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PDB ID	:	6GFW
EMDB ID	:	EMD-4397
Title	:	Cryo-EM structure of bacterial RNA polymerase-sigma54 holoenzyme initial
		transcribing complex
Authors	:	Glyde, R.; Ye, F.Z.; Zhang, X.D.
Deposited on	:	2018-05-02
Resolution	:	3.70 Å(reported)
This is	a l	Full wwPDB EM 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/EMValidationReportHelp 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:

EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $ELECTRON\ MICROSCOPY$

The reported resolution of this entry is 3.70 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f EM} {f structures} \ (\#{f Entries})$
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for $\geq=3, 2, 1$ 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 $\leq=5\%$ The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length		Quality of	chain		
1	А	329	—	54%	15%	•	29%
1	В	329	9%	55%	16%		29%
2	С	1342	8%	77%			23%
3	D	1407	14%	71%			23% • •
4	Е	91	7%	63%		19%	19%
5	F	63	27%	38%	-	13%	• 21%
6	G	63	24% 11%	65%			21%



Mol	Chain	Length			Quality of cha	ain			
7	М	497	22%	59%		14%	•	26%	-
8	R	4			100%				-



2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 28005 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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	AltConf	Trace			
1	А	233	Total	C	N	0	S	0	0
			1763	1096	313	348	6		
1	В	225	Total	\mathbf{C}	Ν	0	\mathbf{S}	0	0
1	D	235	1735	1085	305	340	5	0	0

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

Mol	Chain	Residues		Α	AltConf	Trace			
2	С	1341	Total 9998	C 6268	N 1739	O 1952	S 39	0	0

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

Mol	Chain	Residues		Α	AltConf	Trace			
3	D	1345	Total 9722	C 6102	N 1747	O 1832	S 41	0	0

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

Mol	Chain	Residues		At	oms	AltConf	Trace		
4	Е	74	Total 546	C 337	N 105	O 103	S 1	0	0

• Molecule 5 is a DNA chain called nifH promoter template DNA.

Mol	Chain	Residues		At	oms		AltConf	Trace	
5	F	50	Total 1027	C 484	N 197	O 296	Р 50	0	0

• Molecule 6 is a DNA chain called NifH promoter non-template DNA.



Mol	Chain	Residues		A	toms	AltConf	Trace		
6	G	50	Total 1026	C 486	N 189	O 301	Р 50	0	0

• Molecule 7 is a protein called RNA polymerase sigma-54 factor.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	М	366	Total 2102	C 1295	N 385	0 421	S 1	0	0

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
М	-19	MET	-	initiating methionine	UNP A0A0J4U551
М	-18	GLY	-	expression tag	UNP A0A0J4U551
М	-17	SER	-	expression tag	UNP A0A0J4U551
М	-16	SER	-	expression tag	UNP A0A0J4U551
М	-15	HIS	-	expression tag	UNP A0A0J4U551
М	-14	HIS	-	expression tag	UNP A0A0J4U551
М	-13	HIS	-	expression tag	UNP A0A0J4U551
М	-12	HIS	-	expression tag	UNP A0A0J4U551
М	-11	HIS	-	expression tag	UNP A0A0J4U551
М	-10	HIS	-	expression tag	UNP A0A0J4U551
М	-9	SER	-	expression tag	UNP A0A0J4U551
М	-8	SER	-	expression tag	UNP A0A0J4U551
М	-7	GLY	-	expression tag	UNP A0A0J4U551
М	-6	LEU	-	expression tag	UNP A0A0J4U551
М	-5	VAL	-	expression tag	UNP A0A0J4U551
М	-4	PRO	-	expression tag	UNP A0A0J4U551
М	-3	ARG	-	expression tag	UNP A0A0J4U551
М	-2	GLY	-	expression tag	UNP A0A0J4U551
М	-1	SER	-	expression tag	UNP A0A0J4U551
M	0	HIS	-	expression tag	UNP A0A0J4U551
М	336	ALA	ARG	engineered mutation	UNP A0A0J4U551

• Molecule 8 is a RNA chain called de novo synthesized RNA.

Mol	Chain	Residues	Atoms			AltConf	Trace		
8	R	4	Total 86	C 39	N 17	O 27	Р 3	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 atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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



• Molecule 2: DNA-directed RNA polymerase subunit beta

Chain C: 77%



23%







19%

• Molecule 4: DNA-directed RNA polymerase subunit omega

Chain E: 63% 19%



• Molecule 8: de novo synthesized RNA

Chain R:

100%



There are no outlier residues recorded for this chain.



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	89996	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE	Depositor
	CORRECTION	
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{\AA}^2)$	48	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT $(4k \ge 4k)$	Depositor
Maximum map value	0.287	Depositor
Minimum map value	-0.156	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.035	Depositor
Map size (Å)	276.48, 276.48, 276.48	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	Depositor



5 Model quality (i)

5.1 Standard geometry (i)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with |Z| > 5 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bo	ond lengths	Bond angles		
WIOI	Ullalli	RMSZ	ISZ $\# Z > 5$		# Z > 5	
1	А	0.26	0/1784	0.50	0/2424	
1	В	0.25	0/1754	0.48	0/2388	
2	С	0.24	0/10148	0.46	0/13768	
3	D	0.30	3/9856~(0.0%)	0.50	4/13399~(0.0%)	
4	Е	0.23	0/548	0.45	0/743	
5	F	0.95	5/1153~(0.4%)	1.35	15/1777~(0.8%)	
6	G	0.70	2/1150~(0.2%)	0.92	3/1773~(0.2%)	
7	М	0.30	0/1869	0.57	3/2593~(0.1%)	
8	R	0.12	0/96	0.57	0/149	
All	All	0.35	10/28358~(0.0%)	0.58	25/39014~(0.1%)	

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
2	С	0	1
3	D	0	3
5	F	0	2
All	All	0	6

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(\text{\AA})$	$\operatorname{Ideal}(\operatorname{\AA})$
3	D	426	ALA	C-N	13.35	1.59	1.34
5	F	-5	DG	O3'-P	-11.48	1.47	1.61
6	G	16	DG	O3'-P	-11.36	1.47	1.61
5	F	6	DT	O3'-P	-8.72	1.50	1.61
3	D	858	VAL	C-N	6.85	1.47	1.34
5	F	-2	DC	O3'-P	6.82	1.69	1.61
3	D	1184	ASP	C-N	6.51	1.46	1.34
6	G	16	DG	C3'-O3'	-5.34	1.37	1.44



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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	-1	DC	P-OP1	5.28	1.57	1.49
5	F	-3	DG	O3'-P	-5.21	1.54	1.61

