

Full wwPDB X-ray Structure Validation Report (i)

Feb 21, 2024 – 07:20 AM EST

PDB ID	:	4Q4Z
Title	:	Thermus thermophilus RNA polymerase de novo transcription initiation com-
		plex
Authors	:	Murakami, K.S.
Deposited on	:	2014-04-15
Resolution	:	2.90 Å(reported)

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

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

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

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7(2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 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 2.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R _{free}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain		
1	٨	215	4%		
1	A	515	59% 14%	27%	
	-		4%		
1	В	315	60% 12%	28%	
			7%		
2	С	1119	79%	19%	••
			9%		
3	D	1524	76%	20%	••
			7%		
4	Е	99	82%	13%	5%



Mol	Chain	Length	Qu	ality of chain	
-	Б	100	14%		
5	F.	423	66%	1	.5% 18%
			5%		
6	G	22	36%	41%	5% 18%
			11%		
7	Н	27	48%	33%	11% 7%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	MG	D	2004	-	-	-	Х



2 Entry composition (i)

There are 12 unique types of molecules in this entry. The entry contains 28755 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

• Molecule 1 is a protein called DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues		Ate	oms		ZeroOcc	AltConf	Trace	
1	Δ	021	Total	С	Ν	Ο	S	0	0	0
		201	1809	1155	315	337	2	0	0	0
1	р	227	Total	С	Ν	0	S	0	0	0
	D	221	1789	1143	310	334	2	0	U	0

• Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues		A	toms		ZeroOcc	AltConf	Trace	
2	С	1112	Total 8774	$\begin{array}{c} \mathrm{C} \\ 5550 \end{array}$	N 1565	O 1635	S 24	0	0	0

• Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues		A	toms		ZeroOcc	AltConf	Trace	
3	D	1494	Total 11808	C 7484	N 2083	O 2205	S 36	0	1	0

• Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues		At	oms		ZeroOcc	AltConf	Trace	
4	Е	94	Total 761	C 486	N 132	0 139	$\frac{S}{4}$	0	0	0

• Molecule 5 is a protein called RNA polymerase sigma factor SigA.

Mol	Chain	Residues		At	oms		ZeroOcc	AltConf	Trace	
5	F	346	Total 2807	C 1770	N 509	0 524	$\frac{S}{4}$	0	0	0

• Molecule 6 is a DNA chain called DNA (5'-D(*CP*CP*TP*GP*CP*AP*TP*CP*CP*GP* TP*GP*AP*GP*TP*GP*CP*AP*GP*CP*A)-3').



Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
6	G	18	Total 370	C 175	N 68	O 109	Р 18	0	0	0

• Molecule 7 is a DNA chain called DNA (25-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	Н	25	Total 516	C 246	N 99	0 147	Р 24	0	0	0

• Molecule 8 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
0	C	1	Total	С	Ν	Ο	Р	0	0
0	C	1	31	10	5	13	3	0	0

• Molecule 9 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	D	2	Total Z 2	Zn 2	0	0

• Molecule 10 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	D	3	Total Mg 3 3	0	0



• Molecule 11 is 5'-O-[(S)-hydroxy{[(S)-hydroxy(phosphonooxy)phosphoryl]methyl}phosphoryl]cytidine (three-letter code: 2TM) (formula: $C_{10}H_{18}N_3O_{13}P_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf		
11	D	1	Total	C	N	0	Р	0	0	
	2	-	29	10	3	13	3		-	

• Molecule 12 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	А	4	Total O 4 4	0	0
12	В	1	Total O 1 1	0	0
12	С	22	Total O 22 22	0	0
12	D	26	TotalO2626	0	0
12	Е	2	Total O 2 2	0	0
12	G	1	Total O 1 1	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-directed RNA polymerase subunit alpha



N543 T544 N545 N545 S541

V5 13

9%

3230 2331

T788 S789











• Molecule 6: DNA (5'-D(*CP*CP*TP*GP*CP*AP*TP*CP*CP*GP*TP*GP*AP*GP*TP*GP *CP*AP*GP*CP*CP*A)-3')







4 Data and refinement statistics (i)

Property	Value	Source	
Space group	C 1 2 1	Depositor	
Cell constants	184.49Å 102.16Å 294.72Å	Depositor	
a, b, c, α , β , γ	90.00° 98.96° 90.00°	Depositor	
Bosolution(A)	29.78 - 2.90	Depositor	
Resolution (A)	43.54 - 2.85	EDS	
% Data completeness	89.5 (29.78-2.90)	Depositor	
(in resolution range)	84.3(43.54-2.85)	EDS	
R_{merge}	(Not available)	Depositor	
R _{sym}	(Not available)	Depositor	
$< I/\sigma(I) > 1$	$1.30 (at 2.86 \text{\AA})$	Xtriage	
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor	
D D.	0.256 , 0.275	Depositor	
Π, Π_{free}	0.258 , 0.275	DCC	
R_{free} test set	1753 reflections $(1.57%)$	wwPDB-VP	
Wilson B-factor $(Å^2)$	45.3	Xtriage	
Anisotropy	0.753	Xtriage	
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.27, 18.5	EDS	
L-test for twinning ²	$< L > = 0.43, < L^2 > = 0.26$	Xtriage	
Estimated twinning fraction	No twinning to report.	Xtriage	
F_o, F_c correlation	0.88	EDS	
Total number of atoms	28755	wwPDB-VP	
Average B, all atoms $(Å^2)$	70.0	wwPDB-VP	

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.74% 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: MG, ATP, ZN, 2TM $\,$

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	B	ond angles
WIOI	Ullalli	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.24	0/1841	0.46	0/2504
1	В	0.22	0/1821	0.44	0/2476
2	С	0.31	1/8941~(0.0%)	0.50	6/12092~(0.0%)
3	D	0.35	1/12019~(0.0%)	0.50	4/16248~(0.0%)
4	Ε	0.24	0/775	0.41	0/1045
5	F	0.23	0/2852	0.40	0/3837
6	G	0.72	2/414~(0.5%)	1.16	3/637~(0.5%)
7	Н	0.57	0/580	1.13	3/895~(0.3%)
All	All	0.33	4/29243~(0.0%)	0.52	16/39734 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1093	TYR	CE2-CZ	-6.38	1.30	1.38
6	G	18	DA	O3'-P	-5.67	1.54	1.61
6	G	3	DT	O3'-P	-5.63	1.54	1.61
2	С	769	PRO	N-CD	5.43	1.55	1.47

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	С	761	PHE	O-C-N	-10.43	106.01	122.70
6	G	18	DA	O4'-C1'-N9	9.34	114.54	108.00
3	D	1257	PRO	CA-N-CD	-8.41	99.72	111.50
3	D	1232	PRO	CA-N-CD	-7.58	100.88	111.50
2	С	761	PHE	C-N-CA	7.11	139.47	121.70
2	С	761	PHE	CA-C-N	7.08	132.78	117.20
6	G	18	DA	C4'-C3'-C2'	6.18	108.67	103.10
3	D	1256	LEU	C-N-CD	6.01	141.01	128.40
2	С	766	GLU	C-N-CD	5.84	140.67	128.40



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	С	765	SER	N-CA-C	-5.53	96.06	111.00
3	D	1231	GLU	C-N-CD	5.36	139.65	128.40
6	G	18	DA	O5'-P-OP1	5.31	117.08	110.70
7	Н	15	DT	O4'-C1'-N1	5.30	111.71	108.00
2	С	769	PRO	CA-N-CD	-5.24	104.16	111.50
7	Н	20	DG	C1'-O4'-C4'	-5.24	104.86	110.10
7	Н	12	DC	O4'-C1'-N1	5.20	111.64	108.00

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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	А	1809	0	1863	38	0
1	В	1789	0	1841	24	0
2	С	8774	0	8877	226	3
3	D	11808	0	12041	258	4
4	Е	761	0	778	9	1
5	F	2807	0	2882	101	2
6	G	370	0	202	19	0
7	Н	516	0	283	31	1
8	С	31	0	11	2	0
9	D	2	0	0	0	0
10	D	3	0	0	0	0
11	D	29	0	14	2	0
12	А	4	0	0	9	0
12	В	1	0	0	0	0
12	С	22	0	0	29	0
12	D	26	0	0	26	0
12	Е	2	0	0	1	0
12	G	1	0	0	0	0
All	All	28755	0	28792	605	6

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 11.



Atom-1	Atom-2	Interatomic	Clash
		distance (A)	overlap (A)
2:C:773:LEU:CD2	5:F:373:LYS:HG3	1.14	1.60
5:F:358:LEU:HD13	5:F:370:LYS:NZ	1.33	1.41
2:C:773:LEU:CD2	5:F:373:LYS:CG	2.03	1.36
2:C:778:PHE:HE2	5:F:419:ARG:NH2	1.25	1.35
2:C:764:GLU:O	2:C:766:GLU:N	1.62	1.32
5:F:358:LEU:CD1	5:F:370:LYS:CE	2.09	1.30
5:F:358:LEU:CD1	5:F:370:LYS:NZ	1.92	1.30
2:C:768:THR:O	2:C:771:GLU:N	1.65	1.28
5:F:355:GLU:OE1	5:F:358:LEU:HD12	1.21	1.27
5:F:358:LEU:HD11	5:F:370:LYS:CE	1.64	1.26
1:A:107:LYS:HG3	12:A:404:HOH:O	1.23	1.25
2:C:778:PHE:CE2	5:F:419:ARG:NH2	2.08	1.21
2:C:764:GLU:OE1	3:D:54:LYS:HE2	1.37	1.20
2:C:778:PHE:HE2	5:F:419:ARG:CZ	1.55	1.19
3:D:1091:SER:OG	3:D:1234:THR:OG1	1.61	1.17
2:C:778:PHE:CE2	5:F:419:ARG:CZ	2.26	1.17
2:C:996:LYS:HG2	12:C:1321:HOH:O	1.44	1.17
2:C:878:SER:HB3	12:C:1301:HOH:O	1.44	1.16
2:C:773:LEU:HD23	5:F:373:LYS:HG3	1.25	1.15
5:F:358:LEU:CD1	5:F:370:LYS:HZ1	1.50	1.14
12:C:1314:HOH:O	5:F:331:ASP:HA	1.45	1.14
2:C:773:LEU:HD22	5:F:373:LYS:CG	1.69	1.11
5:F:358:LEU:HD11	5:F:370:LYS:HE2	1.21	1.11
2:C:773:LEU:HD23	5:F:373:LYS:CB	1.80	1.10
2:C:773:LEU:HD12	2:C:777:ILE:HD11	1.29	1.10
7:H:21:DA:H2"	7:H:22:DT:H5'	1.30	1.09
6:G:6:DA:N1	7:H:22:DT:N3	2.01	1.08
2:C:717:LEU:CD2	2:C:763:GLY:HA2	1.86	1.06
2:C:773:LEU:HD23	5:F:373:LYS:CG	1.73	1.06
3:D:1056:PRO:HA	12:D:2114:HOH:O	1.54	1.04
1:A:107:LYS:CG	12:A:404:HOH:O	1.83	1.04
1:A:107:LYS:CD	12:A:404:HOH:O	2.01	1.04
3:D:1044:LEU:HA	12:D:2114:HOH:O	1.57	1.04
1:A:107:LYS:HE2	12:A:404:HOH:O	1.54	1.03
2:C:774:LEU:HA	2:C:777:ILE:HD12	1.39	1.01
3:D:538:SER:HB2	12:D:2119:HOH:O	1.60	1.01
3:D:1223:ILE:O	3:D:1227:GLN:HG3	1.60	1.01
2:C:717:LEU:HD21	2:C:763:GLY:HA2	1.44	1.00
2:C:768:THR:O	2:C:770:GLU:N	1.95	0.99
2:C:728:HIS:HB3	5:F:423:ASP:O	1.61	0.98

