

Full wwPDB X-ray Structure Validation Report (i)

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PDB ID	:	2AJQ
Title	:	Structure of replicative DNA polymerase provides insigts into the mechanisms
		for processivity, frameshifting and editing
Authors	:	Brieba, L.; Ellenberger, T.
Deposited on	:	2005-08-02
Resolution	:	2.60 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 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	:	2.23.2
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)	:	2.23.2

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 2.60 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 $(\#Entries, resolution range(Å))$		
Rfree	130704	3163 (2.60-2.60)		
Clashscore	141614	3518 (2.60-2.60)		
Ramachandran outliers	138981	3455 (2.60-2.60)		
Sidechain outliers	138945	3455 (2.60-2.60)		
RSRZ outliers	127900	3104 (2.60-2.60)		

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 chair	1			
1	Р	22	18%	59%		9%	5%	9%
1	Х	22	27%	59%			9%	5%
2	Т	26	27%	42%	_	15%	159	%
2	Z	26	4%		54%			•
3	А	704	% •	67%		31%		•



Mol	Chain	Length	Quality of chain					
3	F	704	.% 6 6%	29%	••			
4	В	108	<u>6%</u> 54%	40%	•••			
4	Ι	108	29% 36% 529	%	9% •			



2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 14791 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	D	20	Total	С	Ν	0	Р	0	0	1
			390	184	77	110	19	0		
1	1 X	21	Total	С	Ν	0	Р	0	0	0
			432	204	87	120	21		0	0

• Molecule 1 is a DNA chain called DNA Primer.

• Molecule 2 is a DNA chain called DNA Template.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Т	22	Total	С	Ν	0	Р	0	0	0
			453	215	79	137	22	0		
9	7	25	Total	С	Ν	0	Р	0	0	0
		20	514	244	89	156	25	0	0	0

• Molecule 3 is a protein called T7 DNA polymerase.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
3	А	704	Total 5541	$\begin{array}{c} \mathrm{C} \\ 3527 \end{array}$	N 971	O 1019	S 24	0	0	0
3	F	689	Total 5459	C 3480	N 953	O 1003	S 23	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	5	ALA	ASP	engineered mutation	UNP P00581
А	7	ALA	GLU	engineered mutation	UNP P00581
F	5	ALA	ASP	engineered mutation	UNP P00581
F	7	ALA	GLU	engineered mutation	UNP P00581

• Molecule 4 is a protein called thioredoxin 1.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	Р	105	Total	С	Ν	0	S	0	0	0
4	4 D		799	517	129	150	3	0	0	0
4	т	105	Total	С	Ν	0	S	0	0	0
4	4 1	105	789	512	126	148	3		0	0

• Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	Р	16	Total O 16 16	0	0
5	Т	21	TotalO2121	0	0
5	Х	21	Total O 21 21	0	0
5	Ζ	27	TotalO2727	0	0
5	А	158	Total O 158 158	0	0
5	В	13	Total O 13 13	0	0
5	F	142	Total O 142 142	0	0
5	Ι	16	Total O 16 16	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 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: DNA Primer







 \bullet Molecule 4: thio redoxin 1





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants	168.31Å 169.24Å 179.79Å	Deperitor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
$\mathbf{P}_{\text{assolution}}(\hat{\mathbf{A}})$	45.97 - 2.60	Depositor
Resolution (A)	45.97 - 2.38	EDS
% Data completeness	99.8 (45.97-2.60)	Depositor
(in resolution range)	95.7 (45.97-2.38)	EDS
R _{merge}	0.09	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) > 1$	$1.93 (at 2.37 \text{\AA})$	Xtriage
Refinement program	CNS	Depositor
P. P.	0.233 , 0.284	Depositor
n, n_{free}	0.220 , 0.263	DCC
R_{free} test set	4957 reflections $(5.03%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	60.0	Xtriage
Anisotropy	0.315	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.32 , 40.7	EDS
L-test for $twinning^2$	$< L > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.449 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	14791	wwPDB-VP
Average B, all atoms $(Å^2)$	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 2.61% 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: 2DT

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	Chain	Bo	nd lengths	Bond angles	
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5
1	Р	0.66	1/417~(0.2%)	0.90	1/642~(0.2%)
1	Х	0.41	0/465	0.81	0/715
2	Т	0.55	0/506	0.83	0/780
2	Ζ	0.46	0/574	0.77	0/885
3	А	0.39	0/5680	0.59	0/7693
3	F	0.39	0/5594	0.60	0/7570
4	В	0.31	0/814	0.55	0/1104
4	Ι	0.32	0/803	0.55	0/1089
All	All	0.40	1/14853~(0.0%)	0.63	1/20478~(0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	Р	0	2
1	Х	0	2
2	Т	0	4
2	Ζ	0	2
All	All	0	10

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\operatorname{Ideal}(\operatorname{\AA})$
1	Р	803	DA	O3'-P	-7.13	1.52	1.61

All (1) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Ζ	$Observed(^{o})$	$Ideal(^{o})$
1	Р	821	DA	N9-C1'-C2'	-5.54	102.08	112.60

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	Р	820	DC	Sidechain
1	Р	821	DA	Sidechain
2	Т	854	DG	Sidechain
2	Т	855	DA	Sidechain
2	Т	856	DT	Sidechain
2	Т	857	DG	Sidechain
1	Х	920	DC	Sidechain
1	Х	921	DA	Sidechain
2	Ζ	955	DA	Sidechain
2	Ζ	957	DG	Sidechain

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	Р	390	0	212	37	0
1	Х	432	0	234	29	0
2	Т	453	0	250	21	0
2	Ζ	514	0	284	13	0
3	А	5541	0	5382	186	0
3	F	5459	0	5338	179	0
4	В	799	0	814	45	0
4	Ι	789	0	794	92	0
5	А	158	0	0	14	0
5	В	13	0	0	1	0
5	F	142	0	0	7	1
5	Ι	16	0	0	4	0
5	Р	16	0	0	0	0
5	Т	21	0	0	0	0
5	Х	21	0	0	0	0
5	Ζ	27	0	0	0	0
All	All	14791	0	13308	577	1



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 21.

All (577) 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 (Å)	overlap (Å)
4:B:73:ARG:HH11	4:B:73:ARG:HB3	1.11	1.09
2:T:867:DG:H2"	2:T:868:DT:H5'	1.32	1.07
4:I:16:VAL:HA	4:I:23:ILE:HG21	1.36	1.04
1:P:807:DC:H2"	1:P:808:DG:H5'	1.38	1.03
4:B:73:ARG:HB3	4:B:73:ARG:NH1	1.79	0.96
4:I:80:LEU:H	4:I:89:THR:HG22	1.31	0.94
1:X:917:DT:H2"	1:X:918:DG:H5'	1.50	0.93
1:P:817:DT:H2"	1:P:818:DG:H5'	1.51	0.92
4:I:25:VAL:HA	4:I:56:ALA:H	1.33	0.92
1:X:916:DG:H2"	1:X:917:DT:H5'	1.52	0.92
1:P:805:DA:H2"	1:P:806:DA:H5"	1.51	0.92
4:I:27:PHE:HE2	4:I:58:LEU:HD23	1.33	0.91
4:I:24:LEU:HD21	4:I:80:LEU:HD12	1.52	0.91
1:X:920:DC:H2"	1:X:921:DA:H5'	1.53	0.90
2:T:856:DT:H2"	2:T:857:DG:H5"	1.54	0.90
4:I:38:ILE:HD12	4:I:93:ALA:HA	1.54	0.89
4:B:27:PHE:HE2	4:B:58:LEU:HD23	1.37	0.89
3:F:321:VAL:HG21	4:I:94:LEU:HD21	1.55	0.89
4:B:38:ILE:HD12	4:B:93:ALA:HA	1.52	0.88
3:A:189:LYS:HG3	3:A:194:PRO:HG3	1.56	0.88
4:I:25:VAL:HG12	4:I:56:ALA:HB3	1.55	0.87
3:F:279:THR:HG22	3:F:280:GLY:H	1.37	0.86
4:I:24:LEU:HB2	4:I:55:VAL:HG22	1.57	0.85
1:X:920:DC:H2"	1:X:921:DA:C5'	2.07	0.85
4:I:24:LEU:HA	4:I:79:LEU:O	1.76	0.84
3:A:91:THR:HB	3:A:181:LEU:HD12	1.60	0.84
4:I:4:ILE:CG2	4:I:56:ALA:HA	2.08	0.83
3:F:164:ASN:OD1	3:F:166:GLU:HG2	1.78	0.83
3:F:315:LEU:HD23	3:F:316:ASP:H	1.44	0.83
3:A:321:VAL:HG21	4:B:94:LEU:HD21	1.61	0.83
4:I:23:ILE:O	4:I:80:LEU:HA	1.79	0.82
4:I:24:LEU:CB	4:I:55:VAL:HG22	2.09	0.82
1:X:921:DA:H5'	1:X:921:DA:H8	1.44	0.82
3:F:631:GLU:O	3:F:635:GLU:HG2	1.81	0.81
1:P:820:DC:H1'	5:A:5308:HOH:O	1.81	0.80
4:B:73:ARG:HH11	4:B:73:ARG:CB	1.93	0.80
4:B:27:PHE:HE1	4:B:79:LEU:HD22	1.47	0.79