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
5	F	-1	DC	O5'-P-OP2	-12.22	94.71	105.70
6	G	17	DC	O5'-P-OP1	12.01	125.11	110.70
5	F	-5	DG	C5'-C4'-C3'	-11.39	93.59	114.10
5	F	1	DA	O5'-P-OP2	11.08	123.99	110.70
5	F	-5	DG	C4'-C3'-O3'	9.38	133.15	109.70
5	F	-5	DG	O4'-C1'-N9	8.76	114.13	108.00
5	F	-5	DG	O5'-P-OP2	8.46	120.85	110.70
7	М	295	PRO	CA-N-CD	-8.36	99.80	111.50
6	G	16	DG	C2'-C3'-O3'	-7.22	88.77	112.60
5	F	-4	DC	O5'-P-OP2	6.82	118.88	110.70
5	F	-5	DG	O5'-C5'-C4'	6.74	127.85	111.00
5	F	-2	DC	O5'-P-OP2	-6.72	99.65	105.70
3	D	546	ALA	N-CA-C	6.30	128.02	111.00
5	F	-5	DG	N9-C1'-C2'	-6.13	100.95	112.60
5	F	-1	DC	O5'-P-OP1	5.73	117.57	110.70
3	D	1175	LEU	CA-CB-CG	5.72	128.45	115.30
6	G	16	DG	O3'-P-O5'	-5.70	93.17	104.00
3	D	324	LEU	CA-CB-CG	5.58	128.13	115.30
5	F	-4	DC	C5'-C4'-O4'	5.56	119.86	109.30
5	F	-6	DC	P-O3'-C3'	5.44	126.23	119.70
5	F	-10	DC	C1'-O4'-C4'	-5.16	104.94	110.10
5	F	-4	DC	O5'-P-OP1	-5.08	101.12	105.70
3	D	788	LEU	CA-CB-CG	5.08	126.99	115.30
7	М	224	LEU	CA-CB-CG	5.08	126.97	115.30
7	М	109	LEU	C-N-CD	5.01	138.91	128.40

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	С	1263	ALA	Peptide
3	D	1138	LEU	Peptide
3	D	118	LYS	Peptide
3	D	350	SER	Peptide
5	F	-4	DC	Sidechain
5	F	0	DC	Sidechain



5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	1763	0	1756	44	0
1	В	1735	0	1724	41	0
2	С	9998	0	9628	255	0
3	D	9722	0	9413	247	0
4	Ε	546	0	537	14	0
5	F	1027	0	558	96	0
6	G	1026	0	562	175	0
7	М	2102	0	1401	103	0
8	R	86	0	45	0	0
All	All	28005	0	25624	858	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 16.

All (858) 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)
5:F:8:DA:H2"	5:F:9:DT:C5'	1.43	1.47
6:G:-17:DT:C2'	6:G:-16:DT:H72	1.45	1.47
5:F:8:DA:C2'	5:F:9:DT:H5"	1.46	1.45
2:C:372:PRO:HB2	7:M:317:GLN:CB	1.60	1.31
6:G:-17:DT:O5'	7:M:367:LEU:HD11	1.30	1.26
7:M:319:ILE:HD12	7:M:320:ARG:N	1.52	1.24
2:C:540:ARG:O	2:C:541:GLU:HG2	1.40	1.20
6:G:-17:DT:C2'	6:G:-16:DT:C7	2.19	1.20
6:G:-17:DT:H2'	6:G:-16:DT:C7	1.74	1.17
2:C:200:ARG:NE	6:G:2:DG:H5"	1.58	1.17
6:G:-20:DA:H2"	6:G:-19:DC:C6	1.79	1.15
2:C:372:PRO:CB	7:M:317:GLN:CB	2.29	1.10
5:F:3:DG:H8	5:F:3:DG:H5"	1.14	1.09
7:M:295:PRO:HD2	7:M:296:ARG:H	1.02	1.08
5:F:-4:DC:H2"	5:F:-3:DG:OP1	1.43	1.08
2:C:540:ARG:C	2:C:541:GLU:HG2	1.70	1.07
5:F:12:DT:H72	7:M:380:THR:HG22	1.07	1.06
3:D:1327:GLU:OE1	3:D:1327:GLU:N	1.88	1.06



	t a c	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
5:F:7:DG:C2'	5:F:8:DA:H5'	1.85	1.06
3:D:107:LEU:HD12	3:D:240:THR:O	1.56	1.05
6:G:-17:DT:H2"	6:G:-16:DT:C7	1.86	1.05
6:G:-7:DA:H3'	6:G:-6:DC:H5"	1.38	1.03
5:F:7:DG:H2"	5:F:8:DA:C5'	1.89	1.03
7:M:281:UNK:HA	7:M:286:UNK:HA	1.42	1.01
3:D:1313:SER:HG	3:D:1325:PHE:HE2	1.05	1.00
5:F:12:DT:C7	7:M:380:THR:HG22	1.91	1.00
5:F:5:DC:N4	7:M:109:LEU:CB	2.24	0.99
5:F:12:DT:H72	7:M:380:THR:CG2	1.94	0.97
6:G:19:DC:H2"	6:G:20:DA:H5'	1.47	0.96
5:F:8:DA:C1'	5:F:9:DT:H5"	1.95	0.95
3:D:1313:SER:OG	3:D:1325:PHE:CE2	2.20	0.95
5:F:5:DC:H42	7:M:109:LEU:CB	1.80	0.94
2:C:200:ARG:NH2	6:G:2:DG:H4'	1.81	0.94
3:D:523:GLU:O	3:D:546:ALA:HB1	1.66	0.94
5:F:-19:DG:H1	6:G:19:DC:N4	1.66	0.94
2:C:372:PRO:CG	7:M:317:GLN:CB	2.46	0.93
6:G:-17:DT:P	7:M:367:LEU:HG	2.08	0.93
7:M:295:PRO:HD2	7:M:296:ARG:N	1.82	0.93
1:A:165:GLU:OE2	1:A:166:ARG:N	2.02	0.93
3:D:547:ARG:HG3	3:D:547:ARG:HH11	1.34	0.92
3:D:1313:SER:OG	3:D:1325:PHE:HE2	1.51	0.91
1:A:103:ASN:HA	1:A:140:ILE:O	1.70	0.90
6:G:-3:DA:H2"	6:G:-2:DA:O5'	1.71	0.90
5:F:23:DT:H72	7:M:457:THR:CB	2.02	0.90
6:G:-17:DT:OP2	7:M:367:LEU:HG	1.72	0.90
6:G:-17:DT:O5'	7:M:367:LEU:CD1	2.20	0.89
5:F:8:DA:H2"	5:F:9:DT:H5'	1.53	0.89
5:F:7:DG:H2"	5:F:8:DA:H5'	0.93	0.89
6:G:-17:DT:H2"	6:G:-16:DT:C5	2.08	0.89
7:M:281:UNK:CA	7:M:286:UNK:HA	2.03	0.89
5:F:23:DT:C7	7:M:457:THR:CB	2.51	0.88
2:C:1268:GLN:OE1	5:F:0:DC:H5"	1.73	0.88
5:F:3:DG:H5"	5:F:3:DG:C8	2.06	0.88
5:F:12:DT:H2'	5:F:13:DG:C8	2.07	0.88
7:M:279:UNK:CB	7:M:288:UNK:CB	2.51	0.88
3:D:129:ASP:CB	3:D:220:ARG:HH22	1.85	0.88
7:M:295:PRO:CD	7:M:296:ARG:H	1.85	0.87
6:G:-11:DC:H2"	6:G:-10:DT:H5'	1.56	0.87
7:M:281:UNK:CB	7:M:286:UNK:HA	2.05	0.86