All (605) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
3:D:65:ARG:CZ	3:D:68:PHE:CE2	2.47	0.97
1:A:107:LYS:CE	12:A:404:HOH:O	2.08	0.97
2:C:543:ASN:HB3	12:C:1316:HOH:O	0.79	0.96
5:F:358:LEU:HD13	5:F:370:LYS:CE	1.82	0.96
6:G:7:DT:H3	7:H:21:DA:N6	1.65	0.95
2:C:777:ILE:HA	5:F:405:LEU:HD11	1.48	0.94
3:D:538:SER:CB	12:D:2119:HOH:O	2.16	0.93
3:D:1235:GLN:HG3	3:D:1239:ARG:HD3	1.50	0.92
3:D:1081:GLY:O	3:D:1084:THR:OG1	1.85	0.92
2:C:764:GLU:OE1	3:D:54:LYS:CE	2.19	0.91
2:C:1041:GLU:HG2	12:C:1315:HOH:O	1.69	0.91
2:C:268:ASP:HA	12:C:1307:HOH:O	1.71	0.90
2:C:768:THR:C	2:C:770:GLU:H	1.75	0.89
2:C:481:ASP:HA	12:C:1322:HOH:O	1.72	0.88
2:C:880:MET:CE	3:D:1242:HIS:CD2	2.55	0.88
5:F:358:LEU:HD13	5:F:370:LYS:HZ1	0.71	0.88
2:C:774:LEU:HA	2:C:777:ILE:CD1	2.02	0.88
3:D:206:ARG:NH2	5:F:101:GLU:OE2	2.06	0.88
3:D:65:ARG:NH2	3:D:68:PHE:CE2	2.41	0.88
5:F:358:LEU:CD1	5:F:370:LYS:HE3	2.04	0.87
3:D:65:ARG:CZ	3:D:68:PHE:HE2	1.87	0.87
3:D:947:ILE:HA	12:D:2120:HOH:O	1.73	0.86
3:D:1225:ALA:O	3:D:1229:ILE:HD12	1.76	0.85
5:F:355:GLU:OE1	5:F:358:LEU:CD1	2.18	0.85
2:C:764:GLU:CD	3:D:54:LYS:HE2	1.96	0.85
3:D:581:LEU:HD21	12:D:2108:HOH:O	1.77	0.84
2:C:768:THR:C	2:C:770:GLU:N	2.27	0.83
2:C:778:PHE:CZ	5:F:419:ARG:CZ	2.61	0.83
11:D:2006:2TM:H1	11:D:2006:2TM:H10	1.60	0.83
2:C:880:MET:HE1	3:D:1242:HIS:CD2	2.14	0.83
5:F:357:ALA:O	5:F:360:LYS:HB2	1.78	0.82
2:C:802:ARG:HB2	2:C:826:TYR:HB2	1.62	0.81
2:C:717:LEU:HD23	2:C:763:GLY:HA2	1.61	0.81
7:H:21:DA:C2'	7:H:22:DT:H5'	2.09	0.81
2:C:764:GLU:O	2:C:765:SER:C	2.20	0.80
2:C:472:ARG:HD2	12:C:1322:HOH:O	1.83	0.79
2:C:774:LEU:CA	2:C:777:ILE:HD12	2.11	0.79
3:D:1086:LEU:O	3:D:1089:ALA:HB3	1.82	0.78
7:H:20:DG:H2"	7:H:21:DA:C5'	2.14	0.78
2:C:773:LEU:CD1	2:C:777:ILE:HD11	2.13	0.77
3:D:675:ARG:NH2	5:F:420:ASP:O	2.17	0.77



Atom-1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:C:762:LYS:HG2	2:C:784:ASP:O	1.85	0.77
2:C:773:LEU:HD22	5:F:373:LYS:HG3	0.77	0.77
3:D:68:PHE:O	3:D:80:VAL:HG23	1.84	0.77
2:C:773:LEU:HD23	5:F:373:LYS:HB2	1.67	0.77
2:C:880:MET:HE2	3:D:1242:HIS:CD2	2.19	0.77
3:D:65:ARG:NH2	3:D:68:PHE:HE2	1.78	0.77
6:G:7:DT:C2	7:H:21:DA:N1	2.53	0.77
2:C:422:ARG:HD2	7:H:15:DT:OP2	1.84	0.76
5:F:355:GLU:CD	5:F:358:LEU:HD12	2.07	0.76
3:D:1082:ALA:O	3:D:1086:LEU:HD13	1.87	0.74
5:F:358:LEU:CD2	5:F:370:LYS:HE3	2.17	0.74
3:D:1432:LYS:HD3	12:D:2122:HOH:O	1.86	0.74
2:C:409:ARG:HH11	2:C:454:SER:HB2	1.53	0.74
2:C:758:ARG:HH21	2:C:788:THR:HB	1.53	0.73
2:C:165:LEU:HB2	2:C:168:ARG:HG3	1.68	0.73
2:C:1030:GLN:OE1	3:D:628:ARG:NH1	2.20	0.73
6:G:7:DT:O2	7:H:21:DA:N1	2.21	0.73
5:F:361:LEU:HD11	5:F:408:LEU:HG	1.72	0.72
7:H:20:DG:H2"	7:H:21:DA:H5"	1.72	0.72
3:D:1084:THR:O	3:D:1088:THR:OG1	2.07	0.72
2:C:764:GLU:O	2:C:766:GLU:HG3	1.90	0.71
2:C:541:SER:HB2	12:C:1302:HOH:O	1.90	0.71
2:C:167:LYS:HD3	7:H:12:DC:H5	1.55	0.71
2:C:728:HIS:HD2	5:F:423:ASP:HB2	1.54	0.71
3:D:65:ARG:CD	5:F:379:ARG:HB3	2.21	0.71
3:D:63:TYR:HD1	3:D:68:PHE:CE1	2.09	0.70
3:D:266:GLU:HG3	3:D:314:PRO:HB3	1.73	0.70
6:G:4:DG:H2"	6:G:5:DC:OP2	1.91	0.70
1:B:176:ARG:NH2	3:D:888:GLU:OE1	2.25	0.70
3:D:68:PHE:O	3:D:80:VAL:CG2	2.39	0.70
2:C:628:PHE:H	2:C:638:ASP:HB3	1.57	0.69
2:C:717:LEU:CD2	2:C:763:GLY:CA	2.69	0.69
3:D:65:ARG:NH2	3:D:68:PHE:CZ	2.60	0.69
1:B:80:LEU:HD21	3:D:842:VAL:HG12	1.73	0.69
3:D:1255:GLY:O	3:D:1259:VAL:HG23	1.93	0.69
3:D:272:LEU:HB2	3:D:280:ALA:HB3	1.75	0.68
1:A:39:PRO:HG3	1:B:39:PRO:HG3	1.74	0.68
2:C:674:VAL:HG12	2:C:869:VAL:HB	1.75	0.68
2:C:428:ARG:NH2	2:C:447:ALA:O	2.27	0.68
2:C:771:GLU:HB3	2:C:775:ARG:NH2	2.09	0.67
3:D:208:PRO:HA	3:D:390:PRO:HA	1.77	0.67



