2	1.91	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:562:THR:OG1	3:A:581:LEU:HG	2.08	0.53
3:A:494:LEU:O	3:A:498:LEU:HB2	2.09	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:549:LEU:HD22	3:A:560:LEU:CD1	2.39	0.52
3:A:429:LEU:HD21	3:A:724:PHE:HB3	1.90	0.52
3:A:324:LEU:HG	3:A:342:LEU:HD23	1.91	0.52
3:A:321:LEU:HD11	3:A:342:LEU:HD21	1.92	0.51
3:A:802:LEU:O	3:A:806:VAL:HG23	2.10	0.51
3:A:313:ARG:HG3	3:A:315:GLU:OE1	2.10	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: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
3:A:371:ASP:OD2	3:A:413:PHE:CZ	2.64	0.51
3:A:360:ALA:HB2	3:A:367:LEU:HD23	1.93	0.51
3:A:616:LEU:O	3:A:619:LEU:HB3	2.11	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:C:204:DG:C5'	3:A:677:ARG:NE	2.73	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
3:A:428:TRP:O	3:A:432:GLU:HB2	2.11	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
1:B:102:DA:H5"	4:B:3079:HOH:O	2.10	0.51
3:A:683:ALA:O	3:A:684:ILE:HG23	2.11	0.51
3:A:751:MET:SD	3:A:751:MET:C	2.89	0.51
3:A:720:VAL:O	3:A:727:ARG:HA	2.11	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
3:A:373:PRO:O	3:A:376:LEU:N	2.44	0.50
3:A:309:PHE:HA	3:A:402:ALA:HB1	1.93	0.50
1:B:107:DG:OP2	3:A:508:LYS:HB2	2.12	0.50
3:A:682:LEU:HD12	3:A:684:ILE:HG12	1.93	0.50
3:A:633:GLN:C	3:A:635:GLY:H	2.13	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:773:GLU:C	3:A:775:MET:N	2.66	0.49
3:A:530:GLU:O	3:A:533:LEU:HB2	2.12	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:739:SER:HB3	4:A:3006:HOH:O	2.11	0.49
3:A:317:MET:HE1	3:A:362:ARG:HB3	1.94	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
3:A:626:GLU:HA	3:A:629:ILE:HG12	1.93	0.49
3:A:309:PHE:CD1	3:A:309:PHE:N	2.81	0.49
3:A:487:ARG:NH2	3:A:512:ARG:O	2.44	0.49
3:A:386:THR:O	3:A:390:VAL:HG23	2.12	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:C:3012:HOH:O	3:A:677:ARG:NH1	2.46	0.48
2:C:212:DT:C4	2:C:213:DG:C6	3.01	0.48
3:A:829:SER:C	3:A:831:LYS:N	2.65	0.48
3:A:317:MET:HG3	3:A:561:HIS:HB3	1.95	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
3:A:552:LEU:HD13	3:A:579:PRO:HB3	1.96	0.47
3:A:375:LEU:CD2	3:A:434:GLU:HB3	2.43	0.47
2:C:215:DT:H5'	2:C:215:DT:H6	1.79	0.47
3:A:636:ARG:NH1	3:A:636:ARG:HA	2.29	0.47
3:A:513:SER:OG	3:A:515:SER:HB3	2.14	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
3:A:778:ARG:HD2	3:A:790:GLU:OE1	2.15	0.47
3:A:647:PHE:CE1	3:A:658:MET:HG2	2.50	0.47
1:B:111:DC:O4'	3:A:583:ASN:HA	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:CZ	3:A:636:ARG:HA	2.45	0.47
3:A:769:PHE:HA	3:A:772:LEU:HB2	1.97	0.46
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: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:352:LEU:O	3:A:355:ASP:HB2	2.15	0.46
3:A:637:ASP:OD1	3:A:659:ARG:NH2	2.49	0.46
3:A:477:LEU:HD22	3:A:528:ILE:HB	1.96	0.46
3:A:466:GLU:HA	3:A:466:GLU:OE2	2.16	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:A:624:GLY:O	3:A:626:GLU:N	2.49	0.46
3:A:736:ARG:HH11	3:A:736:ARG:HG3	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:665:ILE:CG2	3:A:696:TYR:CD1	2.99	0.46
3:A:518:VAL:O	3:A:522:LEU:HG	2.16	0.46
3:A:595:ARG:HD3	3:A:832:GLU:OE2	2.15	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: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:571:THR:HG21	3:A:754:GLN:NE2	2.31	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:324:LEU:HD22	3:A:325:ALA:H	1.81	0.45
3:A:512:ARG:HB2	3:A:512:ARG:HE	1.60	0.45
3:A:753:VAL:O	3:A:753:VAL:HG23	2.15	0.45
3:A:378:TYR:HB2	3:A:567:THR:HB	1.97	0.45
3:A:567:THR:OG1	3:A:567:THR:O	2.32	0.45
3:A:826:ASP:OD2	3:A:829:SER:HB2	2.16	0.45
