

Full wwPDB X-ray Structure Validation Report (i)

Sep 20, 2023 – 11:22 PM EDT

PDB ID	:	5E17
Title	:	T. thermophilus transcription initiation complex having a RRR discriminator
		sequence and a nontemplate-strand length corresponding to TSS selection at
		position 7 (RPo-GGG-7)
Authors	:	Zhang, Y.; Ebright, R.H.
Deposited on	:	2015-09-29
Resolution	:	3.20 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
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.20 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	Similar resolution
	(#Entries)	(#Entries, resolution range(A))
R_{free}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)
RNA backbone	3102	1010 (3.50-2.90)

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	Qua	lity of chain		
1	А	315	% 57%	16%	27%	
1	В	315	51%	19%	30%	
2	С	1119	% • 76%		22%	
3	D	1524	% 76%		20%	••



Continue contraction contrac	nued fron	<i>i</i> previous	page						
Mol	Chain	Length			Quality of ch	ain			
4	Б	0.0							
4	E	99			83%			12%	5%
			3%						
5	\mathbf{F}	443		e	53%	13%		24%	
			5%						
6	G	21		48%		38%		14%	6
7	Н	27		41%		48%		11	L%
	_		14%						
8	I	7			71%		14%	14%	



2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 28784 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	0	\mathbf{S}	0	1	0
1		2.51	1814	1158	316	338	2	0		0
1	В	າາາ	Total	С	Ν	0	S	0	0	0
	D		1750	1120	303	325	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 8792	C 5562	N 1570	O 1636	S 24	0	3	0

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

Mol	Chain	Residues		A	toms			ZeroOcc	AltConf	Trace
3	D	1486	Total 11759	C 7458	N 2070	O 2195	S 36	0	3	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 758	C 483	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	337	Total 2737	C 1726	N 499	O 508	${f S}{4}$	0	0	0

There are 20 discrepancies between the modelled and reference sequences:



Chain	Residue	Modelled	Actual	Comment	Reference
F	-19	MET	-	initiating methionine	UNP Q5SKW1
F	-18	GLY	-	expression tag	UNP Q5SKW1
F	-17	SER	-	expression tag	UNP Q5SKW1
F	-16	SER	-	expression tag	UNP Q5SKW1
F	-15	HIS	-	expression tag	UNP Q5SKW1
F	-14	HIS	-	expression tag	UNP Q5SKW1
F	-13	HIS	-	expression tag	UNP Q5SKW1
F	-12	HIS	-	expression tag	UNP Q5SKW1
F	-11	HIS	-	expression tag	UNP Q5SKW1
F	-10	HIS	-	expression tag	UNP Q5SKW1
F	-9	SER	-	expression tag	UNP Q5SKW1
F	-8	SER	-	expression tag	UNP Q5SKW1
F	-7	GLY	-	expression tag	UNP Q5SKW1
F	-6	LEU	-	expression tag	UNP Q5SKW1
F	-5	VAL	-	expression tag	UNP Q5SKW1
F	-4	PRO	-	expression tag	UNP Q5SKW1
F	-3	ARG	-	expression tag	UNP Q5SKW1
F	-2	GLY	-	expression tag	UNP Q5SKW1
F	-1	SER	-	expression tag	UNP Q5SKW1
F	0	HIS	-	expression tag	UNP Q5SKW1

• Molecule 6 is a DNA chain called DNA (5'-D(*CP*CP*T*GP*CP*AP*TP*CP*CP*GP*T P*GP*AP*GP*CP*GP*AP*GP*GP*G)-3').

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
6	G	18	Total 372	C 176	N 73	O 106	Р 17	0	0	0

• Molecule 7 is a DNA chain called DNA (27-MER).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
7	Н	24	Total 495	C 236	N 94	0 142	Р 23	0	0	0

• Molecule 8 is a RNA chain called RNA (5'-R(*CP*CP*CP*CP*GP*A)-3').

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace			
8	Ι	7	Total 142	C 65	N 24	0 47	Р 6	0	0	0

• Molecule 9 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	В	1	Total Mg 1 1	0	0
9	D	2	Total Mg 2 2	0	0
9	F	1	Total Mg 1 1	0	0

• Molecule 10 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	D	2	Total Zn 2 2	0	0

• Molecule 11 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	А	12	Total O 12 12	0	0
11	В	12	Total O 12 12	0	0
11	С	49	Total O 49 49	0	0
11	D	62	Total O 62 62	0	0
11	Е	5	Total O 5 5	0	0
11	F	8	Total O 8 8	0	0
11	G	5	Total O 5 5	0	0
11	Н	4	Total O 4 4	0	0
11	Ι	2	Total O 2 2	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







Chain H:

41%

K1021 K1021 V1022 1026 S1036 1036 R1036 1006 R1046 1044 L1044 1044 L1044 1044 R1045 10446 R1045 10446 R1045 10446	K1047 K1047 C1050 E1051 F1053 F1053 F1055 F1055 R1055 S1050 S1050 F1061 F1061 F1061	11002 11065 11066 11067 11072 11072 11072	21074 81074 11084 11088 11088	D1100 V1101 T1102 H1103 R1108	11137 R1137 E1141	
q1184 V1188 81190 81197 81197 11234 11234 11235	MET MET MET MET ARG THR THR THR THR CLY CLY CLY CLY CLY CLY CLY CLY CLY CLY	11252 11252 11259 11259 11264 11268 11268	V1292 V1292 51296 61297 61298 F1299	P1306 K1307 P1324 11330	V1344	
V1355 Q1359 K1366 K1366 E1369 T1370 X1377 Y1378	N1 398 N1 402 E1 405 11 421 11 425 N1 434 K1 455	G1 461 L1 462 K1 463 B1 465 N1 465 V1 465 V1 465 L1 467 L1 467	F1480 11484 01488 11488 K1493 A1494	11495 E1496 E1497 A1498 R1499 A1502	AL GLU ALA LYS GLU	
ARG PRO ALA ARG ARG CLY CLYS CLU CLN CLU CLN PRO CLU	GLN ALA					
• Molecule 4: DNA-	-directed RNA polym	nerase subunit	t omega			
Chain E:	920/			120/ 50/		
	03%			1270 570		
MET A2 D7 D14 D14 D14 L19 K18 K18 K18 K18 K25 K25 K25	T50 R72 GLU GLU GLU GLU					
• Molecule 5: RNA	polymerase sigma fa	actor SigA				
Chain F:	62%		1.20/	240/		
				24%		
	ARRA ARRA ARRA ARRA SECY SEC ALS	ALL GLI GLI GLI GLI GLI GLI CLI CLI CLI CLI CLI CLI CLI CLI CLI C		H A B B B B B B B B B B B B B B B B B B		
GLU ASP ASP ASP ASP ASP CLUU CLUU ASP ASP ASP ASP ASP PPAD		PRO ILE PRO LYS ILE SER SER ST8 S78 D79 D79	Land Control C	T120 G121 L122 V131 K134	8138 8142 H143	
1144 1145 1146 1146 1147 1148 1148 1148 1148 1158 1158 1158 1158	E169 H170 K171 K172 K172 H173 H175 F178 E179 E179 E179 E179	110 1188 1188 1192 1192 1193 1194 1194 1194 1194	12210 D211 P227 R276 R276 Q279	R284 E285 E286 E290	8316 8316 8316	
<mark>1319</mark> PRO ASP GLV CVU CVU CVU CVS SER P339 P339 P339	E353 K356 X356 E365 E365 E365 E365 E365 E378 G378 G378	11387 1337 1337 13398 13398 13398 1400 1400 1400	H411 • R414 • 1415 • R416 • R416 • R416 • R416 • R416 • R417 • P423			
• Molecule 6: DNA GP*AP*GP*GP*G	(5'-D(*CP*CP*T*C)-3')	GP*CP*AP*1	P*CP*CP	*GP*TP*(GP*AP*GP*T	P*CP*
Chain G:	48%	38	%	14%		
DC DC DC DC DC DC DC DC DC DC DC DC DC D	4 9 2					
• Molecule 7: DNA	(27-MER)					