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:T:856:DT:H2"	2:T:857:DG:C5'	2.12	0.79
4:I:12:PHE:HD1	4:I:13:ASP:H	1.30	0.79
3:A:276:HIS:HD2	3:A:279:THR:H	1.30	0.78
4:I:37:MET:O	4:I:40:PRO:HD2	1.81	0.78
2:Z:966:DC:H2"	2:Z:967:DG:C8	2.20	0.77
3:A:237:LYS:HA	3:A:237:LYS:HE2	1.67	0.77
3:A:22:VAL:HB	3:A:175:VAL:HG21	1.67	0.76
3:A:95:SER:OG	3:A:123:HIS:HD2	1.69	0.76
1:X:916:DG:H2"	1:X:917:DT:C5'	2.15	0.75
3:A:575:GLU:HG2	3:A:589:LYS:HG3	1.69	0.75
4:B:27:PHE:CE2	4:B:58:LEU:HD23	2.22	0.74
3:F:343:GLN:HG3	3:F:362:PRO:HG2	1.70	0.74
3:A:189:LYS:CG	3:A:194:PRO:HG3	2.17	0.74
3:A:436:ASN:HB3	3:A:439:GLN:HE21	1.53	0.74
3:F:55:LEU:HD13	3:F:89:ILE:HD11	1.70	0.74
3:A:570:GLN:HE22	3:A:606:PRO:HB3	1.52	0.73
3:F:63:LYS:HE3	3:F:228:GLU:OE2	1.88	0.73
3:F:72:LEU:HA	3:F:75:LEU:CD2	2.18	0.73
3:F:49:GLU:OE2	3:F:54:GLY:HA3	1.88	0.73
1:X:910:DC:H2"	1:X:911:DG:H5"	1.71	0.73
3:F:516:PRO:HG2	3:F:520:ASN:HD22	1.53	0.73
3:A:376:ASP:HB3	3:A:379:LYS:HB2	1.69	0.73
4:I:44:GLU:HG3	4:I:45:ILE:H	1.53	0.73
4:B:53:LEU:HD21	4:B:103:LEU:HD13	1.70	0.72
1:P:805:DA:C2'	1:P:806:DA:H5"	2.19	0.72
1:X:919:DC:H1'	3:F:394:LYS:HE2	1.70	0.72
3:A:189:LYS:HD2	3:A:189:LYS:N	2.04	0.72
3:A:343:GLN:HG2	3:A:347:GLN:HE21	1.54	0.72
3:A:484:LEU:HD22	3:A:529:LEU:HD21	1.71	0.72
4:I:4:ILE:HG21	4:I:56:ALA:HA	1.71	0.72
1:X:910:DC:H2"	1:X:911:DG:C5'	2.20	0.71
4:I:52:LYS:HD2	4:I:107:LEU:HD13	1.72	0.71
3:A:72:LEU:HA	3:A:75:LEU:HD11	1.72	0.71
3:F:388:GLU:O	3:F:392:ILE:HG12	1.90	0.71
3:A:318:ARG:HE	3:A:319:GLU:H	1.37	0.71
1:X:921:DA:H5'	1:X:921:DA:C8	2.25	0.71
3:A:343:GLN:HG3	3:A:362:PRO:HG3	1.71	0.71
3:F:95:SER:OG	3:F:123:HIS:HD2	1.73	0.70
3:A:585:GLN:HG2	5:A:5261:HOH:O	1.91	0.70
3:F:343:GLN:HG3	3:F:362:PRO:CG	2.21	0.70
1:P:807:DC:H2"	1:P:808:DG:C5'	2.20	0.70



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:T:858:DG:H2"	2:T:859:DC:H5'	1.73	0.70
3:A:343:GLN:HG3	3:A:362:PRO:CG	2.20	0.70
3:A:13:GLU:H	3:A:13:GLU:CD	1.96	0.70
4:B:37:MET:O	4:B:40:PRO:HD2	1.92	0.70
4:I:27:PHE:CE2	4:I:58:LEU:HD23	2.21	0.69
3:F:273:MET:HG2	3:F:282:PRO:HB3	1.73	0.69
3:A:129:GLY:HA3	3:A:135:MET:HG2	1.74	0.69
4:I:39:ALA:HB3	4:I:40:PRO:HD3	1.75	0.69
3:A:528:PHE:HZ	3:A:556:LEU:HD21	1.58	0.69
3:F:13:GLU:H	3:F:13:GLU:CD	1.96	0.69
2:T:858:DG:H4'	3:A:432:HIS:O	1.92	0.68
3:A:436:ASN:HB3	3:A:439:GLN:NE2	2.07	0.68
3:F:575:GLU:HG3	3:F:576:SER:N	2.07	0.68
3:A:146:MET:HG2	3:A:150:GLN:HE21	1.57	0.68
3:F:359:LYS:N	3:F:359:LYS:HE2	2.09	0.68
3:A:128:TRP:CE3	3:A:131:ARG:HD2	2.28	0.68
4:I:79:LEU:HA	4:I:89:THR:HB	1.75	0.67
3:F:279:THR:HG22	3:F:280:GLY:N	2.09	0.67
4:I:24:LEU:O	4:I:25:VAL:HG13	1.93	0.67
3:F:484:LEU:HD22	3:F:529:LEU:HD21	1.76	0.67
3:A:519:ASP:O	3:A:523:THR:HG22	1.95	0.67
3:A:579:TRP:CE2	3:A:584:GLN:HG3	2.29	0.67
4:I:24:LEU:C	4:I:55:VAL:HA	2.16	0.66
3:F:519:ASP:O	3:F:523:THR:HG22	1.96	0.66
3:F:145:ARG:HA	3:F:148:GLU:HG2	1.76	0.66
3:A:276:HIS:CD2	3:A:279:THR:H	2.13	0.65
3:F:189:LYS:NZ	3:F:194:PRO:HB3	2.12	0.65
3:A:516:PRO:HG2	3:A:520:ASN:HD22	1.61	0.65
1:P:808:DG:H1	2:T:869:DC:H42	1.44	0.65
3:F:43:LEU:O	3:F:47:GLU:HG3	1.96	0.65
4:I:80:LEU:HB3	4:I:88:ALA:O	1.97	0.65
3:F:22:VAL:HB	3:F:175:VAL:HG21	1.78	0.64
3:A:696:MET:HE3	5:A:5084:HOH:O	1.98	0.64
4:I:88:ALA:HB1	4:I:106:ASN:CB	2.28	0.64
4:B:8:THR:HG22	4:B:11:SER:OG	1.96	0.64
3:A:330:GLU:HG3	3:A:332:VAL:HG13	1.80	0.64
3:F:663:GLU:HB2	3:F:696:MET:SD	2.38	0.64
3:F:516:PRO:HG2	3:F:520:ASN:ND2	2.12	0.64
4:I:8:THR:HA	4:I:63:ASN:HD21	1.62	0.64
3:A:297:ILE:HD12	3:A:297:ILE:N	2.12	0.64
3:F:547:ARG:NH1	3:F:551:LEU:HD13	2.12	0.64