3:A:583:ASN:ND2	3:A:583:ASN:C	2.70	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:756:THR:HG22	3:A:757:ALA:N	2.31	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: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: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:438:SER:HB3	3:A:566:GLN:HE22	1.81	0.45
3:A:667:PHE:HA	3:A:670:LEU:HD12	1.98	0.45
3:A:569:THR:CG2	3:A:571:THR:H	2.30	0.45
3:A:749:PHE:O	3:A:752:PRO:HD2	2.17	0.45
3:A:704:ARG:O	3:A:707:ILE:HB	2.17	0.45
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:A:719:TYR:HB3	3:A:729:TYR:CD2	2.53	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: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:740:VAL:CG2	3:A:741:ARG:N	2.80	0.44
3:A:617:ARG:O	3:A:620:ALA:HB3	2.18	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:578:ASP:HA	3:A:579:PRO:HA	1.86	0.43
3:A:429:LEU:HD21	3:A:724:PHE:HB2	1.99	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:341:ALA:C	3:A:343:ARG:N	2.71	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: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:637:ASP:O	3:A:640:THR:HB	2.19	0.43
3:A:504:GLY:HA2	4:A:3018:HOH:O	2.18	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:595:ARG:HG2	3:A:832:GLU:OE2	2.19	0.42
3:A:553:ILE:HG22	3:A:553:ILE:O	2.18	0.42
1:B:106:DC:P	3:A:508:LYS:HG2	2.59	0.42
3:A:317:MET:HA	3:A:317:MET:CE	2.48	0.42
3:A:417:TRP:O	3:A:420:LEU:HB2	2.19	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:736:ARG:NH1	3:A:736:ARG:HG3	2.34	0.42
3:A:426:LEU:HD23	3:A:426:LEU:HA	1.88	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:A:622:LEU:HA	3:A:622:LEU:HD12	1.88	0.42
3:A:593:ARG:HB3	3:A:593:ARG:HE	1.58	0.42
3:A:476:ARG:C	3:A:478:ALA:H	2.23	0.42
3:A:746:ARG:HA	3:A:749:PHE:CE2	2.54	0.42
3:A:482:PHE:HA	4:A:3055:HOH:O	2.18	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	2.26	0.42
2:C:210:DC:H2"	2:C:211:DG:C8	2.55	0.42
3:A:541:LEU:HA	3:A:545:TYR:HD1	1.85	0.42
3:A:441:LEU:CD1	3:A:566:GLN:HG3	2.49	0.42
3:A:381:ASP:HB3	3:A:384:ASN:ND2	2.34	0.42
2:C:204:DG:C2'	2:C:205:DG:OP2	2.58	0.42
3:A:763:LEU:HA	3:A:763:LEU:HD23	1.72	0.42
3:A:297:ALA:HB3	3:A:333:HIS:CD2	2.55	0.42
3:A:569:THR:HG23	3:A:571:THR:H	1.85	0.42
3:A:717:ARG:NH1	3:A:719:TYR:CE1	2.82	0.42
3:A:549:LEU:HB2	3:A:550:PRO:HD3	2.01	0.42
3:A:637:ASP:O	3:A:640:THR:N	2.46	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:596:ARG:HG3	3:A:828:LEU:HD23	2.02	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:739:SER:OG	3:A:740:VAL:N	2.51	0.41
3:A:675:ALA:HB1	3:A:689:ALA:HB1	2.01	0.41
3:A:601:GLU:OE2	3:A:604:TRP:NE1	2.53	0.41
3:A:433:VAL:O	3:A:436:PRO:HG2	2.20	0.41
1:B:108:DG:N2	3:A:540:LYS:NZ	2.68	0.41
3:A:674:SER:HB2	3:A:677:ARG:HG3	2.02	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
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
3:A:719:TYR:HD2	3:A:729:TYR:CE2	2.39	0.41
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: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
3:A:321:LEU:HD13	3:A:338:PRO:CB	2.51	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:C:205:DG:H22	3:A:573:ARG:HH22	1.67	0.41
3:A:604:TRP:HA	3:A:792:PRO:HA	2.02	0.41
3:A:452:ASP:O	3:A:455:TYR:HB3	2.21	0.41
3:A:693:ILE:HG22	3:A:694:GLU:OE2	2.20	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
3:A:636:ARG:HB2	3:A:641:GLU:HG3	2.01	0.41
3:A:822:GLY:C	3:A:823:ILE:HG13	2.41	0.40
1:B:108:DG:H21	3:A:540:LYS:NZ	2.19	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:655:ASP:N	3:A:656:PRO:HD3	2.36	0.40
3:A:625:ASP:O	3:A:628:LEU:N	2.51	0.40
3:A:828:LEU:HA	3:A:832:GLU:OE1	2.21	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:441:LEU:HD11	3:A:566:GLN:HG3	2.02	0.40
3:A:752:PRO:O	3:A:756:THR:HB	2.21	0.40
3:A:585:PRO:HB2	3:A:591:GLY:HA3	2.02	0.40
3:A:430:TYR:HA	3:A:434:GLU:HB2	2.03	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