Atom_1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
5:F:400:ILE:HA	5:F:403:LYS:HG2	1.77	0.67
3:D:576:GLU:HB3	12:D:2102:HOH:O	1.95	0.67
7:H:21:DA:H2"	7:H:22:DT:C5'	2.18	0.67
2:C:773:LEU:HD12	2:C:777:ILE:CD1	2.17	0.66
3:D:1093:TYR:OH	3:D:1441:GLN:NE2	2.28	0.66
3:D:1228:SER:O	3:D:1232:PRO:HD2	1.95	0.66
3:D:1240:THR:O	3:D:1241:PHE:HB2	1.94	0.66
2:C:709:GLU:OE2	2:C:824:ARG:NH1	2.29	0.66
2:C:721:ARG:HH22	2:C:785:VAL:HG11	1.61	0.66
2:C:230:ARG:HD3	2:C:231:PRO:HD2	1.78	0.66
2:C:768:THR:O	2:C:770:GLU:C	2.35	0.66
3:D:526:PRO:HD2	12:D:2119:HOH:O	1.95	0.66
2:C:670:GLN:HE21	2:C:700:TYR:H	1.42	0.65
2:C:784:ASP:OD2	2:C:784:ASP:N	2.29	0.65
3:D:356:PRO:HG2	3:D:359:ALA:HB2	1.77	0.65
3:D:1044:LEU:O	3:D:1244:GLY:HA2	1.95	0.65
3:D:433:GLY:HA2	3:D:449:SER:H	1.62	0.65
5:F:357:ALA:HA	5:F:360:LYS:CG	2.27	0.65
2:C:936:VAL:HG11	2:C:959:PRO:HB2	1.79	0.65
3:D:411:THR:O	5:F:178:ARG:NH1	2.26	0.65
2:C:778:PHE:HE2	5:F:419:ARG:HH22	1.37	0.65
3:D:947:ILE:HD13	12:D:2120:HOH:O	1.97	0.65
3:D:1231:GLU:OE1	3:D:1232:PRO:HD3	1.97	0.65
3:D:318:ARG:NH1	3:D:338:GLU:OE1	2.30	0.64
2:C:717:LEU:HD21	2:C:763:GLY:CA	2.24	0.64
5:F:355:GLU:O	5:F:358:LEU:HB2	1.97	0.64
3:D:1253:THR:OG1	3:D:1254:GLN:N	2.31	0.64
6:G:7:DT:N3	7:H:21:DA:N6	2.28	0.64
1:A:222:LEU:HD21	1:B:218:LEU:HD23	1.80	0.64
3:D:63:TYR:CD1	3:D:68:PHE:CE1	2.85	0.64
2:C:764:GLU:C	2:C:766:GLU:N	2.49	0.64
3:D:1233:GLY:O	3:D:1237:THR:OG1	2.16	0.63
3:D:1252:ILE:HG13	3:D:1252:ILE:O	1.98	0.63
3:D:561:GLY:HA3	5:F:132:ARG:HD3	1.79	0.63
3:D:316:GLN:NE2	3:D:340:THR:O	2.31	0.63
5:F:365:GLU:HB2	5:F:404:ALA:HB2	1.81	0.63
2:C:172:ILE:HG12	2:C:186:VAL:HG22	1.80	0.63
3:D:711:LEU:HD13	3:D:778:LEU:HD23	1.80	0.63
3:D:1465:ASN:OD1	3:D:1470:ARG:NH1	2.31	0.63
5:F:357:ALA:HA	5:F:360:LYS:HG2	1.81	0.63
3:D:1263:PHE:HD2	3:D:1375:MET:HE2	1.64	0.62



A 4 1	A + D	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
2:C:562:SER:HA	12:C:1316:HOH:O	1.99	0.62
3:D:1083:ASP:OD2	3:D:1253:THR:HG22	2.00	0.62
5:F:361:LEU:HB3	5:F:365:GLU:HG3	1.82	0.62
3:D:569:ASN:ND2	5:F:214:GLN:OE1	2.28	0.62
3:D:895:VAL:HG11	3:D:922:LEU:HD21	1.81	0.62
3:D:65:ARG:HD3	5:F:379:ARG:HB3	1.81	0.61
3:D:356:PRO:HB3	3:D:441:ARG:HA	1.82	0.61
3:D:534:ARG:NH2	5:F:313:GLU:O	2.33	0.61
2:C:939:ARG:HG2	2:C:982:PRO:HD3	1.82	0.61
5:F:358:LEU:HD13	5:F:370:LYS:HE3	1.73	0.61
3:D:671:LYS:NZ	5:F:421:PHE:HA	2.14	0.61
2:C:773:LEU:O	2:C:777:ILE:HG13	2.01	0.61
3:D:260:GLU:OE1	3:D:273:ARG:NH1	2.32	0.61
6:G:6:DA:H2"	6:G:7:DT:C5'	2.30	0.61
2:C:763:GLY:C	2:C:765:SER:H	2.04	0.60
2:C:376:ARG:HE	5:F:276:ARG:HG3	1.66	0.60
2:C:711:GLU:HG2	2:C:822:VAL:HG22	1.83	0.60
2:C:274:ARG:HD2	2:C:288:ARG:HG2	1.83	0.60
12:C:1315:HOH:O	3:D:1462:LEU:HB3	2.01	0.60
3:D:1432:LYS:O	3:D:1455:LYS:NZ	2.34	0.60
1:B:128:HIS:HE1	1:B:131:THR:HG23	1.66	0.60
2:C:764:GLU:O	2:C:766:GLU:CA	2.48	0.60
3:D:959:GLU:OE1	3:D:959:GLU:N	2.30	0.60
3:D:846:PRO:HD2	12:D:2115:HOH:O	2.02	0.60
4:E:32:ARG:O	4:E:95:VAL:HG21	2.01	0.60
3:D:1091:SER:OG	3:D:1234:THR:CB	2.48	0.60
3:D:1231:GLU:HB3	3:D:1232:PRO:CD	2.32	0.59
2:C:960:GLU:CB	12:C:1303:HOH:O	2.51	0.59
1:B:216:GLU:OE1	1:B:219:ARG:NH2	2.32	0.59
1:A:196:THR:HG21	2:C:934:PHE:HE2	1.68	0.59
2:C:768:THR:O	2:C:770:GLU:CA	2.51	0.59
6:G:7:DT:C4	7:H:21:DA:N6	2.57	0.59
7:H:20:DG:H2"	7:H:21:DA:H5'	1.83	0.59
3:D:65:ARG:NE	3:D:68:PHE:HE2	1.99	0.59
3:D:845:ASN:HB2	12:D:2115:HOH:O	2.01	0.58
1:B:100:LEU:HG	1:B:141:GLU:HG2	1.86	0.58
3:D:1231:GLU:HB3	3:D:1232:PRO:HD2	1.85	0.58
1:B:94:LEU:O	1:B:146:ARG:NH2	2.36	0.57
7:H:20:DG:C2'	7:H:21:DA:H5"	2.33	0.57
2:C:422:ARG:CD	7:H:15:DT:OP2	2.51	0.57
2:C:581:THR:HB	12:C:1312:HOH:O	2.04	0.57



Atom-1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:C:376:ARG:NE	5:F:276:ARG:HG3	2.19	0.57
2:C:778:PHE:CE2	5:F:419:ARG:NH1	2.71	0.57
3:D:1495:ILE:HG12	4:E:88:GLU:HG3	1.87	0.57
5:F:358:LEU:CD1	5:F:370:LYS:HZ3	2.12	0.57
3:D:167:GLU:OE2	3:D:198:ARG:NH1	2.38	0.57
3:D:45:PHE:O	3:D:86:ARG:NH2	2.37	0.57
3:D:65:ARG:NE	3:D:68:PHE:CE2	2.71	0.57
5:F:233:PHE:CD2	7:H:2:DA:H1'	2.40	0.57
2:C:168:ARG:HD3	2:C:268:ASP:HB3	1.87	0.57
2:C:164:PRO:HA	2:C:269:LEU:HD23	1.87	0.56
3:D:1364:HIS:CE1	3:D:1366:LYS:HG3	2.41	0.56
2:C:878:SER:CB	12:C:1301:HOH:O	2.24	0.56
3:D:1492:LEU:HD22	4:E:74:VAL:HG21	1.87	0.56
1:A:106:PRO:HD3	1:A:134:GLU:HG2	1.88	0.56
2:C:628:PHE:H	2:C:638:ASP:CB	2.19	0.56
1:A:24:VAL:HG22	1:A:196:THR:HG23	1.88	0.56
1:A:70:GLY:N	2:C:607:ASP:OD1	2.38	0.56
1:B:56:VAL:HG22	1:B:142:VAL:HG12	1.87	0.55
3:D:1045:MET:HE1	3:D:1243:THR:O	2.07	0.55
3:D:474:GLU:HG3	3:D:496:LEU:HD11	1.88	0.55
5:F:120:THR:HG22	5:F:122:LEU:HD13	1.87	0.55
2:C:198:ARG:HE	2:C:227:PHE:HA	1.72	0.55
2:C:728:HIS:CB	5:F:423:ASP:O	2.45	0.55
1:B:128:HIS:CE1	1:B:131:THR:HG23	2.41	0.55
2:C:35:PRO:HG2	2:C:38:LYS:HD2	1.88	0.55
2:C:409:ARG:HD2	12:C:1311:HOH:O	2.06	0.55
2:C:419:THR:HG22	2:C:422:ARG:HE	1.71	0.55
1:B:93:SER:O	1:B:95:GLN:NE2	2.39	0.55
3:D:526:PRO:CD	12:D:2119:HOH:O	2.54	0.55
3:D:1229:ILE:CG2	3:D:1356:TYR:OH	2.55	0.55
3:D:411:THR:HG23	3:D:436:GLU:HA	1.89	0.55
3:D:1143:GLY:O	3:D:1147:ARG:HD2	2.06	0.55
6:G:6:DA:H2"	6:G:7:DT:H5'	1.87	0.55
3:D:63:TYR:CD1	3:D:68:PHE:HE1	2.25	0.55
1:A:31:GLY:HA2	12:A:403:HOH:O	2.06	0.55
3:D:1042:ARG:HB3	3:D:1057:VAL:HB	1.88	0.55
2:C:353:ARG:NH1	2:C:357:GLU:OE2	2.40	0.54
3:D:236:TYR:HB2	3:D:319:ALA:HB3	1.87	0.54
2:C:629:TYR:HB3	12:C:1319:HOH:O	2.08	0.54
3:D:56:TYR:CE2	3:D:66:GLN:HG3	2.42	0.54
1:A:231:ALA:HB2	1:B:12:THR:HG22	1.89	0.54