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
4:B:27:PHE:CE1	4:B:79:LEU:HD22	2.32	0.64
3:A:388:GLU:O	3:A:392:ILE:HG12	1.98	0.63
3:A:91:THR:HB	3:A:181:LEU:CD1	2.28	0.63
3:F:110:LEU:HD21	3:F:117:GLY:HA2	1.80	0.63
3:A:194:PRO:HD2	3:A:195:GLU:OE2	1.98	0.63
3:A:553:LYS:O	3:A:557:GLU:HG3	1.99	0.63
3:F:285:LYS:NZ	3:F:285:LYS:HB3	2.14	0.63
4:B:79:LEU:HD23	4:B:81:PHE:HE1	1.64	0.63
4:I:58:LEU:HD11	4:I:63:ASN:ND2	2.14	0.63
2:T:856:DT:C2'	2:T:857:DG:H5"	2.28	0.62
3:F:633:LEU:HD22	3:F:638:LEU:HD12	1.80	0.62
3:F:336:PRO:HB2	3:F:389:TYR:CD1	2.33	0.62
3:A:35:ARG:HB3	3:A:36:PRO:HD2	1.81	0.62
3:A:135:MET:CE	3:A:173:GLN:HE22	2.12	0.62
3:A:489:ALA:HA	3:A:492:ASP:OD1	2.00	0.62
1:P:821:DA:H5'	1:P:821:DA:H8	1.63	0.62
3:A:516:PRO:HG2	3:A:520:ASN:ND2	2.15	0.62
1:P:820:DC:H2"	1:P:821:DA:OP2	1.99	0.62
3:A:345:LYS:HE2	3:A:345:LYS:HA	1.81	0.61
4:B:26:ASP:OD2	4:B:57:LYS:HD2	2.00	0.61
3:F:297:ILE:HD13	4:I:102:PHE:HA	1.82	0.61
4:I:24:LEU:HG	4:I:80:LEU:HB2	1.81	0.61
4:I:25:VAL:O	4:I:78:LEU:HA	2.01	0.61
3:A:228:GLU:CD	3:A:419:SER:HA	2.19	0.61
3:F:189:LYS:HZ1	3:F:194:PRO:HB3	1.66	0.61
4:I:46:ALA:HA	5:I:5005:HOH:O	1.99	0.61
3:F:321:VAL:HG22	4:I:90:LYS:HE3	1.81	0.61
3:A:55:LEU:HD13	3:A:89:ILE:HD11	1.83	0.61
4:B:8:THR:HG23	4:B:11:SER:H	1.64	0.61
4:B:53:LEU:HD12	4:B:53:LEU:C	2.21	0.61
3:A:146:MET:HG2	3:A:150:GLN:NE2	2.16	0.61
4:I:53:LEU:O	4:I:53:LEU:HD23	1.99	0.61
4:I:5:ILE:HG22	4:I:6:HIS:N	2.16	0.60
3:A:547:ARG:NH1	3:A:551:LEU:HD13	2.17	0.60
4:I:23:ILE:C	4:I:24:LEU:HD12	2.20	0.60
3:A:667:GLN:HE21	3:A:671:GLU:HG3	1.66	0.60
3:A:22:VAL:HG23	3:A:171:ASN:OD1	2.01	0.60
3:F:79:ARG:HD3	5:F:5018:HOH:O	2.00	0.60
3:F:184:LYS:O	3:F:184:LYS:HD3	2.02	0.60
1:P:812:DG:H2"	1:P:813:DC:H5"	1.84	0.60
2:T:867:DG:H2"	2:T:868:DT:C5'	2.19	0.60



	to do pagon	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
3:A:439:GLN:HB2	5:A:5308:HOH:O	2.01	0.60
2:T:868:DT:H1'	2:T:869:DC:H5"	1.84	0.60
1:X:916:DG:H1'	1:X:917:DT:H5"	1.84	0.59
1:P:812:DG:H2"	1:P:813:DC:C5'	2.32	0.59
1:P:806:DA:H1'	1:P:807:DC:OP1	2.02	0.59
3:F:148:GLU:C	3:F:150:GLN:H	2.06	0.59
4:I:4:ILE:HG23	4:I:56:ALA:HA	1.83	0.59
4:B:13:ASP:HA	4:B:17:LEU:HD12	1.84	0.59
4:I:24:LEU:O	4:I:55:VAL:HA	2.02	0.59
4:I:26:ASP:N	4:I:56:ALA:O	2.33	0.59
3:A:285:LYS:NZ	3:A:285:LYS:HB3	2.18	0.59
3:F:496:TYR:O	3:F:500:ILE:HG12	2.03	0.59
3:A:315:LEU:HD23	3:A:315:LEU:H	1.67	0.59
3:A:703:CYS:O	3:A:704:HIS:HB2	2.01	0.59
3:F:28:THR:O	3:F:29:ALA:HB3	2.02	0.59
3:A:676:ALA:O	3:A:680:VAL:HG23	2.03	0.58
3:A:550:GLU:HG3	5:A:5421:HOH:O	2.03	0.58
3:F:289:ILE:HD12	3:F:325:PRO:HB2	1.84	0.58
1:P:807:DC:H5'	5:A:5117:HOH:O	2.04	0.58
3:F:484:LEU:O	3:F:488:MET:HG2	2.03	0.58
3:A:195:GLU:H	3:A:195:GLU:CD	2.06	0.58
4:I:5:ILE:HG22	4:I:6:HIS:H	1.69	0.58
4:B:79:LEU:HD12	4:B:89:THR:HB	1.85	0.58
3:A:391:MET:HE2	3:A:391:MET:O	2.03	0.58
3:F:136:LYS:HG3	3:F:173:GLN:HE21	1.69	0.58
4:B:11:SER:O	4:B:15:ASP:HB2	2.03	0.57
1:P:817:DT:H2"	1:P:818:DG:C5'	2.31	0.57
3:A:132:LEU:HD21	3:A:184:LYS:HG3	1.86	0.57
1:P:812:DG:C2'	1:P:813:DC:H5"	2.35	0.57
1:X:910:DC:C2'	1:X:911:DG:H5"	2.33	0.57
2:Z:974:DT:H2"	2:Z:975:DC:C5	2.39	0.57
3:F:523:THR:HG21	5:F:5095:HOH:O	2.03	0.57
3:A:289:ILE:HD12	3:A:325:PRO:HB2	1.85	0.57
3:A:228:GLU:HG2	3:A:418:GLY:O	2.03	0.57
3:A:467:LYS:HE3	3:A:468:PRO:HD2	1.86	0.57
4:I:95:SER:OG	4:I:98:GLN:HG3	2.05	0.57
1:X:903:DA:H2"	1:X:904:DA:N7	2.19	0.56
3:A:500:ILE:HD13	3:A:505:ILE:HD13	1.87	0.56
3:F:94:LEU:HD21	3:F:214:VAL:HG13	1.87	0.56
4:I:32:CYS:HB3	4:I:35:CYS:HB2	1.87	0.56
4:I:43:ASP:HB2	5:I:5012:HOH:O	2.05	0.56