48%

11%



• Molecule 8: RNA (5'-R(*CP*CP*CP*UP*CP*GP*A)-3')





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants	183.01Å 103.57Å 294.94Å	Denesiter
a, b, c, α , β , γ	90.00° 99.20° 90.00°	Depositor
$\mathbf{B}_{\mathrm{ascolution}}\left(\overset{\mathrm{A}}{\mathbf{\lambda}}\right)$	39.82 - 3.20	Depositor
Resolution (A)	39.82 - 3.18	EDS
% Data completeness	93.2 (39.82-3.20)	Depositor
(in resolution range)	93.2(39.82 - 3.18)	EDS
R_{merge}	0.18	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.69 (at 3.18 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.9	Depositor
P. P.	0.215 , 0.260	Depositor
n, n_{free}	0.213 , 0.254	DCC
R_{free} test set	4268 reflections $(4.99%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	61.3	Xtriage
Anisotropy	0.469	Xtriage
Bulk solvent $k_{sol}(e/A^3), B_{sol}(A^2)$	0.29 , 49.5	EDS
L-test for twinning ²	$< L >=0.47, < L^2>=0.30$	Xtriage
	0.026 for 1/2 *h-3/2 *k,-1/2 *h-1/2 *k,-1/2 *h	
Estimated twinning fraction	$+1/2^{*}k$ -l	Xtriage
	$0.023 \text{ for } 1/2^{h+3/2^{k},1/2^{h-1/2^{k},-1/2^{h-1}}}}}}}}}}}}}}}}}}}}}}}}}}}}}}}}}}}}$	0-
E.E. completion	$\frac{1/2^{k-1}}{2}$	EDC
$\mathbf{F}_{o}, \mathbf{F}_{c}$ correlation	0.91	EDS
Total number of atoms	28784	wwPDB-VP
Average B, all atoms (A^2)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.13% 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, ZN

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	Bo	ond angles
MOI		RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.25	0/1849	0.46	0/2515
1	В	0.23	0/1781	0.45	0/2420
2	С	0.25	0/8969	0.45	0/12129
3	D	0.31	4/11975~(0.0%)	0.49	7/16189~(0.0%)
4	Е	0.24	0/772	0.42	0/1040
5	F	0.30	0/2779	0.44	0/3737
6	G	0.49	0/418	0.83	0/645
7	Н	0.53	0/556	0.90	0/858
8	Ι	0.30	0/157	0.96	0/242
All	All	0.29	4/29256~(0.0%)	0.49	7/39775~(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
3	D	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	921	ARG	C-O	9.12	1.40	1.23
3	D	923	GLY	CA-C	-7.58	1.39	1.51
3	D	917	GLN	C-O	6.03	1.34	1.23
3	D	923	GLY	N-CA	-5.26	1.38	1.46

All (7) bond angle outliers are listed below:



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Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
3	D	924	MET	C-N-CA	-7.41	103.17	121.70
3	D	923	GLY	C-N-CA	-6.01	106.67	121.70
3	D	922	LEU	N-CA-C	-5.57	95.97	111.00
3	D	919	PHE	N-CA-CB	5.19	119.95	110.60
3	D	1041	LEU	CA-CB-CG	5.14	127.12	115.30
3	D	921	ARG	CA-C-N	-5.10	105.98	117.20
3	D	922	LEU	C-N-CA	-5.09	111.61	122.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	D	922	LEU	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	1814	0	1869	38	0
1	В	1750	0	1802	44	0
2	С	8792	0	8902	160	0
3	D	11759	0	12002	231	0
4	Е	758	0	770	10	0
5	F	2737	0	2819	41	0
6	G	372	0	203	10	0
7	Н	495	0	272	13	0
8	Ι	142	0	78	2	0
9	В	1	0	0	0	0
9	D	2	0	0	0	0
9	F	1	0	0	0	0
10	D	2	0	0	0	0
11	А	12	0	0	1	0
11	В	12	0	0	6	0
11	С	49	0	0	0	0
11	D	62	0	0	5	0
11	E	5	0	0	1	0
11	F	8	0	0	0	0
11	G	5	0	0	0	0



• • • • • •	j = j	I I I I I I I I I I I I I I I I I I I	Fagarra			
Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	Н	4	0	0	2	0
11	Ι	2	0	0	0	0
All	All	28784	0	28717	488	0

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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 9.

All (488) 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)
3:D:918:ALA:O	3:D:923:GLY:N	1.80	1.12
3:D:919:PHE:O	3:D:923:GLY:HA2	1.51	1.09
3:D:919:PHE:C	3:D:923:GLY:HA2	1.98	0.84
3:D:921:ARG:O	3:D:923:GLY:HA3	1.80	0.82
6:G:20:DG:H1	8:I:2:C:H42	1.32	0.77
1:B:74:ASP:O	11:B:2101:HOH:O	2.02	0.76
3:D:921:ARG:C	3:D:923:GLY:HA3	2.07	0.75
2:C:628:PHE:H	2:C:638:ASP:HB3	1.54	0.73
3:D:266:GLU:HG3	3:D:314:PRO:HB3	1.73	0.71
3:D:65:ARG:NH1	5:F:378:GLY:O	2.24	0.70
3:D:260:GLU:OE1	3:D:273:ARG:NH1	2.24	0.70
3:D:919:PHE:O	3:D:923:GLY:CA	2.37	0.70
2:C:462:ASP:HB3	2:C:468:ARG:HD2	1.75	0.68
2:C:802:ARG:HB2	2:C:826:TYR:HB2	1.75	0.68
3:D:956:ILE:HD11	3:D:1062:ARG:HG2	1.74	0.68
2:C:12:VAL:HG21	2:C:472:ARG:HD3	1.75	0.68
3:D:124:GLU:OE2	3:D:587:ARG:NH2	2.27	0.68
3:D:224:ARG:NE	3:D:254:GLU:OE2	2.25	0.67
2:C:24:GLU:OE2	2:C:27:ARG:NH2	2.27	0.67
2:C:97:ARG:NH1	2:C:110:GLU:OE1	2.24	0.67
1:B:56:VAL:HG22	1:B:142:VAL:HG12	1.76	0.67
3:D:208:PRO:HA	3:D:390:PRO:HA	1.77	0.67
1:A:24:VAL:HG22	1:A:196:THR:HG23	1.76	0.67
2:C:939:ARG:HG2	2:C:982:PRO:HD3	1.76	0.66
2:C:168:ARG:HD3	2:C:268:ASP:HB3	1.77	0.66
2:C:428:ARG:NH2	2:C:447:ALA:O	2.29	0.66
3:D:1324:PRO:HG3	3:D:1330:ILE:HD11	1.78	0.66
3:D:1046:GLN:NE2	3:D:1050:GLY:O	2.28	0.65
3:D:918:ALA:C	3:D:923:GLY:H	1.90	0.65
3:D:968:ASP:OD1	3:D:1058:ARG:NH2	2.30	0.65
2:C:768:THR:OG1	2:C:771:GLU:OE1	2.16	0.64