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
5:F:12:DT:H3	6:G:-12:DA:H2	1.25	0.85
3:D:297:ARG:NH2	7:M:321:SER:CB	2.39	0.85
6:G:16:DG:H2"	6:G:17:DC:OP2	1.76	0.85
3:D:297:ARG:HH22	7:M:321:SER:CB	1.90	0.84
6:G:-20:DA:C2'	6:G:-19:DC:C6	2.60	0.84
6:G:-15:DT:O4	7:M:379:SER:CB	2.26	0.84
7:M:443:THR:CB	7:M:455:ARG:CB	2.55	0.83
2:C:540:ARG:O	2:C:541:GLU:CG	2.26	0.83
1:A:102:LEU:O	1:A:141:SER:HA	1.79	0.82
6:G:-17:DT:P	7:M:367:LEU:CG	2.67	0.82
5:F:12:DT:H5"	5:F:12:DT:H6	1.45	0.81
6:G:-11:DC:H1'	6:G:-10:DT:H5'	1.63	0.81
6:G:18:DG:H2"	6:G:19:DC:H5'	1.59	0.81
2:C:1067:ALA:O	2:C:1233:LEU:HB2	1.80	0.81
5:F:12:DT:C2'	5:F:13:DG:C8	2.64	0.81
3:D:309:ASN:HB2	3:D:326:SER:HB3	1.63	0.81
6:G:-15:DT:O4	7:M:379:SER:HB3	1.81	0.80
2:C:200:ARG:CZ	6:G:2:DG:H5"	2.11	0.80
4:E:10:VAL:HG21	4:E:16:ARG:HE	1.46	0.80
5:F:8:DA:H2"	5:F:9:DT:H5"	0.80	0.80
3:D:822:MET:HB2	3:D:880:VAL:O	1.81	0.79
6:G:-17:DT:H2'	6:G:-16:DT:H72	0.82	0.79
2:C:673:HIS:HB3	2:C:1109:ILE:HB	1.63	0.79
5:F:3:DG:H5'	5:F:4:DG:OP2	1.81	0.79
3:D:107:LEU:CD1	3:D:240:THR:O	2.31	0.79
5:F:-20:DT:H3	6:G:20:DA:H61	1.31	0.79
6:G:-10:DT:C2'	6:G:-9:DC:H5'	2.13	0.79
3:D:523:GLU:O	3:D:546:ALA:CB	2.31	0.78
3:D:201:LEU:HD11	3:D:220:ARG:HD3	1.65	0.78
6:G:-8:DG:H2"	6:G:-7:DA:C8	2.19	0.78
6:G:-10:DT:H2"	6:G:-9:DC:H5'	1.65	0.78
6:G:-17:DT:H2"	6:G:-16:DT:C6	2.19	0.78
5:F:12:DT:C7	7:M:380:THR:CG2	2.59	0.77
6:G:1:DG:H4'	6:G:1:DG:OP1	1.83	0.77
1:B:19:VAL:HB	1:B:23:HIS:HB2	1.65	0.77
2:C:541:GLU:HG3	2:C:542:ARG:HD3	1.66	0.77
6:G:13:DG:H2"	6:G:14:DT:H71	1.64	0.76
2:C:200:ARG:HE	6:G:2:DG:H5"	1.51	0.76
7:M:319:ILE:HD12	7:M:320:ARG:H	1.44	0.76
3:D:297:ARG:HH22	7:M:321:SER:CA	1.97	0.75
6:G:-10:DT:H3'	6:G:-10:DT:P	2.24	0.75



Atom-1	Atom-2	Interatomic	Clash
		distance (A)	overlap (A)
5:F:3:DG:H8	5:F:3:DG:C5'	1.97	0.75
5:F:-19:DG:H1	6:G:19:DC:H42	0.84	0.75
3:D:937:ILE:O	3:D:939:GLY:N	2.20	0.74
3:D:803:VAL:HG21	3:D:1309:ILE:HG23	1.70	0.74
4:E:20:VAL:O	4:E:24:ALA:HB2	1.86	0.74
6:G:0:DG:H2"	6:G:1:DG:C4'	2.18	0.73
5:F:11:DG:H22	6:G:-11:DC:H42	1.35	0.73
6:G:-8:DG:O3'	6:G:-7:DA:O4'	2.07	0.73
2:C:905:ILE:N	2:C:905:ILE:HD12	2.04	0.73
2:C:183:TRP:CZ2	6:G:1:DG:C6	2.77	0.73
2:C:1269:ARG:HD3	5:F:-1:DC:H5'	1.71	0.73
6:G:-7:DA:H3'	6:G:-6:DC:C5'	2.17	0.73
6:G:-2:DA:H2"	6:G:-1:DG:C8	2.22	0.73
2:C:592:ARG:HB3	2:C:653:MET:HB3	1.70	0.72
3:D:547:ARG:HG3	3:D:547:ARG:NH1	2.04	0.72
6:G:-11:DC:C2'	6:G:-10:DT:H5'	2.18	0.72
6:G:19:DC:C2'	6:G:20:DA:H5'	2.18	0.72
6:G:14:DT:C2'	6:G:15:DT:H72	2.20	0.72
5:F:-20:DT:H3	6:G:20:DA:N6	1.85	0.72
6:G:-11:DC:H1'	6:G:-10:DT:C5'	2.19	0.72
7:M:419:ALA:O	7:M:423:LEU:HG	1.89	0.72
5:F:8:DA:C2'	5:F:9:DT:C5'	2.29	0.72
2:C:1246:ARG:NH1	3:D:348:ASP:OD1	2.21	0.72
3:D:915:ILE:HG23	3:D:916:GLY:H	1.55	0.71
3:D:1239:ASP:OD1	3:D:1242:ARG:NH1	2.24	0.71
6:G:12:DT:H2"	6:G:13:DG:C8	2.25	0.71
2:C:372:PRO:CG	7:M:317:GLN:HA	2.20	0.71
1:A:218:ARG:HH22	1:B:234:LEU:HB3	1.54	0.71
5:F:23:DT:H73	7:M:457:THR:CB	2.19	0.71
6:G:-17:DT:P	7:M:367:LEU:HD11	2.31	0.71
6:G:-15:DT:O4	7:M:379:SER:HB2	1.90	0.71
3:D:310:GLY:O	3:D:311:ARG:HG2	1.90	0.71
5:F:12:DT:N3	6:G:-12:DA:H2	1.89	0.70
6:G:-19:DC:H2"	6:G:-18:DT:H71	1.73	0.70
5:F:1:DA:H2"	5:F:2:DG:OP2	1.91	0.70
6:G:-2:DA:H2"	6:G:-1:DG:O5'	1.91	0.70
3:D:426:ALA:HB1	5:F:-1:DC:H1'	1.74	0.70
2:C:372:PRO:CG	7:M:317:GLN:CA	2.71	0.69
2:C:542:ARG:HB3	6:G:4:DG:O4'	1.92	0.69
2:C:372:PRO:HG3	7:M:317:GLN:HA	1.73	0.69
5:F:23:DT:H3	6:G:-23:DA:H61	1.39	0.69