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
3:F:173:GLN:O	3:F:176:VAL:HG22	2.05	0.56
1:P:816:DG:H1'	1:P:817:DT:H5"	1.86	0.56
3:A:109:LEU:HD22	3:A:114:LYS:HD3	1.88	0.56
3:A:49:GLU:OE2	3:A:54:GLY:HA3	2.05	0.56
4:B:79:LEU:HD23	4:B:81:PHE:CE1	2.41	0.56
3:F:547:ARG:HH12	3:F:551:LEU:HD13	1.71	0.56
3:A:130:TYR:CD1	3:A:135:MET:HG3	2.41	0.55
3:F:470:VAL:HG12	3:F:471:GLN:N	2.21	0.55
3:A:513:ALA:HB3	3:A:515:LEU:HD23	1.87	0.55
4:I:24:LEU:CA	4:I:79:LEU:O	2.51	0.55
2:T:869:DC:H2"	2:T:870:DG:C8	2.42	0.55
3:F:330:GLU:HG3	3:F:332:VAL:HG13	1.87	0.55
2:Z:961:DC:H2'	2:Z:962:DT:H71	1.89	0.55
3:A:74:LYS:O	3:A:78:ASN:HA	2.07	0.55
3:F:687:ARG:HH11	3:F:687:ARG:HB3	1.72	0.55
3:A:597:ASP:OD1	3:A:599:ARG:HD2	2.06	0.55
3:A:138:GLU:HB2	3:A:141:ASP:OD2	2.07	0.55
3:F:129:GLY:HA3	3:F:135:MET:HG2	1.89	0.55
3:F:74:LYS:O	3:F:78:ASN:HA	2.07	0.54
1:P:821:DA:H5'	1:P:821:DA:C8	2.41	0.54
3:F:429:ARG:HD2	3:F:615:GLN:NE2	2.23	0.54
1:X:917:DT:C2'	1:X:918:DG:H5'	2.31	0.54
3:F:489:ALA:HA	3:F:492:ASP:OD1	2.07	0.54
3:F:639:LYS:NZ	3:F:643:ASP:OD1	2.40	0.54
1:X:917:DT:H2"	1:X:918:DG:C5'	2.30	0.54
4:B:3:LYS:HD3	4:B:50:GLN:NE2	2.22	0.54
3:F:528:PHE:HZ	3:F:556:LEU:HD21	1.72	0.54
3:A:343:GLN:HG3	3:A:362:PRO:HG2	1.90	0.54
3:A:336:PRO:HB2	3:A:389:TYR:CD1	2.43	0.54
3:F:703:CYS:O	3:F:704:HIS:ND1	2.40	0.54
4:I:8:THR:CA	4:I:63:ASN:HD21	2.20	0.54
3:F:49:GLU:HA	3:F:52:ARG:NH1	2.23	0.54
4:I:44:GLU:HG3	4:I:45:ILE:N	2.21	0.54
1:X:915:DA:H2"	1:X:916:DG:H5'	1.88	0.53
3:A:224:LEU:HD12	3:A:422:PRO:HB3	1.88	0.53
3:A:499:GLU:HG3	3:A:508:LYS:HE2	1.90	0.53
3:F:129:GLY:C	3:F:135:MET:HG2	2.27	0.53
3:F:130:TYR:CD1	3:F:135:MET:HG3	2.43	0.53
3:F:585:GLN:HE21	3:F:585:GLN:HA	1.73	0.53
3:A:290:LYS:HD2	3:A:328:PRO:HG3	1.89	0.53
1:X:919:DC:C1'	3:F:394:LYS:HE2	2.37	0.53



		Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
2:Z:971:DT:H2"	2:Z:972:DT:H71	1.89	0.53	
3:A:376:ASP:OD2	3:A:379:LYS:HD3	2.08	0.53	
3:F:235:ASP:HB2	3:F:459:HIS:CE1	2.44	0.53	
1:P:807:DC:C2'	1:P:808:DG:H5'	2.27	0.53	
1:P:821:DA:H2'	1:P:822:2DT:H73	1.91	0.53	
2:Z:960:DA:H2"	2:Z:961:DC:H5'	1.90	0.53	
3:A:106:ASP:CG	3:A:131:ARG:HH22	2.10	0.53	
3:A:315:LEU:HD23	3:A:315:LEU:N	2.23	0.53	
3:A:391:MET:HE2	3:A:391:MET:C	2.29	0.53	
4:I:79:LEU:HD12	4:I:89:THR:HG21	1.90	0.53	
1:P:809:DA:H1'	1:P:810:DC:H5'	1.91	0.53	
3:A:546:GLU:HB3	5:A:5202:HOH:O	2.07	0.53	
4:I:16:VAL:CA	4:I:23:ILE:HG21	2.25	0.53	
1:P:805:DA:H2"	1:P:806:DA:O4'	2.09	0.53	
3:A:290:LYS:HD3	3:A:326:TYR:OH	2.08	0.53	
3:F:318:ARG:HH11	3:F:319:GLU:HG2	1.74	0.53	
3:A:318:ARG:HE	3:A:319:GLU:N	2.05	0.52	
3:A:528:PHE:CZ	3:A:556:LEU:HD21	2.42	0.52	
3:F:467:LYS:HE3	3:F:468:PRO:HD2	1.91	0.52	
2:Z:958:DG:H4'	3:F:432:HIS:O	2.09	0.52	
4:B:75:ILE:HB	4:B:76:PRO:HA	1.92	0.52	
3:F:35:ARG:HB3	3:F:36:PRO:HD2	1.90	0.52	
4:B:39:ALA:HB3	4:B:40:PRO:HD3	1.90	0.52	
3:F:700:TRP:HE1	3:F:704:HIS:CE1	2.26	0.52	
3:F:268:LYS:HD2	3:F:330:GLU:CD	2.30	0.52	
3:F:494:GLY:O	3:F:495:GLU:HB3	2.10	0.52	
3:A:28:THR:O	3:A:29:ALA:HB3	2.10	0.52	
4:I:81:PHE:HB3	4:I:84:GLY:H	1.75	0.52	
4:B:39:ALA:N	4:B:40:PRO:CD	2.73	0.52	
3:F:20:CYS:HB2	3:F:168:MET:CE	2.40	0.52	
1:P:808:DG:H2"	1:P:809:DA:C8	2.45	0.52	
3:A:666:ALA:HB3	3:A:696:MET:CE	2.40	0.51	
3:A:164:ASN:OD1	3:A:166:GLU:HB2	2.09	0.51	
3:A:492:ASP:HB3	3:A:561:ALA:HB2	1.91	0.51	
3:F:181:LEU:HD22	3:F:185:LEU:HD11	1.92	0.51	
4:B:38:ILE:HD12	4:B:93:ALA:CA	2.35	0.51	
3:A:13:GLU:CD	3:A:13:GLU:N	2.64	0.51	
3:F:116:PRO:O	3:F:118:LYS:N	2.43	0.51	
4:I:24:LEU:HB3	4:I:55:VAL:HG22	1.90	0.51	
4:I:90:LYS:HD3	4:I:102:PHE:CZ	2.45	0.51	
4:B:40:PRO:HA	4:B:43:ASP:OD2	2.11	0.51	



	jugern	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
3:A:72:LEU:O	3:A:76:GLN:HB2	2.11	0.51	
3:F:181:LEU:O	3:F:185:LEU:HG	2.11	0.51	
4:I:49:TYR:CE2	4:I:103:LEU:HB3	2.46	0.51	
3:A:17:LYS:NZ	3:A:17:LYS:HB3	2.25	0.51	
3:A:338:SER:O	3:A:342:ILE:HG13	2.10	0.51	
3:A:484:LEU:O	3:A:488:MET:HG2	2.11	0.50	
3:F:567:GLU:OE1	3:F:567:GLU:HA	2.10	0.50	
4:B:5:ILE:HG22	4:B:6:HIS:O	2.11	0.50	
4:I:24:LEU:O	4:I:54:THR:O	2.29	0.50	
2:T:865:DC:H2"	2:T:866:DC:O5'	2.11	0.50	
3:A:321:VAL:CG2	4:B:94:LEU:HD21	2.39	0.50	
3:A:331:HIS:HB3	5:A:5066:HOH:O	2.10	0.50	
3:F:132:LEU:HD21	3:F:184:LYS:HG3	1.93	0.50	
3:F:687:ARG:HB3	3:F:687:ARG:NH1	2.26	0.50	
3:F:11:LEU:HB3	3:F:13:GLU:OE1	2.11	0.50	
4:I:100:LYS:NZ	4:I:100:LYS:HB3	2.26	0.50	
1:P:807:DC:H1'	1:P:808:DG:H5"	1.94	0.50	
1:P:808:DG:H1	2:T:869:DC:N4	2.10	0.50	
3:F:655:GLU:OE2	3:F:704:HIS:HE1	1.94	0.50	
3:F:295:GLY:O	3:F:321:VAL:HA	2.12	0.50	
3:F:391:MET:HE2	3:F:391:MET:O	2.11	0.50	
3:A:624:LEU:HD12	3:A:684:TRP:CH2	2.47	0.50	
4:I:107:LEU:HG	5:I:5013:HOH:O	2.12	0.50	
2:T:864:DG:OP2	3:A:268:LYS:NZ	2.39	0.49	
3:A:135:MET:HE2	3:A:173:GLN:HE22	1.75	0.49	
3:F:195:GLU:H	3:F:195:GLU:CD	2.14	0.49	
1:X:920:DC:H5'	3:F:394:LYS:HE3	1.94	0.49	
3:F:315:LEU:CD2	3:F:316:ASP:H	2.19	0.49	
3:F:590:ARG:HD2	3:F:592:TRP:O	2.12	0.49	
3:A:478:GLY:O	3:A:482:ARG:HG3	2.12	0.49	
3:F:139:TYR:CE2	3:F:159:GLU:HB2	2.47	0.49	
2:Z:960:DA:H2"	2:Z:961:DC:C5'	2.43	0.49	
4:I:37:MET:HG3	4:I:38:ILE:N	2.28	0.49	
1:P:806:DA:H2"	1:P:807:DC:C5	2.47	0.49	
3:A:141:ASP:O	3:A:145:ARG:HG2	2.11	0.49	
4:B:25:VAL:HG22	4:B:56:ALA:HB3	1.94	0.49	
3:A:35:ARG:HB3	3:A:36:PRO:CD	2.42	0.49	
3:A:129:GLY:CA	3:A:135:MET:HG2	2.41	0.49	
3:A:535:GLU:O	3:A:539:GLN:HG3	2.13	0.49	
3:F:452:ARG:HD2	5:F:5210:HOH:O	2.13	0.49	
4:I:80:LEU:C	4:I:80:LEU:HD23	2.33	0.49	