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
2:C:469:THR:OG1	2:C:538:GLN:NE2	2.30	0.64
3:D:128:TYR:OH	3:D:579:ASP:OD2	2.14	0.63
1:A:185:ARG:NH2	1:A:187:GLY:O	2.30	0.63
2:C:758:ARG:HH21	2:C:788:THR:HB	1.63	0.63
2:C:884:GLN:O	2:C:888:THR:OG1	2.15	0.63
3:D:272:LEU:HB2	3:D:280:ALA:HB3	1.81	0.62
5:F:131:VAL:HG13	5:F:178:ARG:HD3	1.81	0.62
2:C:711:GLU:HG2	2:C:822:VAL:HG22	1.80	0.62
2:C:223:ASP:OD1	2:C:225:SER:OG	2.16	0.61
2:C:165:LEU:HB2	2:C:168:ARG:HG3	1.81	0.61
3:D:192:ALA:HB3	3:D:195:VAL:HB	1.82	0.61
3:D:224:ARG:H	3:D:251:PHE:HE1	1.48	0.61
2:C:740:GLU:OE1	2:C:805:ARG:NH1	2.33	0.61
1:A:133:GLU:OE1	2:C:610:ARG:NH1	2.34	0.61
3:D:970:LYS:HD3	3:D:995:LEU:HD13	1.83	0.60
2:C:409:ARG:NH2	2:C:442:GLU:OE2	2.33	0.60
3:D:432:TYR:O	11:D:2101:HOH:O	2.16	0.60
2:C:612:VAL:HG22	2:C:622:GLU:HG3	1.82	0.60
3:D:500:ARG:NH1	3:D:1388:ARG:O	2.34	0.60
3:D:1108:ARG:NH2	3:D:1198:TYR:O	2.35	0.59
1:B:83:LYS:HE2	1:B:168:ASP:HB2	1.83	0.59
1:B:108:GLU:HG2	1:B:131:THR:HG22	1.85	0.59
2:C:598:GLU:O	2:C:651:LYS:NZ	2.33	0.59
3:D:1495:ILE:HD13	4:E:80:VAL:HG21	1.84	0.59
5:F:227:PHE:HA	11:H:101:HOH:O	2.01	0.59
3:D:433:GLY:HA2	11:D:2101:HOH:O	2.02	0.59
2:C:160:ALA:HB3	2:C:174:LEU:HB2	1.85	0.59
2:C:1100:GLN:HG3	3:D:9:ARG:HH21	1.67	0.58
2:C:787:ASP:OD2	2:C:791:ARG:NH2	2.33	0.58
1:B:80:LEU:HD21	3:D:842:VAL:HG12	1.83	0.58
2:C:674:VAL:HG12	2:C:869:VAL:HB	1.85	0.58
1:B:78:ILE:HA	1:B:81:ASN:HD22	1.69	0.58
3:D:405:ASP:HB3	3:D:423:ASP:HA	1.86	0.57
3:D:242:LEU:HB3	3:D:311:LEU:HD12	1.86	0.57
7:H:2:DA:N1	11:H:101:HOH:O	2.33	0.57
7:H:10:DA:H2'	7:H:11:DG:O4'	2.04	0.57
3:D:273:ARG:HB3	3:D:278:PRO:HA	1.85	0.57
3:D:922:LEU:O	3:D:927:THR:N	2.37	0.57
1:A:215:VAL:HG13	1:B:222:LEU:HD22	1.85	0.57
2:C:420:ARG:O	2:C:422:ARG:NH2	2.35	0.57
1:A:193:ASP:OD1	2:C:938:LYS:NZ	2.35	0.57



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:51:THR:OG1	1:B:87:VAL:O	2.19	0.57
3:D:449:SER:N	11:D:2101:HOH:O	2.13	0.57
1:A:31:GLY:N	1:A:193:ASP:OD2	2.35	0.57
2:C:35:PRO:HG2	2:C:38:LYS:HD2	1.86	0.57
3:D:308:LYS:NZ	11:D:2113:HOH:O	2.36	0.56
2:C:571:LEU:HB2	2:C:574:ALA:HB2	1.87	0.56
2:C:261:ILE:HG23	2:C:290:LEU:HB2	1.87	0.56
3:D:1184:GLN:O	11:D:2102:HOH:O	2.17	0.56
3:D:132:TYR:OH	3:D:568:ARG:NH1	2.38	0.56
3:D:415:VAL:HG13	3:D:419:ASP:HB2	1.87	0.56
1:A:36:LEU:HD11	1:B:221:HIS:HB3	1.87	0.56
3:D:356:PRO:HG2	3:D:359:ALA:HB2	1.85	0.56
2:C:808:ARG:NH2	5:F:305:GLU:OE2	2.37	0.56
3:D:238:PRO:HD3	3:D:318:ARG:HG3	1.86	0.56
5:F:79:ASP:OD2	7:H:8:DG:N1	2.30	0.56
3:D:643:GLY:HA3	3:D:727:GLN:HB2	1.87	0.56
2:C:12:VAL:HG12	2:C:13:ILE:HG23	1.88	0.56
3:D:256:GLU:HG3	3:D:300:LYS:HG3	1.88	0.56
2:C:94:LEU:HD22	2:C:118:ILE:HD11	1.87	0.55
5:F:171:LYS:O	5:F:175:HIS:ND1	2.37	0.55
1:A:196:THR:HG21	2:C:934:PHE:HE1	1.70	0.55
3:D:231:VAL:O	3:D:236:TYR:OH	2.23	0.55
3:D:1071:PHE:O	3:D:1074:SER:OG	2.13	0.55
1:B:78:ILE:HG23	1:B:129:ILE:HG23	1.88	0.55
3:D:162:ARG:NH1	3:D:451:ASP:OD1	2.40	0.55
3:D:921:ARG:C	3:D:923:GLY:CA	2.74	0.55
3:D:1042:ARG:HB3	3:D:1057:VAL:HB	1.88	0.55
1:B:191:ASP:OD1	1:B:191:ASP:N	2.37	0.54
2:C:13:ILE:HD13	2:C:483:VAL:HG11	1.88	0.54
6:G:16:DC:H2'	6:G:17:DG:H8	1.70	0.54
1:B:8:ALA:HB1	1:B:27:PRO:HD2	1.89	0.54
1:B:8:ALA:HB1	1:B:9:PRO:HA	1.89	0.54
3:D:1190:SER:OG	3:D:1369:GLU:OE1	2.19	0.54
2:C:271:GLU:OE1	2:C:288:ARG:NH1	2.39	0.54
2:C:740:GLU:HB3	2:C:805:ARG:HH12	1.72	0.54
6:G:15:DT:H2'	6:G:16:DC:C6	2.43	0.54
3:D:1495:ILE:HG12	4:E:88:GLU:HG3	1.88	0.54
2:C:324:ASP:HB3	2:C:327:HIS:HB2	1.89	0.54
3:D:455:ARG:HB2	3:D:460:ALA:HB2	1.90	0.54
5:F:365:GLU:HB2	5:F:404:ALA:HB2	1.89	0.54
1:A:209:GLU:O	1:A:213:GLN:HG2	2.08	0.53