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	537/539 (100%)	419 (78%)	102 (19%)	16 (3%)	7 9

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	525	ALA
3	A	625	ASP

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Mol	Chain	Res	Type
3	A	681	GLU
3	A	586	VAL
3	A	597	ALA
3	A	814	ALA
3	A	392	ARG
3	A	496	ASP
3	A	321	LEU
3	A	424	GLU
3	A	300	PRO
3	A	578	ASP
3	A	774	GLU
3	A	585	PRO
3	A	433	VAL
3	A	650	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
3	A	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	A	307	VAL
3	A	314	LYS
3	A	321	LEU
3	A	324	LEU
3	A	342	LEU
3	A	345	LEU
3	A	347	GLU
3	A	349	ARG
3	A	351	LEU
3	A	352	LEU
3	A	354	LYS
3	A	362	ARG
3	A	365	LEU
3	A	397	GLU

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Mol	Chain	Res	Type
3	A	401	GLU
3	A	416	LEU
3	A	421	GLU
3	A	427	LEU
3	A	432	GLU
3	A	444	MET
3	A	460	SER
3	A	462	GLU
3	A	467	ILE
3	A	477	LEU
3	A	480	HIS
3	A	484	LEU
3	A	487	ARG
3	A	508	LYS
3	A	512	ARG
3	A	515	SER
3	A	523	ARG
3	A	526	HIS
3	A	531	LYS
3	A	541	LEU
3	A	553	ILE
3	A	563	ARG
3	A	566	GLN
3	A	576	SER
3	A	577	SER
3	A	578	ASP
3	A	583	ASN
3	A	585	PRO
3	A	588	THR
3	A	595	ARG
3	A	611	TYR
3	A	614	ILE
3	A	622	LEU
3	A	625	ASP
3	A	628	LEU
3	A	636	ARG
3	A	642	THR
3	A	645	TRP
3	A	652	GLU
3	A	655	ASP
3	A	657	LEU
3	A	659	ARG

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Mol	Chain	Res	Type
3	A	663	LYS
3	A	665	ILE
3	A	671	TYR
3	A	677	ARG
3	A	679	SER
3	A	680	GLN
3	A	686	TYR
3	A	698	GLN
3	A	699	SER
3	A	708	GLU
3	A	710	THR
3	A	712	GLU
3	A	715	ARG
3	A	720	VAL
3	A	721	GLU
3	A	723	LEU
3	A	730	VAL
3	A	733	LEU
3	A	736	ARG
3	A	739	SER
3	A	740	VAL
3	A	746	ARG
3	A	749	PHE
3	A	750	ASN
3	A	753	VAL
3	A	761	MET
3	A	763	LEU
3	A	771	ARG
3	A	773	GLU
3	A	775	MET
3	A	778	ARG
3	A	781	LEU
3	A	782	GLN
3	A	789	LEU
3	A	797	GLU
3	A	802	LEU
3	A	815	VAL
3	A	817	LEU
3	A	818	GLU
3	A	831	LYS
3	A	832	GLU

Some 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	A	443	HIS
3	A	480	HIS
3	A	534	GLN
3	A	561	HIS
3	A	566	GLN
3	A	582	GLN
3	A	583	ASN
3	A	627	ASN
3	A	754	GLN

5.3.3 RNA (i)

There are no RNA chains in this entry.

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

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	DOC	B	112	1,2	17,19,20	1.02	1 (5%)	20,26,29	0.91	1 (5%)

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	B	112	1,2	-	0/5/18/19	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	112	DOC	P-OP1	2.52	1.49	1.46

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	112	DOC	C2-N3-C4	3.14	120.12	115.57

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.