Interatomic				
Atom-1	Atom-2	distance $(Å)$	overlan (Å)	
3·A·315·LEU·H	3·A·315·LEU·CD2	2.25	0.49	
3:F:268:LYS:HD2	3:F:330:GLU:OE2	2.12	0.49	
4·I·90·LYS·HD3	$4 \cdot I \cdot 102 \cdot PHE \cdot CE1$	2.48	0.10	
3·F·147·LEU·HD11	3·F·152·GLU·OE1	2.13	0.49	
3:A:391:MET:HE1	3:A:392:ILE:HD13	1.94	0.48	
3:A:663:GLU:O	3:A:696:MET:HE1	2.13	0.48	
3:F:298:PHE:CD2	3:F:315:LEU:HA	2.48	0.48	
3:A:102:LEU:HD12	3:A:123:HIS:CE1	2.48	0.48	
3:A:119:ARG:HG3	3:A:119:ARG:HH11	1.78	0.48	
3:F:39:PHE:CZ	3:F:43:LEU:HD11	2.48	0.48	
3·F·655·GLU·OE2	3·F·704·HIS·CE1	2.67	0.48	
4·I·52·LYS·CD	4:I:107:LEU:HD13	2 43	0.48	
3:A:437:LEU:HA	3: A:440: ILE: CD1	2.42	0.48	
3:F:200:ASP:HB2	5:F:5382:HOH:O	2.12	0.48	
3:F:391:MET:CE	3·F·395·ABG·HG3	2 43	0.48	
4·I·3·LYS·HE2	4·I·50·GLN·HE22	1.77	0.48	
3·A·408·ABG·HG2	3·A·408·ABG·HH11	1.78	0.48	
3:A:667:GLN:HE21	3:A:671:GLU:CG	2.25	0.48	
2:T:868:DT:H2"	2:T:869:DC:C5'	2.44	0.48	
4:I:102:PHE:C	4:I:104:ASP:H	2.15	0.48	
4:I:24:LEU:HG	4:I:80:LEU:CB	2.43	0.48	
1:P:813:DC:H1'	1:P:814:DC:H5'	1.94	0.48	
4:B:37:MET:C	4:B:40:PRO:HD2	2.34	0.48	
1:P:805:DA:H2"	1:P:806:DA:C5'	2.32	0.48	
4:I:80:LEU:HD23	4:I:80:LEU:O	2.13	0.48	
1:P:816:DG:H2"	1:P:817:DT:C5'	2.44	0.47	
1:X:911:DG:H2"	1:X:912:DG:C8	2.49	0.47	
3:F:494:GLY:O	3:F:495:GLU:CB	2.61	0.47	
3:A:292:PRO:HA	5:A:5117:HOH:O	2.15	0.47	
3:F:140:LYS:HE3	3:F:154:TYR:OH	2.14	0.47	
3:F:159:GLU:HG2	3:F:160:TRP:CD1	2.48	0.47	
1:P:805:DA:C3'	1:P:806:DA:H5"	2.45	0.47	
3:A:128:TRP:CZ3	3:A:131:ARG:HD2	2.49	0.47	
4:B:8:THR:HG23	4:B:11:SER:N	2.27	0.47	
3:F:597:ASP:OD1	3:F:599:ARG:HD2	2.14	0.47	
4:I:9:ASP:N	4:I:63:ASN:HD21	2.13	0.47	
1:X:917:DT:H1'	1:X:918:DG:H5"	1.97	0.47	
3:A:75:LEU:HD12	3:A:76:GLN:N	2.29	0.47	
3:A:213:ALA:HA	3:A:597:ASP:OD2	2.15	0.47	
3:A:326:TYR:HB3	4:B:92:GLY:HA2	1.95	0.47	
3:A:9:ASN:HB3	3:A:17:LYS:HG3	1.97	0.47	



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
3:F:570:GLN:HE22	3:F:606:PRO:HB3	1.80	0.47	
3:A:35:ARG:HG3	3:A:35:ARG:HH11	1.79	0.47	
3:F:556:LEU:HD11	3:F:566:ARG:NH2	2.30	0.47	
1:P:816:DG:H2"	1:P:817:DT:H5'	1.96	0.46	
3:F:72:LEU:HA	3:F:75:LEU:HD22	1.97	0.46	
3:F:129:GLY:CA	3:F:135:MET:HG2	2.44	0.46	
2:T:854:DG:H5"	3:A:532:ALA:HA	1.97	0.46	
4:I:35:CYS:SG	4:I:76:PRO:HB3	2.56	0.46	
3:A:114:LYS:HD2	5:A:5256:HOH:O	2.15	0.46	
3:A:285:LYS:HB3	3:A:285:LYS:HZ3	1.79	0.46	
2:T:854:DG:H2"	2:T:855:DA:H8	1.80	0.46	
1:X:916:DG:C2'	1:X:917:DT:C5'	2.89	0.46	
3:A:475:ASP:OD2	3:A:475:ASP:C	2.54	0.46	
5:A:5435:HOH:O	3:F:240:GLU:HG3	2.16	0.46	
3:F:13:GLU:CD	3:F:13:GLU:N	2.63	0.46	
3:F:549:LYS:HD3	5:F:5409:HOH:O	2.15	0.46	
3:A:444:ARG:HB2	5:A:5161:HOH:O	2.16	0.46	
4:I:9:ASP:N	4:I:63:ASN:ND2	2.64	0.46	
4:I:44:GLU:CG	4:I:45:ILE:H	2.20	0.46	
3:A:109:LEU:CD2	3:A:114:LYS:HD3	2.45	0.46	
3:A:159:GLU:HG2	3:A:160:TRP:CD1	2.50	0.46	
3:F:31:TYR:CE2	3:F:176:VAL:HG12	2.50	0.46	
3:F:318:ARG:NH1	3:F:319:GLU:HG2	2.30	0.46	
3:A:31:TYR:OH	3:A:176:VAL:HG12	2.16	0.46	
3:A:645:ASP:HB3	3:A:665:ILE:HD13	1.98	0.46	
3:F:72:LEU:HA	3:F:75:LEU:HD21	1.94	0.46	
3:F:115:LEU:O	3:F:117:GLY:N	2.36	0.46	
1:P:820:DC:H5'	3:A:394:LYS:HE2	1.98	0.46	
3:F:106:ASP:OD2	3:F:131:ARG:NH2	2.48	0.46	
3:F:297:ILE:HD13	4:I:102:PHE:CA	2.46	0.46	
3:F:365:ASP:O	3:F:369:LEU:HB2	2.16	0.46	
3:F:470:VAL:CG1	3:F:471:GLN:N	2.78	0.46	
4:I:8:THR:C	4:I:63:ASN:HD21	2.20	0.46	
2:T:869:DC:H2"	2:T:870:DG:H8	1.81	0.45	
3:F:136:LYS:CG	3:F:173:GLN:HE21	2.28	0.45	
3:F:264:TRP:NE1	3:F:344:LYS:HE2	2.31	0.45	
3:F:315:LEU:HD23	4:I:105:ALA:HB1	1.97	0.45	
3:F:493:ASN:HD22	3:F:687:ARG:HH22	1.63	0.45	
1:P:807:DC:H42	2:T:870:DG:H1	1.65	0.45	
1:P:820:DC:C2'	1:P:821:DA:OP2	2.64	0.45	
2:Z:966:DC:H2"	2:Z:967:DG:H8	1.76	0.45	