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:C:243:ARG:NH1	7:H:9:DG:O6	2.39	0.54
2:C:773:LEU:CD1	2:C:777:ILE:CG1	2.85	0.54
3:D:657:LEU:HG	3:D:661:MET:HE2	1.89	0.54
6:G:7:DT:O2	7:H:21:DA:C2	2.59	0.54
2:C:167:LYS:HD3	7:H:12:DC:C5	2.41	0.54
2:C:778:PHE:CZ	5:F:419:ARG:NE	2.75	0.54
3:D:846:PRO:CD	12:D:2115:HOH:O	2.55	0.54
6:G:5:DC:H1'	6:G:6:DA:C8	2.43	0.54
2:C:937:ASP:OD1	2:C:939:ARG:HD3	2.08	0.54
2:C:838:LYS:NZ	8:C:1201:ATP:O1A	2.41	0.53
5:F:357:ALA:C	5:F:360:LYS:HB2	2.28	0.53
2:C:64:LEU:HB3	2:C:100:LEU:HD11	1.90	0.53
3:D:697:GLY:HA3	12:E:101:HOH:O	2.09	0.53
3:D:618:LEU:HG	3:D:1467:ILE:HG23	1.90	0.53
3:D:1235:GLN:O	3:D:1239:ARG:HB2	2.09	0.53
5:F:358:LEU:HD22	5:F:370:LYS:HE3	1.89	0.53
2:C:261:ILE:HG23	2:C:290:LEU:HB2	1.89	0.53
2:C:778:PHE:HZ	5:F:419:ARG:NE	2.07	0.53
3:D:1372:VAL:HA	3:D:1375:MET:HE3	1.90	0.53
2:C:835:VAL:HG23	12:C:1308:HOH:O	2.09	0.53
3:D:137:PRO:HA	3:D:452:ILE:HG13	1.90	0.53
3:D:1324:PRO:HG3	3:D:1330:ILE:HD11	1.90	0.53
2:C:598:GLU:O	2:C:651:LYS:NZ	2.35	0.53
3:D:894:LYS:H	3:D:894:LYS:HD2	1.74	0.53
1:A:199:ILE:HB	1:A:207:PRO:HB3	1.91	0.52
2:C:422:ARG:CG	7:H:15:DT:OP2	2.57	0.52
2:C:425:PHE:O	2:C:427:VAL:N	2.42	0.52
2:C:557:ARG:HD3	2:C:879:ARG:HB3	1.90	0.52
5:F:163:LEU:HD13	5:F:174:LEU:HD13	1.92	0.52
2:C:260:LEU:HB3	2:C:261:ILE:HD12	1.92	0.52
3:D:439:LEU:CD1	5:F:172:ARG:HG3	2.40	0.52
3:D:658:LEU:HA	3:D:661:MET:HE3	1.92	0.52
3:D:1147:ARG:HD3	3:D:1188:VAL:HG11	1.91	0.52
3:D:65:ARG:C	3:D:66:GLN:O	2.46	0.52
3:D:684:LYS:O	3:D:687:VAL:HG12	2.09	0.52
2:C:223:ASP:OD1	2:C:225:SER:OG	2.24	0.52
5:F:397:ILE:HD12	5:F:400:ILE:HD11	1.90	0.52
6:G:15:DT:H2'	6:G:16:DG:C8	2.44	0.52
3:D:1086:LEU:CD1	3:D:1086:LEU:N	2.72	0.52
2:C:217:LEU:HD12	2:C:217:LEU:H	1.73	0.52
2:C:427:VAL:O	2:C:427:VAL:HG22	2.08	0.52



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
2:C:541:SER:O	2:C:545:ASN:ND2	2.43	0.52
3:D:65:ARG:O	3:D:68:PHE:HB2	2.08	0.52
3:D:1253:THR:O	3:D:1257:PRO:HD2	2.10	0.52
5:F:355:GLU:HA	5:F:358:LEU:HG	1.91	0.52
2:C:675:ALA:HB2	2:C:867:VAL:HG11	1.91	0.52
3:D:439:LEU:HD13	5:F:172:ARG:HG3	1.91	0.52
3:D:1253:THR:O	3:D:1257:PRO:HG2	2.10	0.52
2:C:717:LEU:HD23	2:C:763:GLY:CA	2.37	0.52
3:D:200:ASP:O	3:D:397:LYS:HG2	2.10	0.52
3:D:564:GLU:HG3	12:D:2110:HOH:O	2.09	0.52
3:D:1256:LEU:O	3:D:1260:ILE:HG13	2.10	0.52
2:C:729:LEU:HD11	2:C:791:ARG:HH22	1.75	0.52
3:D:321:GLN:HB2	3:D:336:PHE:HB2	1.92	0.52
12:C:1315:HOH:O	3:D:1462:LEU:HD13	2.10	0.51
1:A:58:ILE:HG12	1:A:140:MET:HG2	1.92	0.51
3:D:231:VAL:O	3:D:236:TYR:OH	2.28	0.51
2:C:281:LEU:HD13	2:C:305:PRO:HB2	1.93	0.51
3:D:1048:PRO:HG3	3:D:1075:HIS:ND1	2.25	0.51
3:D:242:LEU:HB3	3:D:311:LEU:HD12	1.91	0.51
3:D:101:HIS:HB3	3:D:104:PHE:HD2	1.75	0.51
7:H:24:DC:C2	7:H:25:DA:C5	2.99	0.51
3:D:890:VAL:HB	3:D:922:LEU:HD13	1.93	0.51
3:D:1219:GLU:HA	12:D:2117:HOH:O	2.09	0.51
2:C:778:PHE:O	2:C:780:GLU:N	2.44	0.51
3:D:437:VAL:HG11	5:F:175:HIS:CD2	2.46	0.51
2:C:624:PRO:CB	12:C:1313:HOH:O	2.58	0.50
1:B:54:THR:OG1	1:B:145:ASP:OD1	2.27	0.50
3:D:209:ARG:HE	3:D:391:ALA:HB2	1.74	0.50
3:D:671:LYS:HZ3	5:F:421:PHE:HA	1.74	0.50
2:C:173:ASP:HB2	2:C:185:LYS:HB3	1.93	0.50
2:C:177:GLU:HG3	2:C:178:PRO:HD2	1.93	0.50
3:D:1271:LYS:HE2	3:D:1331:ASP:HB2	1.93	0.50
2:C:15:LEU:HD11	2:C:583:LEU:HD11	1.93	0.50
3:D:787:LEU:HD21	3:D:947:ILE:HG21	1.92	0.50
3:D:975:GLU:O	3:D:979:GLU:HG2	2.12	0.50
2:C:610:ARG:HD3	2:C:612:VAL:HG23	1.92	0.50
3:D:1488:ASP:OD1	3:D:1488:ASP:N	2.31	0.50
2:C:543:ASN:C	12:C:1316:HOH:O	2.49	0.49
2:C:374:ASN:OD1	5:F:276:ARG:HD2	2.13	0.49
3:D:809:PRO:HB3	3:D:839:LEU:HD13	1.94	0.49
5:F:160:ASP:O	5:F:164:LYS:HG2	2.12	0.49



Atom-1	Atom-2	Interatomic	Clash
	1100111-2	distance (Å)	overlap (Å)
1:B:154:GLU:HG3	3:D:840:LYS:HZ1	1.76	0.49
2:C:168:ARG:O	2:C:267:TYR:HA	2.13	0.49
1:A:209:GLU:O	1:A:213:GLN:HG2	2.12	0.49
3:D:274:ARG:NH2	3:D:279:VAL:HG21	2.27	0.49
2:C:430:VAL:HG23	3:D:1078:ARG:HG2	1.95	0.49
2:C:773:LEU:CD1	2:C:777:ILE:CD1	2.86	0.49
3:D:181:ASP:HB2	3:D:205:TYR:CD1	2.47	0.49
3:D:508:ARG:HB2	3:D:511:TRP:CE2	2.48	0.49
3:D:1087:ARG:HB2	3:D:1237:THR:CG2	2.42	0.49
5:F:353:GLU:O	5:F:356:LYS:HB2	2.12	0.49
2:C:853:LEU:HB2	2:C:858:MET:HE1	1.95	0.49
2:C:874:LEU:O	3:D:1029:ARG:HG3	2.12	0.49
3:D:155:ASP:OD1	3:D:159:ARG:NH1	2.46	0.49
5:F:238:TYR:HH	7:H:1:DT:H6	1.59	0.48
1:B:54:THR:HG22	1:B:169:ALA:HB2	1.95	0.48
2:C:65:VAL:HG21	2:C:103:LYS:HE3	1.95	0.48
2:C:774:LEU:O	2:C:777:ILE:HD12	2.12	0.48
3:D:22:SER:HB2	3:D:92:HIS:HB3	1.94	0.48
3:D:530:VAL:HG12	3:D:531:ASP:H	1.77	0.48
3:D:1114:THR:OG1	3:D:1195:GLN:NE2	2.45	0.48
7:H:24:DC:N3	7:H:25:DA:C6	2.81	0.48
2:C:1031:ARG:NE	6:G:16:DG:OP1	2.36	0.48
2:C:777:ILE:HA	5:F:405:LEU:CD1	2.33	0.48
2:C:1035:MET:SD	6:G:15:DT:H4'	2.53	0.48
3:D:846:PRO:N	12:D:2115:HOH:O	2.47	0.48
1:A:64:GLU:HG2	1:A:76:VAL:HG22	1.95	0.48
3:D:1128:VAL:HG23	3:D:1130:ARG:H	1.79	0.48
3:D:1189:ARG:HB3	3:D:1204:CYS:HA	1.95	0.48
3:D:1229:ILE:HG23	3:D:1356:TYR:OH	2.14	0.48
2:C:376:ARG:HD3	5:F:276:ARG:HD2	1.94	0.48
2:C:960:GLU:HB2	12:C:1303:HOH:O	2.11	0.48
2:C:1102:LEU:HD11	3:D:9:ARG:HH11	1.78	0.48
5:F:361:LEU:HD11	5:F:408:LEU:CG	2.42	0.48
2:C:343:GLN:HG3	2:C:385:PHE:HB2	1.95	0.48
3:D:57:GLU:HG3	3:D:64:LYS:HG2	1.96	0.48
2:C:767:PRO:O	2:C:769:PRO:HD3	2.14	0.47
3:D:124:GLU:OE2	3:D:587:ARG:NH2	2.47	0.47
5:F:131:VAL:HG13	5:F:178:ARG:HD3	1.95	0.47
2:C:540:PHE:HB3	2:C:544:THR:HB	1.95	0.47
3:D:264:LEU:HB3	12:D:2116:HOH:O	2.13	0.47
3:D:1042:ARG:HG3	3:D:1045:MET:HE3	1.96	0.47