Atom-1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:C:408:ARG:NH1	2:C:456:ALA:O	2.41	0.53
2:C:413:LEU:HD11	2:C:451:LEU:HD13	1.90	0.53
4:E:2:ALA:N	11:E:102:HOH:O	2.41	0.53
7:H:9:DG:H2"	7:H:10:DA:C8	2.44	0.53
2:C:617:ASP:OD1	2:C:617:ASP:N	2.42	0.53
3:D:244:GLU:HG3	3:D:310:LEU:HG	1.89	0.53
1:B:176:ARG:NH2	3:D:888:GLU:OE1	2.34	0.53
2:C:937:ASP:OD1	2:C:939:ARG:HD3	2.09	0.53
5:F:169:GLU:O	5:F:172:ARG:HB3	2.08	0.53
1:A:133:GLU:HG2	1:A:134:GLU:H	1.74	0.53
3:D:1068:LEU:O	3:D:1072:ILE:HG12	2.09	0.53
2:C:1038:TRP:CE2	3:D:1099:VAL:HG11	2.44	0.53
1:B:71:VAL:HG22	1:B:132:LEU:HG	1.91	0.53
3:D:270:LEU:HD12	3:D:284:LEU:HD11	1.91	0.53
3:D:631:ILE:HD11	3:D:743:ASP:HB2	1.90	0.53
2:C:168:ARG:O	2:C:267:TYR:HA	2.09	0.53
3:D:181:ASP:HB2	3:D:205:TYR:CD2	2.44	0.52
2:C:543:ASN:ND2	2:C:566:THR:HG22	2.25	0.52
2:C:715:THR:OG1	2:C:718:GLY:O	2.23	0.52
2:C:537:LYS:HD3	2:C:583:LEU:HD11	1.91	0.52
3:D:787:LEU:HD21	3:D:947:ILE:HG21	1.90	0.52
2:C:616:GLU:OE1	2:C:648:ARG:NH1	2.42	0.52
5:F:276:ARG:O	5:F:279:GLN:HG3	2.10	0.52
2:C:504:GLU:HG2	2:C:509:ALA:HB2	1.92	0.52
3:D:838:ARG:NH1	3:D:874:GLU:OE1	2.41	0.52
6:G:12:DG:N2	7:H:16:DC:O2	2.19	0.52
2:C:1008:ARG:NH2	3:D:624:ASP:OD1	2.35	0.52
5:F:105:LYS:HD3	5:F:179:GLU:HG2	1.92	0.52
2:C:172:ILE:HG12	2:C:186:VAL:HG22	1.92	0.52
3:D:919:PHE:HA	3:D:927:THR:OG1	2.10	0.52
3:D:241:ILE:HA	3:D:312:ARG:HG2	1.92	0.52
2:C:805:ARG:O	2:C:807[A]:ARG:NH2	2.36	0.51
2:C:848:VAL:HG22	3:D:740:PHE:O	2.10	0.51
3:D:701:LEU:HB2	3:D:748:HIS:HB2	1.92	0.51
3:D:921:ARG:C	3:D:923:GLY:N	2.59	0.51
5:F:194:LEU:HB2	7:H:6:DT:C2	2.45	0.51
2:C:872:ASN:ND2	3:D:784:ASP:OD2	2.41	0.51
3:D:187:LYS:N	3:D:200:ASP:OD2	2.36	0.51
2:C:207:LEU:HD13	2:C:221:LEU:HD21	1.92	0.51
1:B:32:PHE:HA	1:B:35:THR:HB	1.92	0.51
5:F:189:GLU:HA	5:F:192:LEU:HG	1.91	0.51



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:B:123:MET:HG2	11:B:2103:HOH:O	2.09	0.51
1:B:136:GLY:N	11:B:2107:HOH:O	2.44	0.51
3:D:1461:GLY:O	3:D:1465:ASN:ND2	2.43	0.51
1:B:90:LEU:HD21	1:B:121:GLU:HB2	1.93	0.51
5:F:187:LEU:O	5:F:191:ASN:ND2	2.42	0.51
2:C:936:VAL:HG11	2:C:959:PRO:HB2	1.92	0.50
3:D:785:ILE:HD13	3:D:935:LYS:HA	1.94	0.50
2:C:536:PRO:HB3	3:D:1067:VAL:HG11	1.94	0.50
2:C:709:GLU:OE2	2:C:824:ARG:NH1	2.44	0.50
1:B:216:GLU:OE1	1:B:219:ARG:NH2	2.28	0.50
5:F:120:THR:HG22	5:F:122:LEU:HD13	1.92	0.50
5:F:163:LEU:HD13	5:F:174:LEU:HD13	1.93	0.50
2:C:584:GLU:HB3	2:C:666:LEU:H	1.76	0.50
3:D:479:GLU:HA	3:D:482:LYS:HE2	1.93	0.50
3:D:1040:GLY:O	3:D:1060:SER:HB3	2.12	0.50
3:D:106:LYS:O	3:D:586:ARG:NH1	2.45	0.50
2:C:657:ASP:OD2	2:C:663:ASN:N	2.42	0.49
3:D:1366:LYS:O	3:D:1370:ILE:HG12	2.12	0.49
2:C:286:SER:OG	2:C:301:GLU:OE2	2.25	0.49
1:A:222:LEU:HD21	1:B:218:LEU:HD23	1.93	0.49
2:C:274:ARG:NH2	2:C:278:GLU:OE2	2.46	0.49
3:D:129:PHE:CD2	3:D:456:MET:HB3	2.47	0.49
3:D:707:THR:HG23	3:D:712:GLY:HA3	1.95	0.49
6:G:16:DC:H2'	6:G:17:DG:C8	2.47	0.49
2:C:1046:ALA:HB1	3:D:1471:LEU:HG	1.94	0.49
5:F:172:ARG:O	5:F:176:ILE:HG12	2.12	0.49
1:B:26:GLU:HB3	1:B:194:LYS:HG3	1.94	0.49
2:C:326:ASP:OD1	7:H:14:DG:N2	2.41	0.49
2:C:915:LYS:NZ	3:D:952:ASP:OD2	2.42	0.49
1:A:58:ILE:HG12	1:A:140:MET:HG2	1.94	0.49
2:C:41:ASN:O	2:C:46:ALA:HB2	2.12	0.49
3:D:555:LYS:HA	5:F:142:ARG:HH12	1.77	0.49
3:D:920:LEU:C	3:D:923:GLY:HA2	2.32	0.49
2:C:1015:LEU:HD11	3:D:528:VAL:HG11	1.93	0.48
3:D:97:THR:HG21	3:D:571:LYS:HG2	1.94	0.48
1:A:216:GLU:OE2	1:A:219:ARG:NH2	2.45	0.48
2:C:670:GLN:HG2	2:C:699:PHE:CD2	2.48	0.48
3:D:1047:LYS:HG2	3:D:1053[A]:PHE:CE2	2.48	0.48
3:D:1350:GLU:O	3:D:1354:LYS:HG3	2.12	0.48
5:F:315:VAL:HG22	5:F:316:SER:H	1.78	0.48
7:H:18:DC:H2"	7:H:19:DG:C8	2.49	0.48