	te de pagem	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
4:B:45:ILE:HG13	4:B:99:LEU:CD1	2.46	0.45	
3:F:693:GLU:OE2	3:F:693:GLU:HA	2.16	0.45	
3:A:75:LEU:HD12	3:A:76:GLN:H	1.81	0.45	
3:A:163:PHE:HE1	3:A:168:MET:HB2	1.80	0.45	
3:F:351:TRP:CZ3	3:F:353:PRO:HG3	2.51	0.45	
4:B:32:CYS:HB3	4:B:35:CYS:HB2	1.99	0.45	
3:F:667:GLN:HE21	3:F:671:GLU:HG3	1.80	0.45	
3:F:436:ASN:OD1	3:F:438:ALA:HB3	2.17	0.45	
3:F:628:LYS:HE2	3:F:679:TRP:CD2	2.51	0.45	
4:I:25:VAL:N	4:I:55:VAL:HG13	2.32	0.45	
4:I:44:GLU:O	4:I:46:ALA:N	2.49	0.45	
3:A:59:HIS:O	3:A:60:ASN:HB3	2.17	0.45	
3:F:449:GLU:HB3	5:F:5043:HOH:O	2.16	0.45	
4:I:4:ILE:HG12	5:I:5003:HOH:O	2.16	0.45	
3:A:285:LYS:HG2	5:A:5041:HOH:O	2.17	0.45	
4:B:53:LEU:CD2	4:B:103:LEU:HD22	2.47	0.45	
3:F:168:MET:O	3:F:168:MET:HG3	2.17	0.45	
2:T:867:DG:C2'	2:T:868:DT:H5'	2.23	0.45	
3:A:547:ARG:O	3:A:551:LEU:HB2	2.17	0.44	
4:B:95:SER:OG	4:B:98:GLN:HG3	2.17	0.44	
3:F:496:TYR:CZ	3:F:505:ILE:HD11	2.52	0.44	
1:P:812:DG:H1'	1:P:813:DC:H5"	1.99	0.44	
2:T:860:DA:H2"	2:T:861:DC:H5'	1.99	0.44	
3:F:276:HIS:HA	3:F:277:PRO:HD3	1.88	0.44	
4:I:44:GLU:CG	4:I:45:ILE:N	2.79	0.44	
1:X:921:DA:O4'	3:F:439:GLN:HA	2.16	0.44	
3:A:146:MET:O	3:A:150:GLN:HG3	2.18	0.44	
3:A:181:LEU:O	3:A:185:LEU:HG	2.17	0.44	
3:F:326:TYR:HB3	4:I:92:GLY:HA2	1.98	0.44	
1:X:903:DA:H2"	1:X:904:DA:C8	2.52	0.44	
3:F:298:PHE:HA	3:F:315:LEU:C	2.38	0.44	
3:F:473:GLY:HA3	3:F:703:CYS:HB3	2.00	0.44	
3:A:94:LEU:HD21	3:A:214:VAL:HG13	1.99	0.44	
3:A:193:PRO:HA	3:A:194:PRO:HD3	1.84	0.44	
3:A:335:ASN:OD1	3:A:337:SER:HB2	2.17	0.44	
3:A:525:ILE:HG23	3:A:526:TYR:N	2.32	0.44	
3:F:234:PHE:CZ	3:F:239:ILE:HG13	2.53	0.44	
1:X:910:DC:H2"	1:X:911:DG:H5'	1.94	0.44	
3:A:267:PRO:HD3	4:B:31:TRP:CZ3	2.53	0.44	
3:F:585:GLN:HA	3:F:585:GLN:NE2	2.31	0.44	
4:I:42:LEU:O	4:I:43:ASP:CB	2.66	0.44	



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
4:I:67:ALA:HB3	4:I:68:PRO:HD3	1.99	0.44	
4:I:99:LEU:HD23	4:I:99:LEU:O	2.18	0.44	
3:A:63:LYS:HE2	3:A:228:GLU:OE1	2.18	0.43	
3·F·71·LYS·O	3·F·75·LEU·HD22	2.17	0.43	
3:A:106:ASP:HA	3:A:109:LEU:HD12	2.00	0.43	
3:F:12:LEU:HD21	3:F:229:ARG:HD3	2.00	0.43	
3:F:28:THR:O	3:F:29:ALA:CB	2.66	0.43	
3:A:135:MET:HE1	3:A:173:GLN:HE22	1.82	0.43	
3:A:318:ARG:NH1	3:A:319:GLU:HG2	2.33	0.43	
3:A:407:LEU:HA	3:A:407:LEU:HD23	1.83	0.43	
3:F:31:TYR:N	3:F:31:TYR:CD1	2.87	0.43	
3:F:622:CYS:SG	3:F:654:ASP:HA	2.59	0.43	
3:A:18:PHE:CD2	3:A:39:PHE:HB2	2.53	0.43	
3:A:235:ASP:HB2	3:A:459:HIS:CE1	2.54	0.43	
3:A:391:MET:HE3	3:A:395:ARG:HG3	1.99	0.43	
1:X:904:DA:H2"	1:X:905:DA:C8	2.54	0.43	
3:A:252:GLU:HG3	3:A:256:LYS:NZ	2.33	0.43	
3:A:506:HIS:CG	3:A:522:LYS:HG2	2.54	0.43	
4:B:107:LEU:HB2	5:B:5187:HOH:O	2.18	0.43	
3:F:373:ARG:HA	3:F:380:GLN:OE1	2.18	0.43	
3:F:233:PRO:HB2	3:F:456:GLY:O	2.18	0.43	
3:A:17:LYS:HB3	3:A:17:LYS:HZ3	1.83	0.43	
3:A:135:MET:HE2	3:A:135:MET:HA	2.01	0.43	
3:A:281:LYS:HA	3:A:282:PRO:HD3	1.93	0.43	
1:P:806:DA:H2"	1:P:807:DC:C6	2.54	0.43	
3:A:217:GLU:CD	3:A:599:ARG:HH22	2.22	0.43	
3:A:223:LEU:O	3:A:226:LYS:HB3	2.19	0.43	
3:A:488:MET:HB2	3:A:561:ALA:HB1	2.01	0.43	
3:A:621:ILE:HD11	3:A:686:PHE:CZ	2.54	0.43	
3:A:633:LEU:HD22	3:A:638:LEU:HD12	2.00	0.43	
4:I:42:LEU:O	4:I:43:ASP:HB2	2.19	0.43	
3:A:15:VAL:HG22	3:A:72:LEU:HD21	2.00	0.43	
3:A:173:GLN:O	3:A:177:VAL:HG23	2.19	0.43	
3:F:297:ILE:O	3:F:297:ILE:HG22	2.19	0.43	
3:F:321:VAL:HG22	4:I:90:LYS:CE	2.47	0.43	
3:F:551:LEU:HD12	3:F:551:LEU:HA	1.84	0.43	
3:A:72:LEU:HA	3:A:75:LEU:CD1	2.46	0.42	
3:A:685:ASN:HB3	5:A:5046:HOH:O	2.19	0.42	
3:F:182:LEU:O	3:F:186:LEU:HG	2.19	0.42	
4:I:45:ILE:CD1	4:I:99:LEU:HD13	2.49	0.42	
4:I:99:LEU:O	4:I:103:LEU:HG	2.19	0.42	