Atom 1	Atom 2	Interatomic	Clash
	Atom-2	distance (Å)	overlap (Å)
3:D:137:PRO:HB3	3:D:147:VAL:HG12	1.96	0.47
3:D:224:ARG:NE	3:D:254:GLU:OE2	2.36	0.47
5:F:360:LYS:HA	5:F:360:LYS:HD3	1.63	0.47
3:D:114:THR:HG23	3:D:495:ARG:HG2	1.97	0.47
3:D:355:VAL:HG11	3:D:385:VAL:HG21	1.96	0.47
1:A:109:VAL:HG22	12:A:404:HOH:O	2.13	0.47
2:C:405:ARG:NE	2:C:442:GLU:OE2	2.37	0.47
2:C:976:ASP:OD1	2:C:978:ARG:HG3	2.15	0.47
3:D:192:ALA:HB3	3:D:195:VAL:HB	1.97	0.47
1:B:90:LEU:HD21	1:B:121:GLU:HB2	1.97	0.47
2:C:763:GLY:C	2:C:765:SER:N	2.68	0.47
2:C:1021:LEU:HD22	5:F:331:ASP:O	2.15	0.47
2:C:1058:ASP:OD1	3:D:621:LYS:HE2	2.14	0.47
3:D:207:PHE:HE2	5:F:98:GLU:HG2	1.79	0.47
3:D:272:LEU:O	3:D:279:VAL:N	2.47	0.47
3:D:658:LEU:HD11	3:D:674[A]:ARG:HH11	1.80	0.47
6:G:6:DA:N1	7:H:22:DT:C4	2.80	0.47
6:G:18:DA:H2"	6:G:19:DG:O5'	2.14	0.47
1:A:196:THR:HG21	2:C:934:PHE:CE2	2.47	0.47
2:C:1083:GLU:OE2	3:D:87:ARG:NH2	2.47	0.47
3:D:683:ILE:HD11	3:D:688:TRP:CZ2	2.50	0.47
2:C:773:LEU:O	2:C:773:LEU:HD13	2.15	0.47
2:C:1110:ASP:OD2	2:C:1114:GLY:N	2.39	0.47
12:C:1315:HOH:O	3:D:1472:ILE:HG21	2.15	0.47
5:F:84:TYR:O	5:F:88:ILE:HG12	2.15	0.47
3:D:806:PHE:HB2	3:D:829:VAL:HG22	1.97	0.46
5:F:153:PRO:HA	5:F:156:VAL:HG22	1.96	0.46
2:C:880:MET:HE1	3:D:1242:HIS:CG	2.49	0.46
3:D:65:ARG:NE	5:F:379:ARG:HB3	2.30	0.46
7:H:21:DA:C2'	7:H:22:DT:C5'	2.86	0.46
3:D:1044:LEU:HD23	3:D:1056:PRO:HB3	1.97	0.46
3:D:1088:THR:HG23	3:D:1238:MET:SD	2.56	0.46
5:F:135:ILE:HD11	5:F:178:ARG:HB3	1.96	0.46
2:C:680:ASP:OD2	2:C:978:ARG:NH2	2.48	0.46
3:D:1239:ARG:O	3:D:1241:PHE:CD1	2.68	0.46
3:D:737:ASN:ND2	3:D:1235:GLN:HE22	2.13	0.46
1:A:193:ASP:OD2	2:C:938:LYS:NZ	2.40	0.46
2:C:247:PRO:HA	2:C:248:PRO:HD3	1.68	0.46
2:C:543:ASN:CB	12:C:1316:HOH:O	1.70	0.46
2:C:773:LEU:HD13	2:C:777:ILE:HG13	1.98	0.46
2:C:774:LEU:C	2:C:777:ILE:HD12	2.36	0.46



Atom_1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:C:118:ILE:HD11	2:C:344:PHE:CE2	2.51	0.46
3:D:879:ARG:HD3	3:D:902:LEU:O	2.16	0.46
1:B:110:LYS:HD3	1:B:128:HIS:HA	1.97	0.45
2:C:299:LYS:HE2	2:C:299:LYS:HA	1.96	0.45
11:D:2006:2TM:H2	12:D:2123:HOH:O	2.16	0.45
1:A:8:ALA:HA	1:A:9:PRO:HD3	1.65	0.45
1:A:90:LEU:HB2	1:A:119:ASP:HB3	1.98	0.45
3:D:1122:LEU:HD13	3:D:1178:ALA:HB2	1.99	0.45
1:A:102:LYS:HB2	1:A:102:LYS:HE3	1.75	0.45
2:C:334:ARG:NH2	2:C:342:ASP:OD2	2.46	0.45
1:A:100:LEU:HD22	1:A:141:GLU:HG2	1.98	0.45
3:D:30:GLU:OE1	3:D:40:GLU:HG2	2.17	0.45
3:D:41:ARG:HE	3:D:48:ARG:CZ	2.30	0.45
3:D:218:LYS:HG2	3:D:338:GLU:HG2	1.98	0.45
5:F:357:ALA:HA	5:F:360:LYS:HB2	1.99	0.45
3:D:158:TYR:CE1	3:D:454:ALA:HB3	2.51	0.45
3:D:1091:SER:OG	3:D:1234:THR:CA	2.64	0.45
2:C:911:GLU:O	2:C:915:LYS:HG2	2.16	0.45
2:C:76:PRO:HG3	2:C:120:LEU:HD12	1.99	0.45
2:C:132:ALA:HB1	2:C:394:PHE:HE1	1.82	0.45
2:C:1118:LYS:HE2	3:D:20:SER:O	2.17	0.45
3:D:487:ALA:O	3:D:491:LYS:HG2	2.16	0.45
1:A:179:PHE:HB3	1:A:197:LEU:HD23	1.99	0.45
1:A:198:ARG:HD3	2:C:934:PHE:CE1	2.52	0.45
1:B:32:PHE:HA	1:B:35:THR:HB	1.98	0.45
2:C:41:ASN:O	2:C:46:ALA:HB2	2.17	0.45
3:D:353:VAL:HG11	3:D:387:LEU:HD11	1.98	0.45
2:C:424:GLY:O	2:C:426:ASP:N	2.49	0.45
2:C:764:GLU:O	2:C:766:GLU:CG	2.61	0.45
3:D:238:PRO:HG3	3:D:318:ARG:HB2	1.99	0.45
1:B:48:ILE:HA	1:B:49:PRO:HD3	1.87	0.44
3:D:264:LEU:CB	12:D:2116:HOH:O	2.65	0.44
3:D:1493:LYS:O	3:D:1497:GLU:HG2	2.16	0.44
4:E:45:ARG:NH1	4:E:56:ASP:OD2	2.50	0.44
1:A:54:THR:HG21	1:A:145:ASP:HB2	2.00	0.44
2:C:118:ILE:HD11	2:C:344:PHE:HE2	1.82	0.44
4:E:95:VAL:O	4:E:95:VAL:HG12	2.16	0.44
2:C:367:LEU:HD13	2:C:372:LEU:HD21	2.00	0.44
2:C:422:ARG:HG2	7:H:15:DT:C6	2.52	0.44
2:C:763:GLY:O	2:C:765:SER:N	2.51	0.44
3:D:717:GLN:NE2	12:D:2118:HOH:O	2.50	0.44



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
3:D:1232:PRO:HB3	3:D:1361:VAL:HG11	1.99	0.44
5:F:109:GLY:O	5:F:113:ILE:HG13	2.17	0.44
5:F:362:SER:OG	5:F:365:GLU:HG2	2.18	0.44
2:C:1001:VAL:HG12	12:C:1317:HOH:O	2.17	0.44
3:D:260:GLU:HB3	3:D:271:VAL:HB	2.00	0.44
2:C:422:ARG:HG2	7:H:15:DT:OP2	2.18	0.44
3:D:67:ARG:HG3	5:F:377:ASP:O	2.18	0.44
1:A:6:LEU:HD11	1:A:27:PRO:HG2	1.99	0.44
1:A:64:GLU:HG3	1:A:79:ILE:HD12	1.99	0.44
3:D:84:ILE:O	3:D:87:ARG:HG2	2.18	0.44
3:D:265:GLU:N	12:D:2116:HOH:O	2.51	0.44
3:D:1176:LYS:HB3	3:D:1176:LYS:HE2	1.79	0.44
3:D:1211:MET:HB2	3:D:1211:MET:HE3	1.89	0.44
3:D:1353:GLN:O	3:D:1357:ARG:HG3	2.17	0.44
7:H:15:DT:H2"	7:H:16:DC:H5'	1.99	0.44
1:A:31:GLY:CA	12:A:403:HOH:O	2.64	0.44
2:C:1095:LEU:O	3:D:101:HIS:NE2	2.39	0.44
8:C:1201:ATP:H5'1	12:D:2123:HOH:O	2.16	0.44
3:D:135:LEU:O	3:D:453:ASP:HB3	2.18	0.44
2:C:324:ASP:HB3	2:C:327:HIS:HB2	2.00	0.44
4:E:14:ASP:OD2	4:E:18:ARG:NH1	2.50	0.44
2:C:194:VAL:HA	2:C:197:LEU:HD12	2.00	0.43
2:C:617:ASP:HB2	2:C:619:ARG:HG2	2.00	0.43
2:C:708:TYR:HB3	2:C:790:LEU:HD21	2.00	0.43
3:D:1263:PHE:CE2	3:D:1371:VAL:HG11	2.53	0.43
3:D:1487:VAL:HG11	3:D:1492:LEU:HD13	2.00	0.43
2:C:768:THR:HB	2:C:770:GLU:HB2	2.01	0.43
1:A:57:TYR:CE1	1:A:161:ARG:HD2	2.53	0.43
1:A:159:LYS:HE3	1:A:164:ALA:O	2.17	0.43
3:D:169:TYR:HA	3:D:170:PRO:HD3	1.73	0.43
3:D:792:ILE:HG13	3:D:793:THR:HG23	2.00	0.43
2:C:101:ILE:HG12	2:C:108:ILE:HG12	2.01	0.43
2:C:154:ARG:H	2:C:154:ARG:HG2	1.68	0.43
2:C:499:ALA:HB2	2:C:533:ASP:HB2	2.00	0.43
2:C:97:ARG:HG2	2:C:112:GLU:HB2	2.00	0.43
3:D:410:SER:H	5:F:164:LYS:NZ	2.16	0.43
3:D:796:ARG:NH1	3:D:862:ASP:OD2	2.47	0.43
2:C:1009:SER:O	3:D:624:ASP:HB3	2.19	0.43
3:D:317:VAL:HG23	3:D:339:TRP:HB3	2.00	0.43
2:C:996:LYS:CG	12:C:1321:HOH:O	2.29	0.43
1:B:94:LEU:HD11	1:B:97:VAL:HG22	2.01	0.43