	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
2:C:806:PRO:HA	2:C:811:ASN:HD21	1.58	0.68
3:D:337:ARG:HH12	3:D:1323:ALA:HB3	1.58	0.68
1:A:158:ARG:HG2	1:A:161:SER:OG	1.92	0.68
2:C:10:ARG:HH22	2:C:791:LEU:HD12	1.59	0.68
2:C:372:PRO:HG2	7:M:317:GLN:CB	2.23	0.68
6:G:-5:DT:H2"	6:G:-4:DA:O4'	1.93	0.68
6:G:-17:DT:P	7:M:367:LEU:CD1	2.82	0.68
7:M:305:ALA:HA	7:M:308:ASN:ND2	2.09	0.68
7:M:380:THR:O	7:M:384:VAL:HG23	1.94	0.68
5:F:-4:DC:C2'	5:F:-3:DG:OP1	2.26	0.68
6:G:-11:DC:C1'	6:G:-10:DT:H5'	2.24	0.68
3:D:1161:GLY:O	3:D:1162:ILE:HG13	1.94	0.68
2:C:93:SER:HA	2:C:128:PRO:HA	1.76	0.67
5:F:5:DC:H2'	5:F:6:DT:H72	1.77	0.67
2:C:133:ASN:O	2:C:527:LYS:NZ	2.26	0.67
6:G:0:DG:H2"	6:G:1:DG:OP1	1.95	0.67
1:A:64:VAL:HG11	1:A:78:ILE:HG13	1.77	0.67
2:C:542:ARG:HD2	2:C:542:ARG:N	2.10	0.67
3:D:1162:ILE:HG22	3:D:1164:SER:H	1.57	0.67
5:F:-19:DG:H2"	5:F:-18:DC:C6	2.30	0.67
2:C:365:GLU:O	2:C:369:MET:CB	2.43	0.67
2:C:905:ILE:HD12	2:C:905:ILE:H	1.56	0.67
3:D:56:LEU:HD22	3:D:250:ARG:HH12	1.59	0.67
1:B:222:THR:O	1:B:226:GLU:HB2	1.96	0.66
2:C:1069:ARG:HH12	2:C:1231:TYR:HB3	1.60	0.66
7:M:319:ILE:CD1	7:M:320:ARG:N	2.45	0.66
2:C:619:ALA:HB1	2:C:657:THR:HG22	1.75	0.66
2:C:670:PHE:HB3	2:C:673:HIS:HD2	1.60	0.66
3:D:841:GLY:HA2	3:D:901:ARG:HD3	1.78	0.65
5:F:8:DA:H1'	5:F:9:DT:H5"	1.75	0.65
2:C:1254:VAL:HG12	2:C:1255:THR:HG23	1.78	0.65
5:F:-1:DC:H5"	5:F:-1:DC:H6	1.61	0.65
5:F:0:DC:H2'	5:F:1:DA:H5'	1.77	0.65
2:C:428:VAL:O	2:C:432:LEU:HB2	1.96	0.65
6:G:-7:DA:C3'	6:G:-6:DC:H5"	2.21	0.65
2:C:499:SER:O	2:C:503:LYS:HB3	1.97	0.65
6:G:14:DT:H2'	6:G:15:DT:H72	1.77	0.65
2:C:895:LEU:HG	2:C:896:THR:H	1.62	0.65
3:D:883:ARG:NH1	3:D:898:CYS:SG	2.69	0.65
6:G:4:DG:OP2	6:G:5:DC:P	2.55	0.65
1:A:11:PRO:HA	1:A:30:PRO:HG2	1.79	0.64



		Interatomic	Clash
Atom-1	Atom-2	distance $(Å)$	overlap (Å)
3:D:899:TYR:HE1	3:D:1251:LYS:HB3	1.62	0.64
2:C:540:ARG:C	2:C:541:GLU:CG	2.57	0.64
5:F:-4:DC:N3	6:G:4:DG:O6	2.30	0.64
6:G:-15:DT:H2"	6:G:-14:DG:OP2	1.97	0.64
2:C:373:GLY:HA2	7:M:319:ILE:HG21	1.79	0.64
3:D:130:MET:HB2	3:D:135:ILE:HD11	1.80	0.64
2:C:176:ILE:HG23	2:C:184:LEU:HB3	1.80	0.64
3:D:246:PRO:HD2	3:D:249:LEU:HD12	1.78	0.64
2:C:200:ARG:NE	6:G:2:DG:C5'	2.48	0.64
3:D:186:GLN:O	3:D:190:LYS:HB2	1.98	0.64
6:G:16:DG:C2'	6:G:17:DC:OP2	2.46	0.64
3:D:161:THR:HG22	3:D:162:GLU:H	1.62	0.63
5:F:12:DT:H6	5:F:12:DT:C5'	2.11	0.63
6:G:-11:DC:H2"	6:G:-10:DT:OP2	1.98	0.63
6:G:16:DG:H2"	6:G:17:DC:C6	2.33	0.63
3:D:810:THR:O	3:D:911:LYS:NZ	2.31	0.63
6:G:14:DT:H2"	6:G:15:DT:C7	2.28	0.63
7:M:319:ILE:HD12	7:M:319:ILE:C	2.19	0.63
2:C:1269:ARG:HB2	5:F:0:DC:OP1	1.98	0.63
7:M:279:UNK:HA	7:M:288:UNK:CB	2.28	0.63
2:C:804:PHE:HB3	2:C:1100:PRO:HG3	1.81	0.63
6:G:0:DG:H2'	6:G:1:DG:H5"	1.80	0.63
2:C:935:THR:HG22	2:C:936:ARG:H	1.64	0.63
3:D:948:SER:HB2	3:D:1022:PRO:HB3	1.81	0.63
3:D:499:ILE:HG23	3:D:500:ILE:HG13	1.80	0.63
2:C:149:LEU:HD21	2:C:451:ARG:HE	1.64	0.62
2:C:372:PRO:HG3	7:M:317:GLN:CA	2.29	0.62
6:G:10:DG:H2"	6:G:11:DC:C5	2.35	0.62
2:C:1065:LYS:HG2	2:C:1237:HIS:HB2	1.81	0.62
3:D:1120:THR:HG22	3:D:1122:ALA:H	1.64	0.62
5:F:-12:DA:H61	6:G:12:DT:H3	1.46	0.62
2:C:1115:THR:HB	2:C:1228:GLY:HA3	1.82	0.62
3:D:901:ARG:O	3:D:1251:LYS:NZ	2.32	0.62
1:A:61:ILE:HG13	1:A:62:ASP:H	1.65	0.62
6:G:-8:DG:H2"	6:G:-7:DA:N9	2.15	0.62
3:D:53:ARG:NH1	3:D:88:CYS:SG	2.73	0.62
7:M:366:VAL:HG12	7:M:368:ALA:H	1.65	0.62
5:F:11:DG:H22	6:G:-11:DC:N4	1.98	0.61
3:D:546:ALA:HB3	3:D:548:VAL:HG23	1.81	0.61
3:D:885:VAL:O	3:D:886:VAL:HG12	1.99	0.61
3:D:918:ILE:O	3:D:922:SER:CB	2.48	0.61