		Interatomic	Clash	
Atom-1	Atom-2	distance $(Å)$	overlap (Å)	
1:X:920:DC:H2"	1:X:921:DA:H5"	1.96	0.42	
3:F:17:LYS:HA	3:F:76:GLN:NE2	2.34	0.42	
4:I:58:LEU:HD11	4:I:63:ASN:CG	2.38	0.42	
3:A:184:LYS:O	3:A:184:LYS:HD3	2.20	0.42	
3:F:213:ALA:HA	3:F:597:ASP:OD2	2.19	0.42	
4:I:54:THR:O	4:I:54:THR:HG22	2.19	0.42	
2:Z:974:DT:H2"	2:Z:975:DC:C6	2.55	0.42	
3:A:182:LEU:O	3:A:186:LEU:HG	2.20	0.42	
3:F:475:ASP:OD2	3:F:475:ASP:N	2.52	0.42	
3:F:556:LEU:HD11	3:F:566:ARG:HH21	1.83	0.42	
3:A:446:PRO:O	3:A:447:TYR:HB2	2.19	0.42	
3:F:488:MET:HE3	3:F:561:ALA:HB3	2.01	0.42	
3:A:297:ILE:N	3:A:297:ILE:CD1	2.81	0.42	
1:P:817:DT:C2'	1:P:818:DG:H5'	2.36	0.42	
3:A:471:GLN:HB3	3:A:697:GLY:O	2.20	0.42	
3:F:102:LEU:HD12	3:F:123:HIS:CE1	2.55	0.42	
3:F:343:GLN:HG3	3:F:362:PRO:HG3	1.98	0.42	
4:I:77:THR:HG22	4:I:79:LEU:HD22	2.02	0.42	
4:B:8:THR:CG2	4:B:11:SER:H	2.30	0.42	
3:F:31:TYR:H	3:F:31:TYR:HD1	1.68	0.42	
3:F:136:LYS:HG3	3:F:173:GLN:NE2	2.34	0.42	
3:F:237:LYS:O	3:F:241:GLU:HG3	2.19	0.42	
3:A:196:ILE:HD12	3:A:196:ILE:N	2.35	0.42	
3:F:264:TRP:CD1	3:F:344:LYS:HE2	2.55	0.42	
4:I:12:PHE:CD1	4:I:13:ASP:N	2.81	0.42	
3:F:356:TYR:HD2	3:F:360:GLY:O	2.03	0.41	
3:F:702:ILE:C	3:F:704:HIS:H	2.22	0.41	
3:F:109:LEU:HD13	3:F:131:ARG:HG2	2.02	0.41	
3:F:285:LYS:HB3	3:F:285:LYS:HZ2	1.85	0.41	
3:F:554:LYS:HD3	3:F:554:LYS:HA	1.83	0.41	
3:F:621:ILE:HD11	3:F:686:PHE:CZ	2.55	0.41	
2:Z:971:DT:H2"	2:Z:972:DT:C7	2.51	0.41	
3:A:211:LEU:HD21	3:A:598:GLY:C	2.41	0.41	
3:F:196:ILE:HD12	3:F:196:ILE:N	2.36	0.41	
3:F:254:LEU:O	3:F:258:THR:HG23	2.19	0.41	
3:F:591:ARG:HD2	5:F:5316:HOH:O	2.18	0.41	
1:P:807:DC:C2'	1:P:808:DG:C5'	2.95	0.41	
2:T:868:DT:H2"	2:T:869:DC:H5'	2.02	0.41	
3:A:628:LYS:HE2	3:A:679:TRP:CD2	2.56	0.41	
3:F:525:ILE:HG23	3:F:526:TYR:N	2.35	0.41	
3:F:635:GLU:HA	3:F:635:GLU:OE2	2.20	0.41	



	A h o	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
3:A:276:HIS:HA	3:A:277:PRO:HD3	1.94	0.41	
3:A:290:LYS:HD2	3:A:328:PRO:CG	2.51	0.41	
3:A:490:ARG:HD3	3:A:491:PHE:CZ	2.55	0.41	
3:A:525:ILE:O	3:A:529:LEU:HB2	2.21	0.41	
3:F:473:GLY:O	3:F:694:GLY:HA2	2.20	0.41	
3:F:558:ASN:C	3:F:560:PRO:HD3	2.41	0.41	
3:A:139:TYR:CE2	3:A:159:GLU:HB2	2.56	0.41	
3:A:558:ASN:C	3:A:560:PRO:HD3	2.41	0.41	
4:B:45:ILE:HG13	4:B:99:LEU:HD12	2.02	0.41	
3:F:346:LEU:HD13	3:F:372:VAL:HG11	2.03	0.41	
3:F:391:MET:HE3	3:F:395:ARG:HG3	2.02	0.41	
4:I:49:TYR:HE2	4:I:107:LEU:HD12	1.85	0.41	
2:Z:967:DG:H2'	2:Z:968:DT:H72	2.02	0.41	
4:I:79:LEU:HD22	4:I:79:LEU:N	2.36	0.41	
3:A:193:PRO:HB3	3:A:195:GLU:OE1	2.21	0.41	
3:A:488:MET:HE3	3:A:561:ALA:HB3	2.03	0.41	
3:A:590:ARG:HD2	3:A:592:TRP:O	2.21	0.41	
4:B:48:GLU:OE2	4:B:96:LYS:NZ	2.49	0.41	
3:F:343:GLN:O	3:F:347:GLN:HG3	2.21	0.41	
3:A:168:MET:O	3:A:168:MET:HG3	2.20	0.41	
4:I:20:ASP:HA	4:I:23:ILE:HG13	2.03	0.41	
3:A:551:LEU:HD12	3:A:551:LEU:HA	1.91	0.40	
3:F:106:ASP:HA	3:F:109:LEU:HD12	2.03	0.40	
3:F:158:MET:HB2	3:F:161:TRP:CZ3	2.56	0.40	
3:F:228:GLU:OE1	3:F:420:VAL:N	2.47	0.40	
3:A:530:TYR:CD1	3:A:611:ASN:HB2	2.56	0.40	
4:B:32:CYS:SG	4:B:34:PRO:HD2	2.61	0.40	
3:F:633:LEU:HD22	3:F:638:LEU:CD1	2.47	0.40	
4:I:10:ASP:CG	4:I:11:SER:N	2.75	0.40	
1:X:906:DA:H2	2:Z:972:DT:O2	2.04	0.40	
1:X:915:DA:H2"	1:X:916:DG:C5'	2.50	0.40	
3:A:57:VAL:HG21	3:A:182:LEU:HD22	2.03	0.40	
3:A:356:TYR:HD2	3:A:360:GLY:O	2.04	0.40	
3:F:35:ARG:HB3	3:F:36:PRO:CD	2.50	0.40	
4:I:98:GLN:HA	4:I:101:GLU:HB3	2.02	0.40	
2:Z:952:DT:O2	2:Z:952:DT:C2'	2.69	0.40	
3:A:31:TYR:CD1	3:A:31:TYR:N	2.90	0.40	
3:A:554:LYS:HD3	3:A:554:LYS:HA	1.85	0.40	
3:F:345:LYS:HE2	3:F:345:LYS:HA	2.02	0.40	
3:F:411:ALA:HB3	3:F:413:ASP:OD1	2.21	0.40	
1:X:917:DT:C2'	1:X:918:DG:C5'	2.96	0.40	



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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:189:LYS:HG3	3:A:194:PRO:CG	2.40	0.40
3:A:274:PHE:HE1	4:B:37:MET:HE2	1.86	0.40
4:B:7:LEU:HB2	4:B:58:LEU:HD13	2.02	0.40
4:B:13:ASP:CG	4:B:17:LEU:HD12	2.42	0.40
3:F:125:LEU:HA	3:F:125:LEU:HD23	1.86	0.40
4:I:24:LEU:HD12	4:I:24:LEU:N	2.37	0.40
4:I:102:PHE:C	4:I:104:ASP:N	2.75	0.40

All (1) 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)
5:F:5072:HOH:O	5:F:5072:HOH:O[3_555]	1.46	0.74

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
3	А	702/704~(100%)	657 (94%)	39~(6%)	6 (1%)	17	35
3	F	685/704~(97%)	635~(93%)	43 (6%)	7 (1%)	15	32
4	В	103/108~(95%)	89~(86%)	10 (10%)	4 (4%)	3	4
4	Ι	101/108 (94%)	71 (70%)	19 (19%)	11 (11%)	0	0
All	All	1591/1624 (98%)	1452 (91%)	111 (7%)	28 (2%)	8	16

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	А	302	LYS
3	А	310	ARG
4	В	18	LYS