Atom-1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:C:642:ARG:HD3	2:C:642:ARG:HA	1.87	0.43
3:D:526:PRO:N	12:D:2119:HOH:O	2.51	0.43
3:D:840:LYS:HE3	3:D:841:TYR:CZ	2.53	0.43
3:D:1263:PHE:CD2	3:D:1375:MET:HE2	2.48	0.43
5:F:355:GLU:HA	5:F:358:LEU:CG	2.49	0.43
2:C:773:LEU:HD23	5:F:373:LYS:HB3	1.91	0.43
7:H:23:DG:H2"	7:H:24:DC:C6	2.53	0.43
3:D:81:THR:OG1	3:D:82:LYS:N	2.52	0.42
3:D:103:TRP:HB3	3:D:1448:THR:HG21	2.01	0.42
3:D:1086:LEU:N	3:D:1086:LEU:HD12	2.33	0.42
4:E:37:ASN:OD1	4:E:37:ASN:N	2.44	0.42
2:C:562:SER:CA	12:C:1316:HOH:O	2.63	0.42
3:D:12:LEU:HD21	3:D:104:PHE:CZ	2.54	0.42
3:D:12:LEU:HD23	3:D:12:LEU:HA	1.85	0.42
3:D:1255:GLY:HA2	3:D:1355:VAL:HG13	2.01	0.42
3:D:1402:ALA:O	3:D:1405:GLU:HG2	2.19	0.42
4:E:68:LEU:HD12	4:E:68:LEU:HA	1.77	0.42
3:D:1031:ASN:O	3:D:1035:ILE:HG12	2.19	0.42
3:D:1254:GLN:O	3:D:1257:PRO:HB2	2.19	0.42
3:D:560:GLN:HE22	5:F:222:ARG:HH12	1.68	0.42
3:D:1108:ARG:NH2	3:D:1198:TYR:O	2.50	0.42
2:C:546:LEU:HB2	2:C:565:GLN:HE22	1.84	0.42
2:C:1091:GLU:OE2	3:D:606:ILE:HG21	2.19	0.42
3:D:795:VAL:HG12	3:D:876:SER:HB3	2.00	0.42
2:C:218:VAL:O	2:C:222:MET:HG2	2.19	0.42
2:C:878:SER:N	12:C:1301:HOH:O	2.44	0.42
3:D:131:LYS:NZ	3:D:154:THR:HG22	2.34	0.42
5:F:355:GLU:O	5:F:356:LYS:C	2.58	0.42
2:C:792:VAL:HA	2:C:793:PRO:HD3	1.92	0.42
3:D:372:ASP:HA	3:D:373:PRO:HD3	1.88	0.42
3:D:706:PRO:HG3	6:G:14:DG:H21	1.84	0.42
3:D:1036:ARG:NH2	3:D:1042:ARG:O	2.52	0.42
2:C:624:PRO:CA	12:C:1313:HOH:O	2.68	0.42
2:C:1090:LYS:HA	2:C:1090:LYS:HD3	1.80	0.42
3:D:483:HIS:CG	3:D:484:PRO:HD2	2.54	0.42
3:D:838:ARG:HD3	3:D:874:GLU:OE1	2.20	0.42
1:A:57:TYR:CD1	1:A:161:ARG:HD2	2.55	0.42
1:A:115:LEU:HA	1:A:116:PRO:HD3	1.87	0.42
2:C:954:THR:HA	2:C:955:PRO:HD3	1.91	0.42
1:A:133:GLU:HG2	1:A:134:GLU:N	2.35	0.42
2:C:239:PHE:CD2	2:C:253:ALA:HA	2.54	0.42



Atom 1	Atom 2	Interatomic	Clash
Atom-1	1100m-1 1100m-2		overlap (Å)
5:F:355:GLU:HA	5:F:358:LEU:HB2	2.02	0.42
2:C:545:ASN:HB3	2:C:583:LEU:HD22	2.02	0.41
3:D:801:GLY:HA3	3:D:821:VAL:HG13	2.01	0.41
3:D:1117:TYR:HB2	3:D:1188:VAL:O	2.20	0.41
2:C:768:THR:OG1	2:C:771:GLU:HG3	2.20	0.41
2:C:1092:LEU:HD13	2:C:1099:VAL:HG21	2.01	0.41
3:D:644:LEU:HD12	3:D:645:PRO:HD2	2.01	0.41
1:A:80:LEU:HD23	1:A:80:LEU:HA	1.95	0.41
1:B:83:LYS:HE2	1:B:168:ASP:HB2	2.02	0.41
3:D:1253:THR:O	3:D:1257:PRO:CD	2.68	0.41
2:C:486:MET:HB3	2:C:490:GLU:HB3	2.01	0.41
3:D:176:ASP:OD1	3:D:177:ALA:N	2.44	0.41
3:D:185:VAL:N	3:D:201:GLY:O	2.45	0.41
3:D:455:ARG:HB2	3:D:460:ALA:HB2	2.02	0.41
5:F:208:SER:HB3	5:F:211:ASP:OD2	2.20	0.41
2:C:124:ASP:HB3	2:C:592:LEU:HD12	2.02	0.41
3:D:760:ARG:O	3:D:764:LEU:HB2	2.21	0.41
3:D:889:ALA:HB1	3:D:930:LEU:HA	2.02	0.41
5:F:285:GLU:HA	5:F:286:PRO:HD3	1.84	0.41
2:C:771:GLU:HB3	2:C:775:ARG:HH21	1.83	0.41
3:D:66:GLN:C	3:D:68:PHE:N	2.73	0.41
5:F:321:ILE:O	5:F:327:SER:HB3	2.20	0.41
5:F:358:LEU:HD11	5:F:370:LYS:NZ	1.97	0.41
1:B:56:VAL:HG21	1:B:82:LEU:HD13	2.02	0.41
2:C:765:SER:O	2:C:767:PRO:HD3	2.21	0.41
3:D:68:PHE:O	3:D:80:VAL:HG21	2.19	0.41
3:D:106:LYS:HD2	3:D:106:LYS:HA	1.75	0.41
3:D:704:ARG:HB2	3:D:745:MET:HG2	2.03	0.41
4:E:3:GLU:HA	4:E:4:PRO:HD3	1.96	0.41
5:F:88:ILE:CG2	5:F:193:ARG:HG2	2.50	0.41
6:G:5:DC:H1'	6:G:6:DA:H8	1.85	0.41
2:C:408:ARG:NH1	2:C:456:ALA:O	2.53	0.41
2:C:571:LEU:HD23	2:C:702:SER:HB3	2.03	0.41
2:C:1102:LEU:HD11	3:D:9:ARG:HB2	2.03	0.41
3:D:538:SER:HB3	12:D:2119:HOH:O	2.03	0.41
3:D:707:THR:HG23	3:D:712:GLY:HA3	2.01	0.41
1:B:124:ASN:OD1	1:B:124:ASN:N	2.53	0.41
2:C:13:ILE:HD13	2:C:483:VAL:HG11	2.03	0.41
2:C:749:VAL:HB	2:C:792:VAL:HG21	2.03	0.41
2:C:773:LEU:CD1	2:C:773:LEU:C	2.89	0.41
2:C:946:ARG:HG3	12:C:1320:HOH:O	2.20	0.41



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
3:D:171:LEU:HD11	3:D:393:ILE:HD11	2.03	0.41
3:D:192:ALA:HB1	3:D:193:PRO:HD2	2.02	0.41
3:D:525:ARG:C	12:D:2119:HOH:O	2.59	0.41
3:D:639:LEU:HA	3:D:729:HIS:CD2	2.56	0.41
3:D:675:ARG:HH22	5:F:420:ASP:HB3	1.85	0.41
3:D:843:PHE:HE1	3:D:864:VAL:HG21	1.86	0.41
1:A:109:VAL:CG2	12:A:404:HOH:O	2.69	0.41
2:C:773:LEU:HD13	2:C:777:ILE:CG1	2.51	0.41
2:C:942:GLU:HG3	2:C:945:ARG:HH21	1.85	0.41
3:D:613:ARG:HG3	3:D:618:LEU:HD22	2.03	0.41
1:B:143:ARG:NH1	1:B:158:ILE:HD12	2.35	0.40
3:D:226:PRO:HD3	3:D:249:TYR:CE2	2.56	0.40
5:F:373:LYS:HA	5:F:373:LYS:HD3	1.93	0.40
7:H:21:DA:H1'	7:H:22:DT:C5'	2.51	0.40
2:C:848:VAL:HB	3:D:740:PHE:O	2.21	0.40
2:C:1104:GLU:HA	3:D:7:LYS:HE3	2.03	0.40
3:D:50:PHE:CD2	3:D:522:PRO:HD3	2.55	0.40
3:D:517:VAL:HA	3:D:518:PRO:HD3	1.95	0.40
5:F:162:LYS:O	5:F:165:SER:OG	2.34	0.40
1:A:64:GLU:OE2	2:C:830:LYS:NZ	2.51	0.40
2:C:773:LEU:HD22	5:F:373:LYS:CD	2.42	0.40
2:C:1054:THR:OG1	2:C:1055:LEU:N	2.53	0.40
3:D:403:PHE:CD2	3:D:444:VAL:HG23	2.57	0.40
3:D:784:ASP:HB2	3:D:939:PHE:CE2	2.56	0.40
3:D:1366:LYS:O	3:D:1370:ILE:HG12	2.21	0.40
6:G:15:DT:H2'	6:G:16:DG:H8	1.87	0.40
2:C:1097:LEU:HD11	3:D:103:TRP:HZ3	1.86	0.40
3:D:34:TYR:CZ	3:D:35:ARG:HG3	2.57	0.40
2:C:704:HIS:CD2	2:C:831:ARG:HD2	2.57	0.40
2:C:858:MET:HG2	2:C:867:VAL:O	2.22	0.40
2:C:1035:MET:HG2	2:C:1038:TRP:CZ3	2.57	0.40
3:D:907:GLU:HB2	3:D:1026:SER:HA	2.03	0.40

All (6) 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)
3:D:306:GLU:OE1	7:H:1:DT:O5'[4_745]	1.70	0.50
2:C:318:PRO:CB	4:E:87:LYS:CG[1_545]	1.77	0.43
3:D:34:TYR:OH	3:D:327:GLU:OE1[4_755]	1.89	0.31



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:328:GLY:O	5:F:303:ARG:NH2[4_745]	2.11	0.09
2:C:37:GLU:OE1	3:D:1151:ARG:NH1[3_545]	2.12	0.08
2:C:49:ARG:NH2	5:F:390:PHE:O[1_545]	2.18	0.02