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:64:GLU:HG3	1:A:79:ILE:HD12	1.94	0.48
2:C:143:SER:O	2:C:147:TYR:OH	2.29	0.48
5:F:284:ARG:NH2	5:F:290:GLU:OE2	2.46	0.48
2:C:904:PRO:HB2	2:C:907:ASP:HB3	1.94	0.48
3:D:101:HIS:HB3	3:D:104:PHE:HD2	1.78	0.48
3:D:487:ALA:O	3:D:491:LYS:HG2	2.13	0.48
2:C:198:ARG:HE	2:C:227:PHE:HA	1.78	0.48
3:D:171:LEU:HD12	3:D:390:PRO:HG2	1.94	0.48
1:B:150:TYR:CE1	1:B:170:VAL:HG22	2.49	0.48
3:D:236:TYR:HB2	3:D:319:ALA:HB3	1.96	0.48
3:D:1099:VAL:O	3:D:1103:HIS:HB3	2.13	0.48
3:D:411:THR:HG23	3:D:436:GLU:HA	1.96	0.48
3:D:1084:THR:O	3:D:1088:THR:HG23	2.14	0.48
2:C:721:ARG:HH22	2:C:785:VAL:HG11	1.79	0.48
3:D:63:TYR:OH	3:D:74:GLU:OE2	2.30	0.48
3:D:1103:HIS:CE1	3:D:1463:LYS:H	2.32	0.48
3:D:355:VAL:HG11	3:D:385:VAL:HG21	1.95	0.47
2:C:615:TYR:OH	2:C:623:TYR:OH	2.17	0.47
3:D:96:ALA:HB3	3:D:554:LEU:HD23	1.96	0.47
3:D:966:GLU:O	3:D:969:ARG:HG2	2.15	0.47
3:D:1259:VAL:HG23	3:D:1355:VAL:HG11	1.95	0.47
5:F:189:GLU:O	5:F:192:LEU:HB2	2.15	0.47
1:A:55:SER:HB3	1:A:143:ARG:HB3	1.96	0.47
1:B:46:SER:O	1:B:148:VAL:HB	2.14	0.47
3:D:1047:LYS:N	3:D:1051:GLU:O	2.38	0.47
3:D:158:TYR:CE1	3:D:454:ALA:HB3	2.49	0.47
3:D:176:ASP:OD1	3:D:177:ALA:N	2.47	0.47
3:D:1480:PHE:O	4:E:18:ARG:NH2	2.47	0.47
1:B:190:THR:O	11:B:2102:HOH:O	2.20	0.47
2:C:1009:SER:HB3	3:D:651:GLU:O	2.14	0.47
3:D:218:LYS:HG2	3:D:338:GLU:HG2	1.96	0.47
3:D:923:GLY:O	3:D:927:THR:HB	2.15	0.47
3:D:1053[B]:PHE:CE2	3:D:1055:VAL:HB	2.50	0.47
2:C:1016:ILE:O	3:D:87:ARG:NH1	2.48	0.47
3:D:923:GLY:O	3:D:927:THR:CB	2.62	0.47
3:D:923:GLY:O	3:D:924:MET:C	2.49	0.47
3:D:563:PRO:HD2	3:D:566:ILE:HD12	1.96	0.47
3:D:841:TYR:HB2	3:D:864:VAL:HG22	1.96	0.47
3:D:1377:LYS:HE2	3:D:1378:TYR:CZ	2.50	0.47
1:B:83:LYS:NZ	3:D:842:VAL:O	2.48	0.47
3:D:483:HIS:CE1	3:D:488:ARG:HD3	2.50	0.47



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
3:D:924:MET:HB3	4:E:7:ASP:OD1	2.15	0.47
3:D:770:LEU:HD11	3:D:919:PHE:CD1	2.50	0.47
3:D:890:VAL:HG21	3:D:922:LEU:HD13	1.97	0.47
3:D:1484:THR:O	4:E:25:LYS:NZ	2.27	0.47
2:C:1009:SER:O	3:D:624:ASP:HB3	2.14	0.46
3:D:417:PRO:HD3	3:D:432:TYR:HA	1.98	0.46
2:C:86:LYS:HB2	2:C:88:LEU:HG	1.96	0.46
2:C:727:PRO:HB3	2:C:783:ARG:HD3	1.97	0.46
3:D:915:VAL:O	3:D:919:PHE:HB2	2.15	0.46
2:C:224:GLU:CD	2:C:224:GLU:H	2.18	0.46
2:C:367:LEU:HD13	2:C:372:LEU:HD21	1.98	0.46
2:C:1090:LYS:HA	2:C:1090:LYS:HD3	1.72	0.46
3:D:55:ASP:OD1	3:D:83:SER:OG	2.31	0.46
5:F:101:GLU:HG2	5:F:105:LYS:HE2	1.97	0.46
5:F:144:ILE:HB	5:F:147:LEU:HD13	1.98	0.46
2:C:87:ASP:HA	2:C:131:GLY:HA3	1.97	0.46
2:C:541:SER:O	2:C:545:ASN:ND2	2.41	0.46
1:B:128:HIS:CE1	1:B:131:THR:HG23	2.50	0.46
2:C:456:ALA:HB3	2:C:459:ALA:HB2	1.98	0.46
3:D:319:ALA:HA	3:D:337:LEU:HD23	1.98	0.46
3:D:975:GLU:O	3:D:979:GLU:HG2	2.16	0.46
2:C:63:GLY:HA3	2:C:100:LEU:HD21	1.98	0.46
2:C:129:ILE:HB	2:C:134:ARG:HD2	1.97	0.46
3:D:22:SER:HB2	3:D:92:HIS:HB3	1.98	0.46
3:D:314:PRO:HB2	3:D:317:VAL:HG12	1.98	0.46
3:D:411:THR:O	5:F:178:ARG:NH1	2.44	0.46
2:C:704:HIS:CD2	2:C:831:ARG:HD2	2.51	0.46
5:F:353:GLU:HA	5:F:356:LYS:HD2	1.98	0.46
1:A:124:ASN:OD1	1:A:124:ASN:N	2.49	0.46
3:D:996:TRP:CD2	3:D:1056:PRO:HG3	2.51	0.46
3:D:1236:LEU:HA	3:D:1359:GLN:HG3	1.98	0.46
1:B:190:THR:HG21	3:D:722:GLU:OE2	2.15	0.46
2:C:1054:THR:OG1	2:C:1055:LEU:N	2.48	0.46
7:H:12:DC:H1'	7:H:13:DT:C4	2.51	0.46
2:C:843:HIS:NE2	2:C:887:GLU:OE2	2.41	0.45
2:C:1031:ARG:HA	3:D:622:ARG:HA	1.98	0.45
3:D:353:VAL:HG12	3:D:355:VAL:H	1.81	0.45
3:D:875:THR:OG1	3:D:876:SER:N	2.48	0.45
3:D:1264:GLU:OE2	3:D:1425:THR:OG1	2.31	0.45
1:A:221:HIS:O	1:A:224:TYR:N	2.50	0.45
1:B:73:GLU:HB3	1:B:77:GLU:HB3	1.98	0.45



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:78:ILE:N	11:B:2101:HOH:O	2.15	0.45
3:D:1197:ARG:HB2	3:D:1398:TRP:CH2	2.51	0.45
2:C:243:ARG:NH1	7:H:9:DG:O6	2.49	0.45
2:C:602:GLU:HB2	2:C:648:ARG:HH21	1.82	0.45
2:C:1037:VAL:HG13	2:C:1049:LEU:HD11	1.98	0.45
3:D:58:CYS:HB2	3:D:76:CYS:SG	2.57	0.45
3:D:58:CYS:SG	3:D:62:LYS:N	2.90	0.45
3:D:252:ARG:HA	3:D:303:PRO:HA	1.99	0.45
3:D:1296:SER:HB3	3:D:1299:PHE:HB2	1.99	0.45
5:F:80:PRO:HB2	5:F:210:LEU:HD11	1.99	0.45
5:F:89:GLY:HA3	7:H:7:DG:C6	2.51	0.45
1:A:228:PRO:HB3	1:B:13:VAL:HG21	1.98	0.45
2:C:556:ASN:O	2:C:559:LEU:HB3	2.16	0.45
3:D:743:ASP:OD1	3:D:743:ASP:N	2.50	0.45
3:D:951:ILE:HG13	3:D:1062:ARG:HD2	1.98	0.45
3:D:483:HIS:CG	3:D:484:PRO:HD2	2.52	0.45
3:D:1455:LYS:HB2	3:D:1455:LYS:HE3	1.84	0.45
1:A:70:GLY:N	2:C:607:ASP:OD1	2.48	0.45
3:D:63:TYR:HB2	3:D:80:VAL:HG21	1.98	0.45
3:D:618:LEU:HG	3:D:1467:ILE:HG23	1.98	0.45
3:D:1344:VAL:HG11	3:D:1421:LEU:HD22	1.98	0.45
1:B:143:ARG:NH1	1:B:158:ILE:HD12	2.31	0.45
2:C:976:ASP:OD1	2:C:978:ARG:HD3	2.17	0.45
2:C:1092:LEU:HD13	2:C:1099:VAL:HG21	1.97	0.45
3:D:38:LYS:HA	3:D:38:LYS:HD3	1.84	0.45
3:D:703:ASN:HB2	3:D:713:ILE:HG12	1.99	0.45
3:D:1488:ASP:OD1	3:D:1488:ASP:N	2.40	0.45
3:D:96:ALA:HB2	3:D:555:LYS:HG2	1.99	0.44
3:D:760:ARG:O	3:D:764:LEU:HB2	2.17	0.44
2:C:675:ALA:HB2	2:C:867:VAL:HG11	1.99	0.44
3:D:921:ARG:H	3:D:921:ARG:HG2	1.60	0.44
2:C:440:PRO:HB2	3:D:1074:SER:HB2	2.00	0.44
2:C:957:LYS:HD3	2:C:961:GLU:HB3	2.00	0.44
3:D:890:VAL:O	3:D:926:LYS:HD3	2.17	0.44
1:A:179:PHE:HB3	1:A:197:LEU:HD23	2.00	0.44
3:D:750:PRO:HG2	3:D:756:GLN:NE2	2.32	0.44
3:D:879:ARG:HD3	3:D:902:LEU:O	2.17	0.44
1:A:222:LEU:HD11	1:B:218:LEU:HG	1.98	0.44
2:C:88:LEU:O	2:C:131:GLY:N	2.50	0.44
3:D:1036:ARG:NH2	3:D:1042:ARG:O	2.43	0.44
1:A:64:GLU:OE2	2:C:830:LYS:NZ	2.50	0.44