	t i c	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
5:F:4:DG:O6	7:M:109:LEU:CB	2.49	0.61
5:F:20:DT:H3	6:G:-20:DA:H61	1.48	0.61
6:G:17:DC:O5'	6:G:17:DC:H2'	2.00	0.61
3:D:365:GLN:HA	3:D:438:GLU:O	2.01	0.61
5:F:1:DA:C2'	5:F:2:DG:OP2	2.49	0.61
1:B:80:GLU:O	1:B:84:ASN:ND2	2.34	0.61
2:C:297:VAL:HA	2:C:335:THR:HG22	1.83	0.61
2:C:1261:GLY:O	2:C:1266:GLY:N	2.34	0.61
1:A:61:ILE:HG21	1:A:64:VAL:HB	1.83	0.61
7:M:278:UNK:CB	7:M:291:UNK:O	2.48	0.61
6:G:-2:DA:C2'	6:G:-1:DG:O5'	2.49	0.61
2:C:853:ASP:HB2	2:C:862:LEU:HD22	1.83	0.60
3:D:362:ARG:NH1	3:D:626:TYR:OH	2.34	0.60
1:A:25:LYS:HA	1:A:203:ILE:O	2.02	0.60
2:C:564:PRO:HG2	2:C:568:ASN:HB2	1.84	0.60
2:C:1295:SER:O	2:C:1301:ARG:NH1	2.34	0.60
6:G:15:DT:OP2	6:G:15:DT:H6	1.84	0.60
3:D:341:ASN:OD1	3:D:342:LEU:N	2.31	0.60
6:G:13:DG:H2"	6:G:14:DT:C7	2.32	0.60
6:G:2:DG:P	6:G:3:DC:H5"	2.41	0.60
1:B:28:LEU:HD12	1:B:201:LEU:HD23	1.83	0.60
2:C:105:TYR:HA	2:C:113:THR:HG22	1.83	0.60
3:D:51:PRO:HB2	3:D:58:CYS:HA	1.82	0.60
5:F:12:DT:H2"	5:F:13:DG:C8	2.37	0.60
5:F:20:DT:H3	6:G:-20:DA:N6	2.00	0.60
3:D:129:ASP:CA	3:D:220:ARG:HH22	2.14	0.60
3:D:350:SER:HA	3:D:468:VAL:O	2.01	0.60
1:A:231:PHE:HE2	1:B:39:LEU:HD23	1.67	0.59
3:D:598:LYS:HA	3:D:601:ILE:HG22	1.84	0.59
5:F:10:DC:H5"	5:F:10:DC:O2	2.02	0.59
7:M:319:ILE:HD12	7:M:320:ARG:CA	2.29	0.59
1:B:56:VAL:HA	1:B:146:VAL:HG12	1.85	0.59
4:E:58:LEU:HD12	4:E:59:ILE:HG12	1.83	0.59
4:E:27:ALA:O	4:E:31:GLN:HB2	2.03	0.59
2:C:540:ARG:HG3	2:C:541:GLU:H	1.68	0.59
3:D:279:LEU:O	3:D:283:LEU:HB2	2.03	0.59
3:D:918:ILE:O	3:D:922:SER:HB3	2.02	0.59
3:D:309:ASN:ND2	3:D:323:PRO:O	2.34	0.59
3:D:554:GLU:OE2	3:D:570:LYS:NZ	2.35	0.59
6:G:0:DG:C2'	6:G:1:DG:H5"	2.32	0.59
6:G:-17:DT:OP2	7:M:367:LEU:CG	2.46	0.59



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:C:887:VAL:HB	2:C:913:VAL:HG11	1.84	0.59
3:D:1268:ASN:OD1	3:D:1269:ALA:N	2.35	0.59
2:C:385:PHE:O	2:C:389:PHE:HB2	2.02	0.58
2:C:932:GLN:HB3	2:C:1051:LYS:HB2	1.83	0.58
2:C:967:LEU:HB3	2:C:1021:LEU:HD13	1.84	0.58
2:C:592:ARG:HB2	2:C:655:VAL:HG22	1.85	0.58
3:D:109:SER:HB3	3:D:296:LYS:HE2	1.83	0.58
2:C:937:ASP:HB2	2:C:1039:GLY:HA3	1.86	0.58
2:C:592:ARG:NH2	2:C:601:ASP:OD1	2.36	0.58
3:D:309:ASN:HB2	3:D:326:SER:CB	2.33	0.58
3:D:920:ALA:O	3:D:923:ILE:N	2.36	0.58
1:A:159:ILE:HD13	1:A:159:ILE:O	2.04	0.58
2:C:1061:GLN:HB2	2:C:1062:PRO:HD2	1.86	0.58
2:C:371:ARG:HG2	2:C:373:GLY:H	1.67	0.58
4:E:27:ALA:O	4:E:31:GLN:CB	2.52	0.58
3:D:270:ARG:HH12	5:F:9:DT:H72	1.68	0.58
3:D:123:ARG:HH21	3:D:1334:GLU:HG2	1.68	0.57
1:A:53:GLY:O	1:A:148:ARG:HA	2.04	0.57
3:D:1221:LEU:HD13	3:D:1306:LEU:HB3	1.87	0.57
3:D:450:HIS:HD2	3:D:453:VAL:HG23	1.70	0.57
6:G:-11:DC:H2"	6:G:-10:DT:C5'	2.32	0.57
6:G:-4:DA:H4'	6:G:-3:DA:OP1	2.04	0.57
2:C:1269:ARG:HD3	5:F:-1:DC:C5'	2.34	0.57
3:D:259:ARG:NH1	7:M:273:UNK:O	2.37	0.57
3:D:509:GLY:O	3:D:513:MET:HB2	2.05	0.57
3:D:1238:GLN:NE2	3:D:1248:ILE:O	2.36	0.57
3:D:1263:LYS:HZ2	3:D:1279:GLN:HG2	1.70	0.57
2:C:1300:GLY:O	2:C:1304:MET:HB3	2.04	0.57
3:D:120:LEU:HB3	3:D:121:PRO:HD2	1.85	0.57
1:B:57:THR:HB	1:B:147:GLN:HG2	1.87	0.57
4:E:20:VAL:O	4:E:24:ALA:CB	2.52	0.57
2:C:785:ASP:OD2	2:C:791:LEU:N	2.37	0.57
6:G:-17:DT:C2'	6:G:-16:DT:C5	2.76	0.57
6:G:-10:DT:H2"	6:G:-9:DC:C5'	2.35	0.57
7:M:281:UNK:CB	7:M:286:UNK:CA	2.82	0.57
1:A:39:LEU:O	1:A:43:LEU:CB	2.53	0.56
3:D:107:LEU:O	3:D:108:ALA:HB3	2.06	0.56
5:F:11:DG:OP2	5:F:11:DG:H2'	2.05	0.56
2:C:542:ARG:CD	2:C:542:ARG:H	2.18	0.56
1:A:100:LEU:O	1:A:143:ARG:HA	2.05	0.56
2:C:664:GLY:O	2:C:686:GLN:NE2	2.37	0.56