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	ntiles
1	А	229/315~(73%)	226 (99%)	3 (1%)	0	100	100
1	В	225/315~(71%)	222 (99%)	3 (1%)	0	100	100
2	С	1108/1119 (99%)	1076 (97%)	26 (2%)	6 (0%)	29	61
3	D	1491/1524 (98%)	1454 (98%)	33 (2%)	4 (0%)	41	71
4	Е	92/99~(93%)	89 (97%)	3 (3%)	0	100	100
5	F	344/423~(81%)	336 (98%)	7 (2%)	1 (0%)	41	71
All	All	3489/3795~(92%)	3403 (98%)	75 (2%)	11 (0%)	41	71

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	С	425	PHE
2	С	765	SER
2	С	769	PRO
3	D	1240	THR
2	С	779	GLY
3	D	66	GLN
5	F	360	LYS
2	С	763	GLY
3	D	1253	THR
2	С	768	THR
3	D	1257	PRO



5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
1	А	200/273~(73%)	196~(98%)	4 (2%)	55	82
1	В	200/273~(73%)	196 (98%)	4 (2%)	55	82
2	С	936/941~(100%)	907~(97%)	29 (3%)	40	74
3	D	1260/1279~(98%)	1229 (98%)	31 (2%)	47	78
4	Ε	83/88~(94%)	83 (100%)	0	100	100
5	F	301/371~(81%)	296~(98%)	5 (2%)	60	86
All	All	2980/3225~(92%)	2907 (98%)	73 (2%)	47	79

All (73) residues with a non-rotameric side chain are listed below:

Mol	Chain	Res	Type
1	А	6	LEU
1	А	66	SER
1	А	96	THR
1	А	219	ARG
1	В	7	LYS
1	В	14	ARG
1	В	91	ASN
1	В	154	GLU
2	С	81	ASP
2	С	141	HIS
2	С	194	VAL
2	С	219	GLN
2	С	285	LEU
2	С	299	LYS
2	С	360	LEU
2	С	397	GLU
2	С	405	ARG
2	С	464	LEU
2	С	513	VAL
2	С	557	ARG
2	С	595	LEU
2	С	610	ARG



Mol	Chain	Res	Type
2	С	617	ASP
2	С	640	ARG
2	С	698	ASP
2	С	728	HIS
2	C	729	LEU
2	С	765	SER
2	С	767	PRO
2	С	768	THR
2	С	769	PRO
2	С	773	LEU
2	С	775	ARG
2	С	778	PHE
2	С	784	ASP
2	С	848	VAL
2	C	1078	GLU
3	D	66	GLN
3	D	67	ARG
3	D	87	ARG
3	D	134	VAL
3	D	276	ASP
3	D	354	VAL
3	D	406	ASP
3	D	415	VAL
3	D	420	VAL
3	D	530	VAL
3	D	618	LEU
3	D	632	VAL
3	D	683	ILE
3	D	709	HIS
3	D	754	PHE
3	D	784	ASP
3	D	907	GLU
3	D	1083	ASP
3	D	1084	THR
3	D	1236	LEU
3	D	1237	THR
3	D	1238	MET
3	D	1243	THR
3	D	1252	ILE
3	D	1254	GLN
3	D	1256	LEU
3	D	1288	GLU



00000			us puye
Mol	Chain	Res	Type
3	D	1307	LYS
3	D	1433	SER
3	D	1455	LYS
3	D	1488	ASP
5	F	95	THR
5	F	141	VAL
5	F	279	GLN
5	F	356	LYS
5	F	369	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	95	GLN
2	С	390	GLN
2	С	434	HIS
2	С	506	ASN
2	С	565	GLN
2	С	670	GLN
2	С	728	HIS
2	С	860	HIS
3	D	316	GLN
3	D	560	GLN
3	D	669	ASN
3	D	717	GLN
3	D	737	ASN
3	D	768	ASN
3	D	855	HIS
3	D	976	GLN
3	D	1124	GLN
3	D	1195	GLN
3	D	1242	HIS
3	D	1254	GLN
3	D	1441	GLN
5	F	83	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.



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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 7 ligands modelled in this entry, 5 are monoatomic - leaving 2 for Mogul analysis.

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	al Trung Chain Deg Link		Bond lengths			Bond angles				
	туре	Chain	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
11	2TM	D	2006	-	27,30,30	2.15	7 (25%)	39,47,47	1.76	10 (25%)
8	ATP	С	1201	10	26,33,33	0.92	1 (3%)	31,52,52	1.19	4 (12%)

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
11	2TM	D	2006	-	-	5/19/38/38	0/2/2/2
8	ATP	С	1201	10	-	8/18/38/38	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms		Observed(Å)	$\operatorname{Ideal}(\operatorname{\AA})$
11	D	2006	2TM	C5-C4	-4.50	1.32	1.42
11	D	2006	2TM	PB-O3B	4.39	1.63	1.58
11	D	2006	2TM	PB-O1B	-4.10	1.46	1.56
11	D	2006	2TM	PA-O2A	-3.53	1.48	1.56
11	D	2006	2TM	C6-N1	-3.38	1.29	1.38
11	D	2006	2TM	O4'-C4'	-2.40	1.39	1.45



001000	Contributed from precious page								
Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	Ideal(Å)		
11	D	2006	2TM	C4-N3	-2.34	1.30	1.34		
8	C	1201	ATP	C5-C4	2.26	1.46	1.40		

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
11	D	2006	2TM	O4'-C1'-N1	3.92	117.33	108.36
11	D	2006	2TM	C2'-C1'-N1	-3.81	102.43	113.22
11	D	2006	2TM	O3G-PG-O1G	3.81	125.58	110.68
11	D	2006	2TM	O1B-PB-O2B	3.63	122.18	110.07
11	D	2006	2TM	O2-C2-N3	-3.26	117.03	122.33
8	С	1201	ATP	N3-C2-N1	-3.00	123.99	128.68
11	D	2006	2TM	O2A-PA-C1	2.59	117.16	106.58
11	D	2006	2TM	C6-N1-C2	-2.52	116.11	120.49
8	С	1201	ATP	N6-C6-N1	2.48	123.73	118.57
8	С	1201	ATP	PB-O3B-PG	-2.17	125.38	132.83
11	D	2006	2TM	O2B-PB-C1	2.15	114.76	109.07
11	D	2006	2TM	C1'-N1-C2	2.12	123.16	118.42
11	D	2006	2TM	N4-C4-N3	2.04	121.55	117.97
8	С	1201	ATP	C2-N1-C6	2.01	122.19	118.75

There are no chirality outliers.

Mol	Chain	\mathbf{Res}	Type	Atoms
8	С	1201	ATP	PB-O3B-PG-O3G
8	С	1201	ATP	C5'-O5'-PA-O3A
11	D	2006	2TM	O4'-C4'-C5'-O5'
11	D	2006	2TM	PB-O3B-PG-O2G
11	D	2006	2TM	PA-C1-PB-O2B
8	С	1201	ATP	C5'-O5'-PA-O1A
8	С	1201	ATP	PA-O3A-PB-O2B
8	С	1201	ATP	PB-O3A-PA-O1A
8	С	1201	ATP	PB-O3A-PA-O2A
11	D	2006	2TM	C3'-C4'-C5'-O5'
11	D	2006	2TM	PB-O3B-PG-O1G
8	С	1201	ATP	PA-O3A-PB-O1B
8	С	1201	ATP	PB-O3B-PG-O1G

All (13) torsion outliers are listed below:

There are no ring outliers.

2 monomers are involved in 4 short contacts:



Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	D	2006	2TM	2	0
8	С	1201	ATP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<rsrz></rsrz>	#RSRZ>2	$OWAB(Å^2)$	Q<0.9
1	А	231/315~(73%)	0.44	12 (5%) 27 23	36, 68, 92, 101	0
1	В	227/315~(72%)	0.43	12 (5%) 26 22	41, 69, 100, 122	0
2	С	1112/1119 (99%)	0.48	73 (6%) 18 14	25, 58, 115, 135	0
3	D	1494/1524~(98%)	0.59	135 (9%) 9 7	19, 58, 122, 214	0
4	Е	94/99~(94%)	0.53	7 (7%) 14 11	34, 73, 111, 114	0
5	F	346/423~(81%)	0.93	61 (17%) 1 1	43, 79, 152, 176	0
6	G	18/22~(81%)	0.19	1 (5%) 24 20	55, 81, 139, 140	0
7	Н	25/27 (92%)	0.39	3(12%) 4 3	70, 100, 149, 169	0
All	All	3547/3844~(92%)	0.57	304 (8%) 10 8	19, 64, 124, 214	0

All (304) RSRZ outliers are listed below:

Mol	Chain	\mathbf{Res}	Type	RSRZ
3	D	173	PRO	8.7
2	С	311	PHE	7.6
2	С	300	ASP	7.5
3	D	211	VAL	7.1
3	D	427	VAL	7.0
5	F	149	GLU	6.9
2	С	207	LEU	6.8
3	D	1499	ARG	6.6
5	F	373	LYS	6.4
5	F	150	THR	6.3
5	F	381	HIS	6.3
3	D	241	ILE	6.1
2	С	107	LEU	6.0
5	F	386	VAL	5.9
3	D	1297	GLU	5.8
3	D	322	VAL	5.7



Mol	Chain	Res	Type	RSRZ
5	F	375	LEU	5.6
3	D	324	ALA	5.5
1	А	231	ALA	5.4
1	В	2	LEU	5.2
3	D	1298	GLY	5.2
3	D	1127	GLU	5.2
5	F	382	THR	5.1
5	F	146	GLY	5.1
2	С	365	ASP	5.1
3	D	1500	LYS	5.0
5	F	369	LEU	5.0
3	D	267	GLY	5.0
3	D	1305	LEU	5.0
3	D	203	ALA	4.9
3	D	977	ALA	4.9
3	D	976	GLN	4.8
5	F	414	ARG	4.7
2	С	219	GLN	4.7
5	F	423	ASP	4.6
2	С	64	LEU	4.6
3	D	268	ALA	4.6
4	Е	85	LEU	4.5
3	D	1495	ILE	4.5
5	F	356	LYS	4.5
3	D	422	ALA	4.5
3	D	821	VAL	4.5
5	F	376	ILE	4.4
3	D	1497	GLU	4.4
2	С	769	PRO	4.3
5	F	388	ALA	4.3
5	F	145	PRO	4.3
5	F	359	SER	4.3
2	С	811	PRO	4.3
5	F	151	LEU	4.3
2	С	104	ASP	4.3
2	С	629	TYR	4.3
5	F	147	LEU	4.2
3	D	1299	PHE	4.2
3	D	368	VAL	4.2
1	А	94	LEU	4.2
2	С	208	ALA	4.2
3	D	195	VAL	4.1