Atom-1	Atom-2	Interatomic	Clash
		distance (A)	overlap (A)
2:C:256:TYR:HE1	7:H:11:DG:H22	1.65	0.44
2:C:405:ARG:HD3	2:C:566:THR:HG21	1.98	0.44
3:D:800:LYS:HB3	3:D:822:ALA:HB2	2.00	0.44
3:D:1267:ARG:HA	3:D:1268:PRO:HD3	1.87	0.44
1:B:94:LEU:HD11	1:B:97:VAL:HG22	1.98	0.44
2:C:237:ARG:O	2:C:240:THR:OG1	2.29	0.44
3:D:127:LEU:HA	3:D:457:GLY:HA2	1.98	0.44
6:G:17:DG:H2'	6:G:18:DA:C8	2.53	0.44
1:B:155:LYS:HA	1:B:155:LYS:HD3	1.74	0.44
2:C:670:GLN:HG2	2:C:699:PHE:CG	2.52	0.44
3:D:317:VAL:HG23	3:D:339:TRP:HB3	2.00	0.44
2:C:587:VAL:HG11	2:C:666:LEU:HD22	2.00	0.43
2:C:1110:ASP:OD2	2:C:1114:GLY:N	2.49	0.43
2:C:1115:LEU:HB3	3:D:85:VAL:HG12	2.00	0.43
3:D:8:VAL:HG12	3:D:1434:TRP:HZ2	1.82	0.43
3:D:180:LYS:NZ	3:D:357:GLU:OE1	2.46	0.43
3:D:926:LYS:H	3:D:926:LYS:HG3	1.50	0.43
3:D:1362:LYS:HB2	3:D:1362:LYS:HE2	1.75	0.43
2:C:1090:LYS:HE2	2:C:1112:PHE:CZ	2.53	0.43
2:C:1094:ALA:HA	3:D:518:PRO:HB2	2.01	0.43
3:D:959:GLU:OE1	3:D:959:GLU:N	2.36	0.43
2:C:35:PRO:HA	2:C:36:PRO:HD3	1.85	0.43
2:C:724:ARG:NH2	2:C:734:LEU:O	2.51	0.43
3:D:517:VAL:HA	3:D:518:PRO:HD3	1.84	0.43
1:A:196:THR:HG21	2:C:934:PHE:CE1	2.52	0.43
2:C:947:ALA:HA	2:C:950:LEU:HB2	1.99	0.43
3:D:704:ARG:HD2	3:D:738:ALA:HB2	2.01	0.43
1:B:141:GLU:OE1	1:B:161:ARG:NH2	2.52	0.43
1:A:20:TYR:OH	1:A:198:ARG:HD2	2.18	0.43
2:C:63:GLY:N	2:C:367:LEU:HD12	2.34	0.43
2:C:247:PRO:HA	2:C:248:PRO:HD3	1.68	0.43
5:F:153:PRO:HA	5:F:156:VAL:HG22	1.99	0.43
2:C:396:ASP:HA	2:C:633:GLN:NE2	2.33	0.43
3:D:730:PRO:O	3:D:733:CYS:HB2	2.19	0.43
3:D:860:LEU:O	3:D:876:SER:HB2	2.19	0.43
2:C:928:LYS:HB2	2:C:928:LYS:HE3	1.82	0.43
3:D:137:PRO:HA	3:D:452:ILE:HG23	2.00	0.43
3:D:236:TYR:CE2	3:D:242:LEU:HD12	2.53	0.43
5:F:208:SER:HB3	5:F:211:ASP:OD2	2.19	0.43
6:G:19:DG:H2'	6:G:20:DG:C8	2.53	0.43
1:B:124:ASN:OD1	1:B:124:ASN:N	2.50	0.43



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
3:D:171:LEU:HD11	3:D:393:ILE:HD11	2.01	0.43
3:D:699:VAL:O	3:D:756:GLN:NE2	2.48	0.43
3:D:1101:VAL:HG13	3:D:1102:THR:HG23	2.01	0.43
5:F:134:LYS:NZ	5:F:157:GLU:OE1	2.37	0.43
1:A:91:ASN:HA	1:A:92:PRO:HD3	1.83	0.43
2:C:304:LEU:HB3	2:C:305:PRO:HD3	2.01	0.43
2:C:435:TYR:OH	2:C:533:ASP:OD2	2.23	0.43
2:C:755:LEU:HD22	2:C:825:VAL:HG11	2.01	0.43
3:D:142:LEU:HB2	3:D:161:LEU:HD21	2.00	0.43
3:D:921:ARG:O	3:D:922:LEU:C	2.57	0.43
3:D:1045[B]:MET:HE3	3:D:1072:ILE:HG21	2.01	0.43
3:D:1493:LYS:O	3:D:1497:GLU:HG2	2.18	0.43
1:A:221:HIS:HA	1:A:224:TYR:CD2	2.53	0.42
2:C:895:TYR:HB2	2:C:991:GLN:HG3	1.99	0.42
3:D:310:LEU:H	3:D:310:LEU:HD12	1.84	0.42
3:D:771:SER:HA	3:D:772:PRO:HD3	1.85	0.42
2:C:139:GLN:NE2	2:C:413:LEU:O	2.49	0.42
2:C:399:ASN:OD1	2:C:401:LEU:HB3	2.19	0.42
2:C:875:GLY:O	2:C:879:ARG:HD3	2.19	0.42
3:D:1137:ARG:O	3:D:1141:GLU:HG3	2.19	0.42
1:B:110:LYS:HD3	1:B:128:HIS:HA	2.02	0.42
2:C:229:MET:HB2	2:C:233:GLU:HB2	2.01	0.42
2:C:535:SER:O	2:C:538:GLN:HG2	2.18	0.42
3:D:125:GLN:O	3:D:130:SER:N	2.52	0.42
3:D:657:LEU:HG	3:D:661:MET:HE2	2.00	0.42
3:D:860:LEU:HD22	3:D:878:GLY:HA2	2.01	0.42
2:C:905:ILE:C	2:C:907:ASP:H	2.23	0.42
2:C:1065:ALA:HB1	2:C:1077:PRO:HG3	2.01	0.42
1:A:11:PHE:O	1:B:228:PRO:HA	2.18	0.42
3:D:1072:ILE:HA	3:D:1075:HIS:HD2	1.83	0.42
3:D:169:TYR:HA	3:D:170:PRO:HD3	1.82	0.42
3:D:772:PRO:O	3:D:1209:LEU:HD12	2.18	0.42
3:D:892:ASP:OD1	3:D:894:LYS:HD2	2.20	0.42
4:E:13:VAL:HG21	4:E:19:LEU:HB2	2.01	0.42
1:A:102:LYS:HE3	1:A:102:LYS:HB2	1.89	0.42
1:A:103:ALA:HB1	1:A:107:LYS:HD3	2.02	0.42
2:C:374:ASN:OD1	5:F:276:ARG:HD2	2.20	0.42
3:D:372:ASP:HA	3:D:373:PRO:HD3	1.90	0.42
3:D:917:GLN:O	3:D:918:ALA:C	2.58	0.42
3:D:200:ASP:O	3:D:397:LYS:HG2	2.20	0.42
3:D:1053[A]:PHE:CE2	3:D:1072:ILE:HG23	2.55	0.42