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
2:C:1154:ASP:O	2:C:1155:VAL:HG22	2.04	0.56
5:F:12:DT:N3	6:G:-12:DA:C2	2.59	0.56
6:G:-20:DA:C2'	6:G:-19:DC:C5	2.88	0.56
6:G:-2:DA:C2	7:M:310:ALA:HB1	2.41	0.56
7:M:209:GLU:O	7:M:210:THR:HG23	2.05	0.56
2:C:541:GLU:HG3	2:C:542:ARG:CD	2.34	0.56
1:A:45:ARG:O	1:A:49:SER:HB3	2.05	0.56
2:C:905:ILE:H	2:C:905:ILE:CD1	2.18	0.56
5:F:5:DC:H2'	5:F:6:DT:C7	2.35	0.56
2:C:797:GLY:N	2:C:1231:TYR:OH	2.39	0.56
2:C:1101:LEU:HD23	3:D:725:MET:HE3	1.87	0.56
3:D:268:LEU:HD13	3:D:306:LEU:HA	1.87	0.56
6:G:8:DA:C8	6:G:9:DT:H72	2.41	0.56
2:C:499:SER:O	2:C:503:LYS:CB	2.54	0.56
3:D:60:ARG:H	3:D:90:VAL:HG22	1.70	0.56
6:G:0:DG:H2'	6:G:0:DG:N3	2.20	0.56
3:D:628:GLY:O	3:D:632:ALA:HB2	2.06	0.55
2:C:1157:GLN:HG2	2:C:1159:VAL:HG12	1.88	0.55
6:G:2:DG:H8	6:G:2:DG:OP2	1.89	0.55
2:C:200:ARG:HE	6:G:2:DG:C5'	2.17	0.55
3:D:94:GLN:O	3:D:95:THR:OG1	2.24	0.55
3:D:1148:ARG:NH2	6:G:7:DC:H5"	2.21	0.55
2:C:967:LEU:HD13	2:C:1021:LEU:HD22	1.86	0.55
6:G:1:DG:H2"	6:G:2:DG:H5'	1.87	0.55
7:M:279:UNK:CA	7:M:288:UNK:CB	2.84	0.55
2:C:516:ASP:HA	2:C:761:GLN:HE22	1.70	0.55
3:D:1319:PHE:HB3	3:D:1340:LYS:HD2	1.88	0.55
3:D:628:GLY:O	3:D:632:ALA:CB	2.54	0.55
1:A:110:VAL:HG11	1:A:140:ILE:HD11	1.88	0.55
3:D:120:LEU:HG	3:D:1330:ARG:HD3	1.88	0.55
3:D:917:VAL:O	3:D:921:GLN:HB2	2.07	0.55
3:D:1367:GLN:O	3:D:1370:MET:HB3	2.06	0.55
6:G:14:DT:H2"	6:G:15:DT:OP2	2.06	0.55
2:C:1007:LYS:HA	2:C:1011:LEU:HD12	1.89	0.55
1:A:135:ASP:HB3	2:C:726:TYR:HE1	1.71	0.54
3:D:156:ARG:NH2	3:D:191:SER:OG	2.40	0.54
5:F:-12:DA:N6	6:G:12:DT:H3	2.04	0.54
2:C:74:ARG:N	2:C:97:ARG:O	2.37	0.54
2:C:538:LEU:HD11	2:C:543:ALA:CB	2.37	0.54
2:C:617:ALA:HB2	2:C:650:VAL:HG21	1.89	0.54
3:D:885:VAL:HB	3:D:1258:ARG:HD2	1.90	0.54



	t i a	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:31:LEU:HD11	1:A:201:LEU:HB2	1.89	0.54
2:C:1247:SER:HB3	3:D:375:GLU:HG3	1.89	0.54
2:C:1340:GLU:OE2	3:D:21:LYS:NZ	2.32	0.54
3:D:824:PRO:HD3	3:D:835:LEU:HD13	1.89	0.54
6:G:-17:DT:OP2	7:M:367:LEU:CD1	2.55	0.54
7:M:295:PRO:CD	7:M:296:ARG:N	2.50	0.54
2:C:530:ILE:HD11	2:C:575:LEU:HG	1.89	0.54
2:C:883:LEU:HD23	2:C:884:VAL:HG23	1.89	0.54
3:D:510:LEU:HB3	3:D:596:LEU:HD23	1.90	0.54
5:F:12:DT:C2	6:G:-12:DA:H2	2.25	0.54
6:G:-18:DT:H2"	6:G:-17:DT:C6	2.43	0.54
5:F:23:DT:H3	6:G:-23:DA:N6	2.04	0.54
6:G:-27:DT:H2"	6:G:-26:DG:C8	2.42	0.54
3:D:45:ASN:ND2	3:D:52:GLU:OE1	2.41	0.54
3:D:523:GLU:HG3	3:D:524:GLY:H	1.73	0.54
1:A:158:ARG:HG2	1:A:158:ARG:O	2.06	0.54
1:B:43:LEU:O	1:B:47:LEU:CB	2.55	0.54
3:D:710:ASP:OD1	3:D:711:GLY:N	2.40	0.54
3:D:1326:GLN:CB	3:D:1327:GLU:OE1	2.56	0.54
2:C:500:ALA:O	2:C:504:GLU:HB2	2.08	0.53
3:D:360:TYR:CD2	3:D:361:LEU:HG	2.43	0.53
3:D:916:GLY:HA2	3:D:919:ALA:HB3	1.90	0.53
3:D:966:VAL:HG21	3:D:976:THR:HG23	1.90	0.53
6:G:-20:DA:H2'	6:G:-19:DC:C5	2.43	0.53
1:A:118:ASP:OD1	1:A:119:GLY:N	2.40	0.53
5:F:-5:DG:C4'	5:F:-4:DC:OP1	2.55	0.53
2:C:1174:GLU:HA	2:C:1177:ARG:HG3	1.90	0.53
3:D:918:ILE:O	3:D:922:SER:OG	2.25	0.53
5:F:12:DT:H5"	5:F:12:DT:C6	2.35	0.53
6:G:-2:DA:C2	7:M:310:ALA:CB	2.92	0.53
1:B:192:VAL:HG12	1:B:193:GLU:OE1	2.08	0.53
2:C:915:ASP:OD2	2:C:919:ARG:NH1	2.42	0.53
2:C:1119:MET:HG2	2:C:1228:GLY:HA2	1.91	0.53
3:D:754:ILE:HG22	3:D:755:ILE:H	1.72	0.53
1:A:39:LEU:O	1:A:43:LEU:HB2	2.08	0.53
2:C:95:PRO:HB3	2:C:123:TYR:HE1	1.73	0.53
3:D:422:LEU:HA	3:D:436:ALA:HA	1.91	0.53
3:D:553:THR:HG22	3:D:567:THR:HB	1.90	0.53
1:B:185:TYR:HA	1:B:202:VAL:O	2.09	0.53
2:C:143:ARG:HD2	2:C:512:SER:HB2	1.90	0.53
2:C:591:TYR:OH	2:C:611:GLU:OE1	2.22	0.53