Mol	Chain	Res	Type	RSRZ
3	D	202	VAL	4.1
1	А	230	ALA	4.1
3	D	339	TRP	4.1
3	D	393	ILE	4.1
3	D	310	LEU	4.0
2	С	217	LEU	4.0
2	С	296	GLY	4.0
2	С	766	GLU	4.0
5	F	349	LEU	3.9
5	F	143	HIS	3.9
3	D	830	ALA	3.9
3	D	1319	VAL	3.9
3	D	982	PHE	3.9
5	F	392	VAL	3.9
3	D	983	LEU	3.9
5	F	385	GLU	3.8
1	А	97	VAL	3.8
3	D	191	LEU	3.8
5	F	415	THR	3.8
3	D	974	ILE	3.7
2	С	299	LYS	3.7
2	С	729	LEU	3.7
3	D	488	ARG	3.6
5	F	390	PHE	3.6
2	С	307	LEU	3.6
3	D	1490	LYS	3.6
5	F	127	ILE	3.6
7	Н	24	DC	3.6
2	С	763	GLY	3.6
3	D	428	LYS	3.5
3	D	1313	VAL	3.5
3	D	212	ARG	3.5
3	D	335	LEU	3.5
3	D	1058	ARG	3.5
3	D	387	LEU	3.4
3	D	1300	SER	3.4
3	D	667	ALA	3.4
3	D	378	ILE	3.4
3	D	666	ILE	3.4
3	D	345	TYR	3.4
3	D	973	GLN	3.4
3	D	174	GLY	3.4



Mol	Chain	Res	Type	RSRZ
3	D	674[A]	ARG	3.4
2	С	226	VAL	3.4
5	F	383	LEU	3.3
2	С	242	LEU	3.3
2	С	281	LEU	3.3
3	D	367	ILE	3.3
3	D	213	VAL	3.3
5	F	361	LEU	3.3
2	С	174	LEU	3.3
3	D	1242	HIS	3.3
2	С	52	PHE	3.2
2	С	778	PHE	3.2
5	F	377	ASP	3.2
5	F	410	TYR	3.2
2	С	189	ARG	3.2
2	С	228	ALA	3.2
3	D	1306	PRO	3.2
2	С	159	ILE	3.1
2	С	315	ALA	3.1
5	F	173	TYR	3.1
3	D	831	GLY	3.1
2	С	102	HIS	3.1
2	С	200	LEU	3.0
3	D	1287	GLU	3.0
1	В	122	ILE	3.0
3	D	377	VAL	3.0
3	D	1405	GLU	3.0
5	F	397	ILE	3.0
5	F	345	ALA	3.0
3	D	410	SER	3.0
3	D	320	ALA	3.0
1	В	3	ASP	3.0
3	D	1283	ILE	3.0
5	F	421	PHE	3.0
1	В	118	ALA	3.0
2	С	304	LEU	3.0
4	Е	32	ARG	3.0
3	D	1491	THR	2.9
1	В	120	VAL	2.9
3	D	409	VAL	2.9
3	D	1130	ARG	2.9
2	C	298	PHE	2.9



Mol	Chain	Res	Type	RSRZ
1	В	82	82 LEU	
2	С	511	GLU	2.9
3	D	374	GLU	2.9
1	А	100	LEU	2.9
5	F	391	GLY	2.9
2	С	275	TYR	2.9
7	Н	23	DG	2.9
3	D	807	ALA	2.9
5	F	413	SER	2.9
2	С	775	ARG	2.9
1	В	6	LEU	2.8
3	D	373	PRO	2.8
3	D	969	ARG	2.8
3	D	1327	ARG	2.8
4	Е	89	MET	2.8
3	D	205	TYR	2.8
1	А	99	LEU	2.8
5	F	153	PRO	2.7
1	А	233	VAL	2.7
7	Н	25	DA	2.7
5	F	310	ILE	2.7
3	D	269	PHE	2.7
3	D	336	PHE	2.7
5	F	393	THR	2.7
3	D	142	LEU	2.7
1	А	142	VAL	2.7
3	D	144	GLY	2.7
3	D	217	LYS	2.7
3	D	316	GLN	2.6
5	F	419	ARG	2.6
3	D	531	ASP	2.6
3	D	1128	VAL	2.6
3	D	1054	GLU	2.6
3	D	198	ARG	2.6
3	D	340	THR	2.6
3	D	1239	1239 ARG	
2	С	762	762 LYS	
2	С	196	LEU	2.6
3	D	687	VAL	2.6
3	D	805	GLU	2.6
3	D	833	GLU	2.6
3	D	135	LEU	2.6



Mol	Chain	Res	Type	RSRZ	
2	С	617	ASP	2.6	
5	F	342	VAL	2.6	
5	F	379	ARG	2.6	
2	С	297	GLU	2.5	
3	D	1408	ILE	2.5	
2	С	1070	ILE	2.5	
3	D	337	LEU	2.5	
2	С	100	LEU	2.5	
3	D	240	GLU	2.5	
1	В	138	LEU	2.5	
1	А	115	LEU	2.5	
3	D	270	LEU	2.5	
3	D	1277	ILE	2.5	
3	D	338	GLU	2.4	
5	F	136	LEU	2.4	
5	F	346	THR	2.4	
2	С	422	ARG	2.4	
1	A	62	LEU	2.4	
2	С	185	LYS	2.4	
3	D	54	LYS	2.4	
2	С	105	THR	2.4	
2	С	41	ASN	2.4	
5	F	93	LEU	2.4	
2	С	227	PHE	2.4	
3	D	216	VAL	2.4	
3	D	1292	VAL	2.4	
3	D	70	GLY	2.4	
3	D	143	ASN	2.4	
1	A	234	ALA	2.4	
1	B	111	ALA	2.4	
3	D	350	HIS	2.4	
4	E	51	LEU	2.4	
3	D	239	GLY	2.4	
3	D	1325	LEU	2.4	
3	D	1133	ARG	2.4	
3	D	161	LEU	2.4	
3	D	470	LEU	2.4	
3	D	189	GLN	2.4	
5	F	422	LEU	2.3	
5	F	411	HIS	2.3	
3	D	225	LEU	2.3	
5	F	159	ILE	2.3	



Mol	Chain	Res	Type	RSRZ	
4	Е	79 LEU		2.3	
2	С	1040	LEU	2.3	
2	С	764	GLU	2.3	
2	С	1	MET	2.3	
3	D	980	MET	2.3	
1	В	119	ASP	2.3	
5	F	420	ASP	2.3	
1	А	232	ALA	2.3	
3	D	1238	MET	2.3	
4	Е	54	LEU	2.3	
3	D	452	ILE	2.3	
3	D	1304	LYS	2.3	
3	D	321	GLN	2.3	
3	D	394	LEU	2.2	
3	D	1174	LEU	2.2	
3	D	401	TYR	2.2	
3	D	463	GLN	2.2	
3	D	484	PRO	2.2	
3	D	304	304 LEU		
2	С	975 TYR		2.2	
3	D	490 ALA		2.2	
3	D	1275 SER		2.2	
5	F	401 GLU		2.2	
1	В	189	189 ARG		
2	С	351	LEU	2.2	
3	D	1225	ALA	2.2	
3	D	80	VAL	2.2	
3	D	219	GLU	2.2	
2	С	157	ARG	2.2	
3	D	426	LYS	2.2	
5	F	148	LYS	2.2	
5	F	394	ARG	2.2	
2	С	66	LEU	2.2	
5	F	96	LEU	2.2	
5	F	352	GLU	2.2	
5	F	125 ASP		2.2	
3	D	380	GLU	2.2	
1	В	89 PHE		2.1	
3	D	314	PRO	2.1	
3	D	676	MET	2.1	
2	С	63	GLY	2.1	
2	С	147	TYR	2.1	



Mol	Chain	Res	Type	RSRZ	
3	D	152	LEU	2.1	
3	D	804 LEU		2.1	
2	С	153 ALA		2.1	
5	F	400 ILE		2.1	
2	С	176	VAL	2.1	
2	С	757	GLY	2.1	
3	D	1129	THR	2.1	
6	G	3	DT	2.1	
2	С	21	ILE	2.1	
3	D	343	LYS	2.1	
3	D	242	LEU	2.1	
5	F	138	SER	2.1	
2	С	202	TYR	2.1	
4	Е	87	LYS	2.1	
2	С	245	245 GLY		
2	С	254 VAL		2.1	
2	С	367 LEU		2.1	
3	D	1273	VAL	2.1	
5	F	142	ARG	2.1	
2	С	739	GLU	2.1	
3	D	1281	VAL	2.1	
2	С	375 SER		2.0	
2	С	183	SER	2.0	
3	D	317	VAL	2.0	
3	D	360	ARG	2.0	
2	С	188	LYS	2.0	
2	С	649	VAL	2.0	
2	С	99	GLN	2.0	
3	D	1044	LEU	2.0	
5	F	122	LEU	2.0	
5	F	416	ARG	2.0	
2	С	205	GLU	2.0	
5	F	229	TYR	2.0	
2	С	361	MET	2.0	
5	F	389	PHE	2.0	
2	С	372	LEU	2.0	

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

There are no non-standard protein/DNA/RNA residues in this entry.



6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} extsf{-factors}(\mathbf{A}^2)$	Q<0.9
10	MG	D	2004	1/1	0.41	0.66	$54,\!54,\!54,\!54$	0
11	2TM	D	2006	29/29	0.85	0.19	38,51,69,94	0
8	ATP	С	1201	31/31	0.88	0.19	38,47,75,83	0
10	MG	D	2003	1/1	0.95	0.26	38,38,38,38	0
10	MG	D	2005	1/1	0.96	0.31	45,45,45,45	0
9	ZN	D	2001	1/1	0.97	0.17	38,38,38,38	0
9	ZN	D	2002	1/1	0.97	0.02	59, 59, 59, 59, 59	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.







6.5 Other polymers (i)

There are no such residues in this entry.