Atom-1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:88:ARG:N	11:B:2103:HOH:O	2.52	0.42
2:C:420:ARG:HE	2:C:420:ARG:HB2	1.61	0.42
3:D:566:ILE:HD11	5:F:192:LEU:HD21	2.02	0.42
4:E:44:GLU:OE1	4:E:72:ARG:NH2	2.49	0.42
1:B:213:GLN:O	1:B:217:ILE:HG13	2.19	0.42
2:C:124:ASP:OD2	2:C:407:LYS:NZ	2.36	0.42
2:C:721:ARG:HH12	2:C:785:VAL:HG11	1.85	0.42
3:D:171:LEU:HD23	3:D:171:LEU:HA	1.90	0.42
3:D:1044:LEU:HD23	3:D:1056:PRO:HB3	2.01	0.42
1:A:150:TYR:CD1	2:C:696:LYS:HG2	2.55	0.41
2:C:203:ASP:OD1	2:C:204:GLN:N	2.53	0.41
2:C:896:PHE:HB2	2:C:921:ALA:HB1	2.01	0.41
3:D:475:LYS:O	3:D:479:GLU:HG2	2.20	0.41
3:D:889:ALA:HB1	3:D:930:LEU:HA	2.01	0.41
6:G:20:DG:H2'	6:G:21:DG:O4'	2.20	0.41
1:A:39:PRO:HG3	1:B:39:PRO:HG3	2.02	0.41
1:A:150:TYR:CE2	1:A:152:PRO:HG3	2.55	0.41
2:C:954:THR:HA	2:C:955:PRO:HD3	1.93	0.41
3:D:803:GLY:HA2	3:D:827:ILE:HA	2.02	0.41
1:A:63:HIS:CE1	1:A:65:PHE:HB2	2.56	0.41
2:C:173:ASP:HB2	2:C:185:LYS:HB3	2.01	0.41
2:C:740:GLU:OE1	2:C:807[B]:ARG:NH2	2.53	0.41
3:D:209:ARG:O	3:D:346:ARG:HD3	2.21	0.41
3:D:414:ARG:HD3	3:D:451:ASP:HB2	2.01	0.41
3:D:437:VAL:HG11	5:F:175:HIS:CD2	2.55	0.41
3:D:790:TYR:CE1	3:D:1022:VAL:HG13	2.55	0.41
3:D:1018:ASN:HA	3:D:1019:PRO:HD3	1.90	0.41
4:E:44:GLU:OE2	4:E:72:ARG:NH1	2.49	0.41
1:A:80:LEU:O	1:A:83:LYS:HB2	2.21	0.41
1:A:148:VAL:O	11:A:402:HOH:O	2.21	0.41
1:A:172:SER:HA	1:A:173:PRO:HD2	1.87	0.41
2:C:164:PRO:HA	2:C:269:LEU:HD23	2.03	0.41
2:C:1043:TYR:CG	3:D:763:MET:HG2	2.55	0.41
3:D:646:LYS:HB3	3:D:688:TRP:CZ3	2.56	0.41
3:D:814:ALA:O	3:D:818:ARG:HG3	2.21	0.41
1:B:150:TYR:HE1	1:B:170:VAL:HG22	1.86	0.41
2:C:607:ASP:HB3	2:C:610:ARG:H	1.85	0.41
2:C:906:PHE:CG	3:D:1067:VAL:HG12	2.56	0.41
3:D:890:VAL:HA	3:D:926:LYS:HB3	2.02	0.41
5:F:88:ILE:HG23	5:F:193:ARG:HG2	2.03	0.41
1:A:115:LEU:HA	1:A:116:PRO:HD3	1.88	0.41



Atom 1	Atom 2	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
2:C:6:PHE:CD1	2:C:909:ALA:HB2	2.55	0.41	
3:D:318:ARG:NH1	3:D:338:GLU:OE1	2.53	0.41	
3:D:408:GLU:HA	5:F:171:LYS:NZ	2.36	0.41	
3:D:881:LEU:O	3:D:885:ILE:HG13	2.21	0.41	
3:D:1020:LEU:HB3	3:D:1035:ILE:HD12	2.03	0.41	
2:C:45:GLN:O	2:C:49:ARG:HG2	2.20	0.41	
2:C:276:LYS:HE3	2:C:276:LYS:HB3	1.89	0.41	
2:C:328:LEU:HD23	2:C:328:LEU:HA	1.89	0.41	
2:C:611:ILE:HD11	2:C:641:PRO:HB3	2.03	0.41	
2:C:690:ILE:HB	2:C:694:LEU:HD12	2.01	0.41	
2:C:944:LEU:O	2:C:948:GLU:HB2	2.21	0.41	
3:D:923:GLY:O	3:D:927:THR:OG1	2.39	0.41	
5:F:338:LEU:HA	5:F:339:PRO:HD3	1.84	0.41	
1:A:198:ARG:HD3	2:C:934:PHE:CZ	2.56	0.41	
3:D:618:LEU:HD13	3:D:618:LEU:HA	1.85	0.41	
3:D:743:ASP:HA	8:I:7:A:H4'	2.02	0.41	
3:D:784:ASP:HB2	3:D:939:PHE:HE1	1.86	0.41	
3:D:920:LEU:O	3:D:923:GLY:HA2	2.20	0.41	
3:D:1072:ILE:HA	3:D:1075:HIS:CD2	2.55	0.41	
3:D:1045[B]:MET:HE1	3:D:1057:VAL:HG23	2.03	0.41	
5:F:397:ILE:HD12	5:F:400:ILE:HD12	2.02	0.41	
6:G:15:DT:C4	6:G:16:DC:N4	2.89	0.41	
4:E:14:ASP:OD1	4:E:18:ARG:NH1	2.48	0.41	
2:C:30:LEU:O	2:C:71:TYR:OH	2.28	0.40	
2:C:55:GLU:HG2	2:C:65:VAL:HG22	2.01	0.40	
3:D:226:PRO:HG2	3:D:245:LEU:HD11	2.02	0.40	
3:D:935:LYS:HE2	3:D:935:LYS:HB3	1.94	0.40	
3:D:1065:LEU:HD23	3:D:1069:GLU:HB3	2.03	0.40	
2:C:807[A]:ARG:NH1	2:C:810:ASP:OD2	2.45	0.40	
2:C:976:ASP:HB3	2:C:979:THR:OG1	2.21	0.40	
2:C:1018:GLN:O	2:C:1058:ASP:HA	2.21	0.40	
3:D:573:MET:SD	5:F:210:LEU:HB3	2.61	0.40	
3:D:956:ILE:H	3:D:956:ILE:HG12	1.61	0.40	
5:F:383:LEU:HD13	5:F:398:ARG:HB2	2.03	0.40	
7:H:12:DC:H1'	7:H:13:DT:C5	2.56	0.40	
1:B:94:LEU:O	1:B:146:ARG:NH2	2.54	0.40	
2:C:76:PRO:HG3	2:C:120:LEU:HD12	2.03	0.40	
3:D:622:ARG:NH1	6:G:17:DG:OP1	2.35	0.40	
3:D:786:ILE:HG22	3:D:1026:SER:HB2	2.03	0.40	
3:D:1274:ILE:HG22	3:D:1324:PRO:HA	2.03	0.40	
2:C:683:ASN:HB2	2:C:872:ASN:HB2	2.04	0.40	