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:C:930:ASP:HB3	2:C:1053:TYR:HD2	1.74	0.53
5:F:14:DC:H5	7:M:377:HIS:NE2	2.07	0.53
1:A:104:LYS:HD3	1:A:110:VAL:HG12	1.91	0.53
2:C:151:ARG:NH1	2:C:445:ILE:O	2.42	0.53
6:G:4:DG:OP2	6:G:4:DG:O3'	2.26	0.53
2:C:40:GLU:O	2:C:73:TYR:OH	2.26	0.52
3:D:309:ASN:ND2	3:D:324:LEU:HD12	2.24	0.52
3:D:317:THR:OG1	3:D:321:LYS:O	2.26	0.52
3:D:1268:ASN:HB3	3:D:1300:ALA:HB1	1.90	0.52
2:C:372:PRO:HG2	7:M:317:GLN:HA	1.91	0.52
2:C:728:ASP:OD1	2:C:729:ALA:N	2.42	0.52
7:M:239:THR:HG21	7:M:246:LEU:HD11	1.91	0.52
7:M:425:LYS:O	7:M:429:ALA:HB2	2.09	0.52
1:B:25:LYS:HA	1:B:203:ILE:O	2.10	0.52
2:C:895:LEU:O	2:C:896:THR:OG1	2.25	0.52
3:D:593:ASN:O	3:D:594:GLN:HG3	2.08	0.52
3:D:886:VAL:HG21	3:D:1261:LEU:HD12	1.91	0.52
1:B:43:LEU:O	1:B:47:LEU:HB2	2.09	0.52
2:C:808:ASN:HD22	2:C:810:TYR:HE1	1.57	0.52
2:C:998:LEU:HB3	2:C:1011:LEU:HD22	1.90	0.52
3:D:545:HIS:O	3:D:546:ALA:HB3	2.09	0.52
5:F:12:DT:C5'	5:F:12:DT:C6	2.90	0.52
2:C:402:ARG:NH2	2:C:419:ILE:O	2.43	0.52
6:G:3:DC:H4'	6:G:4:DG:OP1	2.10	0.52
6:G:0:DG:C2'	6:G:1:DG:C5'	2.88	0.52
1:B:222:THR:O	1:B:226:GLU:CB	2.56	0.52
2:C:1327:LEU:O	2:C:1331:ARG:HG2	2.10	0.52
3:D:355:ILE:HG22	3:D:461:PHE:HE1	1.75	0.52
2:C:1259:LEU:HD13	2:C:1264:GLN:HE21	1.75	0.52
7:M:281:UNK:CB	7:M:286:UNK:CB	2.87	0.52
3:D:425:ARG:HG2	3:D:427:PRO:HD2	1.91	0.52
3:D:884:SER:O	3:D:887:SER:OG	2.24	0.52
5:F:12:DT:H71	5:F:12:DT:OP2	2.10	0.52
6:G:-19:DC:C2'	6:G:-18:DT:H71	2.40	0.52
6:G:12:DT:H2"	6:G:13:DG:N7	2.25	0.52
2:C:200:ARG:HH21	6:G:2:DG:H4'	1.70	0.51
3:D:647:PRO:HG2	3:D:650:LYS:HB2	1.91	0.51
3:D:147:ILE:HG22	3:D:188:LEU:HD12	1.92	0.51
3:D:905:ARG:HE	4:E:16:ARG:NH2	2.08	0.51
3:D:1159:ILE:HG22	3:D:1160:SER:H	1.75	0.51
2:C:696:ASP:OD2	2:C:827:ARG:NH1	2.42	0.51



	h a	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
6:G:14:DT:H2"	6:G:15:DT:C6	2.46	0.51
1:A:59:VAL:HG22	1:A:144:ILE:HG12	1.91	0.51
1:B:209:GLY:O	1:B:210:THR:HG22	2.10	0.51
2:C:1300:GLY:O	2:C:1304:MET:CB	2.58	0.51
5:F:15:DA:C2	6:G:-15:DT:O2	2.63	0.51
7:M:155:THR:C	7:M:156:ILE:HG13	2.30	0.51
6:G:-17:DT:OP1	7:M:367:LEU:HD21	2.11	0.51
3:D:287:ALA:HB1	3:D:288:PRO:HD2	1.91	0.51
3:D:547:ARG:NH1	3:D:547:ARG:CG	2.73	0.51
3:D:746:LEU:HD13	3:D:754:ILE:HG21	1.93	0.51
5:F:0:DC:C2'	5:F:1:DA:C5'	2.88	0.51
6:G:10:DG:C4	6:G:11:DC:C4	2.99	0.51
7:M:364:PRO:HD3	7:M:415:ALA:HB1	1.93	0.51
1:B:62:ASP:OD1	1:B:63:GLY:N	2.43	0.51
2:C:673:HIS:ND1	3:D:763:PHE:O	2.39	0.51
2:C:765:ILE:HG22	2:C:787:PRO:HG3	1.93	0.51
1:A:158:ARG:CG	1:A:161:SER:OG	2.58	0.51
3:D:342:LEU:HD11	3:D:1348:LYS:HZ2	1.76	0.51
3:D:1265:THR:N	3:D:1303:SER:O	2.44	0.51
1:B:236:ASP:OD1	1:B:237:VAL:N	2.44	0.51
2:C:718:ALA:HB3	2:C:781:ASP:HB3	1.93	0.51
2:C:781:ASP:OD1	2:C:782:VAL:N	2.40	0.51
3:D:114:ILE:HD12	3:D:304:ASP:HB3	1.93	0.51
2:C:164:THR:HG23	2:C:165:HIS:H	1.75	0.51
3:D:611:ILE:HG22	3:D:612:LEU:HD12	1.93	0.51
3:D:1368:ASP:O	3:D:1371:ARG:HG2	2.11	0.51
6:G:-2:DA:H2	7:M:310:ALA:O	1.94	0.51
6:G:19:DC:H1'	6:G:20:DA:H5'	1.93	0.51
1:B:99:ILE:HG13	1:B:145:LYS:HG3	1.92	0.50
2:C:18:ARG:O	2:C:1156:ARG:NE	2.43	0.50
2:C:411:ARG:HH22	2:C:424:ASP:HA	1.76	0.50
3:D:297:ARG:HH22	7:M:321:SER:HA	1.75	0.50
3:D:974:VAL:HG12	3:D:975:ILE:H	1.76	0.50
6:G:-18:DT:C2	6:G:-17:DT:C2	2.98	0.50
7:M:188:VAL:HG12	7:M:202:GLN:HG2	1.94	0.50
4:E:10:VAL:HG21	4:E:16:ARG:NE	2.20	0.50
2:C:720:ARG:HE	2:C:736:VAL:HG21	1.77	0.50
2:C:968:GLU:HA	2:C:971:LEU:HB3	1.93	0.50
3:D:514:THR:HG22	3:D:576:ARG:HG2	1.93	0.50
3:D:332:LYS:HB2	3:D:336:GLY:O	2.11	0.50
2:C:1281:TYR:OH	3:D:434:ILE:O	2.29	0.50