Mol	Chain	Res	Type
4	В	19	ALA
3	F	114	LYS
4	Ι	11	SER
4	Ι	20	ASP
4	Ι	44	GLU
3	А	308	GLU
3	А	313	CYS
4	В	15	ASP
3	F	116	PRO
3	F	117	GLY
3	F	154	TYR
4	Ι	87	ALA
3	А	152	GLU
4	Ι	46	ALA
3	А	156	ASP
4	В	84	GLY
3	F	495	GLU
4	Ι	13	ASP
4	Ι	16	VAL
4	Ι	21	GLY
3	F	653	HIS
4	Ι	18	LYS
4	Ι	43	ASP
3	F	296	GLY
4	Ι	45	ILE

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 sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Perce	entiles
3	А	563/582~(97%)	533~(95%)	30~(5%)	22	45
3	F	559/582~(96%)	528 (94%)	31 (6%)	21	43
4	В	84/87~(97%)	79~(94%)	5~(6%)	19	39
4	Ι	81/87~(93%)	79~(98%)	2 (2%)	47	73
All	All	1287/1338 (96%)	1219 (95%)	68 (5%)	22	45



All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	А	17	LYS
3	А	62	HIS
3	А	75	LEU
3	А	86	GLU
3	А	125	LEU
3	А	173	GLN
3	А	189	LYS
3	А	232	PHE
3	А	241	GLU
3	А	285	LYS
3	А	343	GLN
3	А	358	ASP
3	А	368	VAL
3	A	379	LYS
3	А	391	MET
3	А	410	VAL
3	А	420	VAL
3	А	423	ASN
3	А	426	VAL
3	А	449	GLU
3	А	501	LEU
3	А	529	LEU
3	А	554	LYS
3	А	567	GLU
3	А	584	GLN
3	А	599	ARG
3	А	624	LEU
3	А	630	GLU
3	А	654	ASP
3	А	686	PHE
4	В	15	ASP
4	В	37	MET
4	В	53	LEU
4	В	73	ARG
4	В	80	LEU
3	F	17	LYS
3	F	62	HIS
3	F	75	LEU
3	F	85	ARG
3	F	86	GLU
3	F	110	LEU
3	F	125	LEU



Mol	Chain	Res	Type
3	F	136	LYS
3	F	168	MET
3	F	169	ASP
3	F	171	ASN
3	F	181	LEU
3	F	232	PHE
3	F	285	LYS
3	F	315	LEU
3	F	343	GLN
3	F	359	LYS
3	F	391	MET
3	F	493	ASN
3	F	499	GLU
3	F	523	THR
3	F	529	LEU
3	F	551	LEU
3	F	559	THR
3	F	566	ARG
3	F	575	GLU
3	F	584	GLN
3	F	599	ARG
3	F	624	LEU
3	F	630	GLU
3	F	686	PHE
4	Ι	25	VAL
4	Ι	49	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
3	А	101	ASN
3	А	123	HIS
3	А	150	GLN
3	А	171	ASN
3	А	173	GLN
3	А	276	HIS
3	А	343	GLN
3	А	347	GLN
3	А	423	ASN
3	А	439	GLN
3	А	520	ASN
3	А	558	ASN



Mol	Chain	Res	Type
3	А	570	GLN
3	А	584	GLN
3	А	667	GLN
4	В	50	GLN
4	В	83	ASN
3	F	123	HIS
3	F	173	GLN
3	F	276	HIS
3	F	450	GLN
3	F	460	HIS
3	F	493	ASN
3	F	520	ASN
3	F	539	GLN
3	F	570	GLN
3	F	584	GLN
3	F	585	GLN
3	F	615	GLN
3	F	667	GLN
4	Ι	50	GLN
4	Ι	63	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

2 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	Turne	Chain	Dec Link		Bo	ond leng	$_{\rm ths}$	B	ond ang	gles
	туре	Chain	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	2DT	Р	822	1,2	14,20,21	1.18	2 (14%)	12,28,31	<mark>4.36</mark>	1 (8%)
1	2DT	Х	922	1,2	14,20,21	1.15	2 (14%)	12,28,31	4.43	1 (8%)



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	2DT	Р	822	1,2	-	1/4/18/19	0/2/2/2
1	2DT	Х	922	1,2	-	1/4/18/19	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Х	922	2DT	C4-N3	3.04	1.38	1.33
1	Р	822	2DT	C4-N3	2.83	1.38	1.33
1	Р	822	2DT	C6-C5	-2.34	1.33	1.40
1	Х	922	2DT	C6-C5	-2.27	1.33	1.40

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms		$Observed(^{o})$	$Ideal(^{o})$
1	Х	922	2DT	C4-N3-C2	14.85	127.68	115.14
1	Р	822	2DT	C4-N3-C2	14.72	127.57	115.14

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	Р	822	2DT	O4'-C1'-N1-C6
1	Х	922	2DT	O4'-C1'-N1-C6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	Р	822	2DT	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)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
4	Ι	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Ι	81:PHE	С	82:LYS	N	5.61



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	Р	19/22~(86%)	-0.58	0 100 100	50, 100, 170, 171	0
1	X	20/22~(90%)	-0.38	0 100 100	48, 100, 201, 201	0
2	Т	22/26~(84%)	-0.64	0 100 100	49, 90, 145, 153	0
2	Z	25/26~(96%)	-0.29	1 (4%) 38 31	49, 97, 183, 192	0
3	А	704/704~(100%)	-0.09	10 (1%) 75 71	38, 61, 116, 153	0
3	F	689/704~(97%)	-0.11	7 (1%) 82 80	38, 60, 105, 143	0
4	В	105/108~(97%)	0.23	7 (6%) 17 13	50, 93, 113, 116	0
4	Ι	105/108~(97%)	1.81	31 (29%) 0 0	51, 108, 147, 153	0
All	All	1689/1720~(98%)	0.02	56 (3%) 46 39	38, 64, 135, 201	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	Ι	16	VAL	17.9
4	Ι	84	GLY	11.7
4	Ι	53	LEU	11.5
4	Ι	87	ALA	9.7
4	Ι	83	ASN	9.4
4	Ι	82	LYS	7.8
4	Ι	19	ALA	6.7
3	F	299	LYS	6.5
4	Ι	86	VAL	6.5
4	Ι	102	PHE	6.4
4	Ι	22	ALA	5.7
4	Ι	105	ALA	5.2
4	Ι	106	ASN	5.1
4	Ι	18	LYS	4.8
4	Ι	23	ILE	4.5
2	Ζ	976	DG	4.4



Mol	Chain	Res	Type	RSRZ
4	Ι	17	LEU	4.4
4	Ι	94	LEU	4.3
3	А	318	ARG	4.1
4	Ι	107	LEU	3.9
4	Ι	85	GLU	3.8
4	Ι	104	ASP	3.8
3	А	301	PRO	3.5
3	F	297	ILE	3.5
4	В	22	ALA	3.5
4	Ι	80	LEU	3.5
4	Ι	21	GLY	3.3
4	Ι	24	LEU	3.3
4	В	80	LEU	3.3
3	А	324	ALA	3.2
4	В	16	VAL	3.1
4	Ι	20	ASP	3.1
3	А	298	PHE	3.1
4	Ι	4	ILE	3.1
4	Ι	6	HIS	3.1
4	Ι	79	LEU	3.1
4	Ι	3	LYS	3.1
3	F	136	LYS	3.0
3	А	319	GLU	3.0
3	F	530	TYR	3.0
3	А	300	LYS	2.9
4	Ι	101	GLU	2.8
4	Ι	9	ASP	2.4
4	Ι	26	ASP	2.4
3	F	318	ARG	2.3
4	В	4	ILE	2.3
3	F	161	TRP	2.3
3	А	299	LYS	2.3
4	В	102	PHE	2.3
4	В	94	LEU	2.3
3	А	294	VAL	2.2
3	F	315	LEU	2.2
3	А	302	LYS	2.1
4	В	53	LEU	2.1
4	Ι	99	LEU	2.1
3	А	182	LEU	2.0

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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	B-factors(Å ²)	Q<0.9
1	2DT	Р	822	19/20	0.97	0.14	48,50,55,56	0
1	2DT	Х	922	19/20	0.97	0.14	48,52,57,59	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.