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1032:PHE:CZ	2:C:1036:GLU:HB3	2.57	0.40
5:F:285:GLU:HA	5:F:286:PRO:HD3	1.83	0.40
5:F:362:SER:OG	5:F:365:GLU:HG2	2.21	0.40
3:D:916:TYR:O	3:D:919:PHE:HB3	2.22	0.40
3:D:1402:ALA:O	3:D:1405:GLU:HG2	2.22	0.40
5:F:184:ARG:O	5:F:188:ILE:HG13	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
1	А	230/315~(73%)	228 (99%)	2(1%)	0	100	100
1	В	218/315~(69%)	210 (96%)	7 (3%)	1 (0%)	29	67
2	С	1111/1119 (99%)	1081 (97%)	29 (3%)	1 (0%)	51	83
3	D	1485/1524~(97%)	1445 (97%)	40 (3%)	0	100	100
4	Е	92/99~(93%)	90~(98%)	2(2%)	0	100	100
5	F	333/443~(75%)	329 (99%)	4 (1%)	0	100	100
All	All	3469/3815 (91%)	3383 (98%)	84 (2%)	2(0%)	51	83

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	С	925	TYR
1	В	8	ALA



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	Percentil	es
1	А	201/273~(74%)	199~(99%)	2(1%)	76 90	
1	В	195/273~(71%)	192 (98%)	3 (2%)	65 85	
2	С	939/941~(100%)	922~(98%)	17 (2%)	59 82]
3	D	1256/1279~(98%)	1234 (98%)	22 (2%)	59 82	Γ
4	Ε	82/88~(93%)	81 (99%)	1 (1%)	71 88]
5	F	293/388~(76%)	290 (99%)	3 (1%)	76 90	
All	All	2966/3242~(92%)	2918 (98%)	48 (2%)	62 84	

All (48) residues with a non-rotameric side chain are listed below:

Mol	Chain	Res	Type
1	А	6	LEU
1	А	74	ASP
1	В	55	SER
1	В	96	THR
1	В	154	GLU
2	С	100	LEU
2	С	141	HIS
2	С	174	LEU
2	С	177	GLU
2	С	230	ARG
2	С	342	ASP
2	С	353	ARG
2	С	358	ARG
2	С	402	SER
2	С	429	ASP
2	С	566	THR
2	С	575	GLN
2	С	610	ARG
2	С	617	ASP
2	С	670	GLN
2	С	807[A]	ARG
2	С	807[B]	ARG



Mol	Chain	Res	Type
3	D	35	ARG
3	D	149	LYS
3	D	270	LEU
3	D	273	ARG
3	D	288	MET
3	D	632	VAL
3	D	709	HIS
3	D	743	ASP
3	D	754	PHE
3	D	864	VAL
3	D	894	LYS
3	D	907	GLU
3	D	921	ARG
3	D	956	ILE
3	D	1014	ASN
3	D	1041	LEU
3	D	1129	THR
3	D	1184	GLN
3	D	1188	VAL
3	D	1234	THR
3	D	1307	LYS
3	D	1488	ASP
4	E	50	THR
5	F	88	ILE
5	F	369	LEU
5	F	417	LYS

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

Mol	Chain	Res	Type
1	В	81	ASN
2	С	99	GLN
2	С	117	HIS
2	С	506	ASN
2	С	538	GLN
2	С	962	GLN
3	D	66	GLN
3	D	143	ASN
3	D	669	ASN
3	D	1124	GLN
5	F	83	GLN



5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
8	Ι	6/7~(85%)	1 (16%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
8	Ι	2	С

There are no RNA pucker outliers to report.

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 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ $>$	#RSRZ>2	$\mathbf{OWAB}(\mathbf{\AA}^2)$	Q < 0.9
1	А	231/315~(73%)	-0.36	4 (1%) 70 57	40, 54, 82, 135	0
1	В	222/315~(70%)	-0.29	0 100 100	38, 61, 96, 118	0
2	С	1112/1119 (99%)	-0.34	7 (0%) 89 83	20, 49, 113, 153	0
3	D	1486/1524~(97%)	-0.18	17 (1%) 80 69	18, 53, 118, 151	1 (0%)
4	Ε	94/99~(94%)	-0.41	0 100 100	24, 49, 86, 107	0
5	F	337/443~(76%)	-0.03	15 (4%) 33 21	42, 73, 124, 149	0
6	G	18/21~(85%)	-0.17	1 (5%) 24 13	36, 64, 143, 151	0
7	Н	24/27~(88%)	-0.01	0 100 100	59, 83, 139, 168	0
8	Ι	7/7~(100%)	-0.08	1 (14%) 2 1	33, 35, 85, 108	0
All	All	3531/3870 (91%)	-0.24	45 (1%) 77 65	18, 55, 116, 168	1 (0%)

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	С	63	GLY	5.1
5	F	146	GLY	5.0
1	А	232	ALA	4.5
5	F	149	GLU	4.5
5	F	377	ASP	3.8
3	D	422	ALA	3.8
3	D	173	PRO	3.7
3	D	144	GLY	3.6
3	D	922	LEU	3.5
5	F	414	ARG	3.1
2	С	365	ASP	3.1
3	D	1237	THR	3.1
3	D	531	ASP	3.0
5	F	138	SER	2.9
2	С	362	GLY	2.9



Mol	Chain	Res	Type	RSRZ
2	С	766	GLU	2.8
3	D	316	GLN	2.8
3	D	1499	ARG	2.8
5	F	170	HIS	2.6
3	D	1297	GLU	2.5
5	F	415	THR	2.5
3	D	1306	PRO	2.4
3	D	174	GLY	2.4
3	D	321	GLN	2.4
1	А	230	ALA	2.4
1	А	234	ALA	2.3
5	F	191	ASN	2.3
5	F	381	HIS	2.3
8	Ι	1	С	2.3
5	F	145	PRO	2.3
5	F	150	THR	2.3
2	С	739	GLU	2.3
3	D	923	GLY	2.3
2	С	104	ASP	2.3
3	D	345	TYR	2.3
3	D	235	ALA	2.3
3	D	1292	VAL	2.3
5	F	416	ARG	2.3
5	F	376	ILE	2.2
5	F	411	HIS	2.2
1	А	233	VAL	2.2
3	D	1298	GLY	2.2
5	F	142	ARG	2.1
2	С	600	ASP	2.0
6	G	5	DC	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	$\mathbf{B} ext{-factors}(\mathbf{A}^2)$	Q<0.9
9	MG	В	2001	1/1	0.69	0.27	64,64,64,64	0
10	ZN	D	1603	1/1	0.90	0.07	45,45,45,45	0
9	MG	F	2001	1/1	0.94	0.14	62,62,62,62	0
9	MG	D	1601	1/1	0.97	0.18	37,37,37,37	0
10	ZN	D	1602	1/1	0.98	0.03	6,6,6,6	0
9	MG	D	1604	1/1	0.98	0.12	19,19,19,19	0

6.5 Other polymers (i)

There are no such residues in this entry.