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
3:D:126:LEU:O	3:D:220:ARG:NH2	2.44	0.50
3:D:201:LEU:CD1	3:D:220:ARG:CD	2.90	0.50
1:A:59:VAL:O	1:A:171:LEU:HB2	2.10	0.50
1:B:44:ARG:HE	1:B:185:TYR:HE1	1.60	0.50
2:C:551:HIS:CG	2:C:552:PRO:HD2	2.47	0.50
6:G:-10:DT:C1'	6:G:-9:DC:H5'	2.42	0.50
6:G:4:DG:H2'	6:G:5:DC:O4'	2.11	0.50
6:G:8:DA:C2'	6:G:9:DT:H72	2.41	0.50
2:C:675:ASP:OD1	2:C:676:ALA:N	2.44	0.50
3:D:43:THR:HG22	3:D:56:LEU:HD12	1.92	0.50
2:C:27:LEU:HD11	2:C:663:VAL:HG11	1.94	0.49
2:C:188:PHE:HE1	2:C:194:LEU:HG	1.77	0.49
2:C:956:ALA:O	2:C:960:LEU:CB	2.59	0.49
3:D:723:TYR:O	3:D:727:ASP:CB	2.60	0.49
3:D:1149:ARG:HE	3:D:1218:HIS:CD2	2.30	0.49
2:C:798:GLN:HB3	2:C:827:ARG:NH2	2.27	0.49
3:D:925:GLU:HB3	3:D:926:PRO:HD3	1.94	0.49
5:F:-5:DG:H4'	5:F:-4:DC:OP1	2.11	0.49
6:G:19:DC:H1'	6:G:20:DA:C5'	2.42	0.49
1:A:219:ARG:HH22	1:B:6:THR:HG23	1.77	0.49
2:C:18:ARG:NH1	2:C:1188:ASP:OD1	2.45	0.49
2:C:677:ASN:OD1	2:C:678:ARG:N	2.45	0.49
2:C:1116:HIS:CD2	2:C:1208:GLY:HA3	2.47	0.49
3:D:201:LEU:CD1	3:D:220:ARG:HD3	2.39	0.49
5:F:0:DC:C2'	5:F:1:DA:H5'	2.43	0.49
2:C:1142:ARG:HG3	2:C:1161:LEU:HD23	1.93	0.49
3:D:555:TYR:HB2	3:D:586:GLY:HA2	1.94	0.49
3:D:1209:VAL:HG12	3:D:1210:ILE:H	1.78	0.49
1:B:29:GLU:HB3	1:B:200:LYS:HG3	1.93	0.49
2:C:542:ARG:HD2	2:C:542:ARG:H	1.77	0.49
3:D:548:VAL:N	3:D:572:THR:O	2.45	0.49
1:A:160:HIS:C	1:A:160:HIS:CD2	2.85	0.49
3:D:332:LYS:HE3	3:D:340:GLN:HB2	1.93	0.49
3:D:1168:GLU:O	3:D:1169:THR:C	2.50	0.49
6:G:13:DG:C2'	6:G:14:DT:H71	2.38	0.49
3:D:499:ILE:HG13	3:D:500:ILE:H	1.77	0.49
6:G:-3:DA:C2'	6:G:-2:DA:O5'	2.51	0.49
2:C:538:LEU:HD11	2:C:543:ALA:HB1	1.94	0.49
3:D:104:HIS:HA	3:D:243:PRO:HA	1.94	0.49
3:D:317:THR:HG23	3:D:324:LEU:HD23	1.95	0.49
3:D:515:ARG:HD2	3:D:544:LEU:HD22	1.95	0.49



		Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
3:D:975:ILE:HG21	3:D:980:THR:HG21	1.93	0.49	
3:D:1209:VAL:HG12	3:D:1210:ILE:N	2.27	0.49	
2:C:106:GLU:HA	2:C:114:VAL:HG13	1.95	0.49	
3:D:1042:ASP:HA	3:D:1046:ILE:HB	1.95	0.49	
5:F:0:DC:H2"	5:F:1:DA:C5'	2.43	0.49	
2:C:935:THR:HG23	2:C:1048:LYS:HE2	1.94	0.48	
3:D:97:VAL:HG22	3:D:101:ARG:HG3	1.94	0.48	
6:G:-17:DT:OP1	7:M:367:LEU:CD2	2.60	0.48	
6:G:0:DG:H2"	6:G:1:DG:C5'	2.42	0.48	
7:M:239:THR:HG23	7:M:241:LEU:H	1.77	0.48	
7:M:364:PRO:HB3	7:M:416:SER:CB	2.44	0.48	
3:D:201:LEU:HD11	3:D:220:ARG:CD	2.39	0.48	
3:D:600:ALA:O	3:D:604:MET:HB2	2.13	0.48	
2:C:500:ALA:O	2:C:504:GLU:CB	2.62	0.48	
6:G:10:DG:C5	6:G:11:DC:N4	2.81	0.48	
7:M:162:VAL:HA	7:M:165:ILE:HD12	1.96	0.48	
2:C:956:ALA:O	2:C:960:LEU:HB2	2.14	0.48	
2:C:1268:GLN:O	3:D:346:ARG:HD2	2.13	0.48	
3:D:546:ALA:CB	3:D:548:VAL:HG23	2.44	0.48	
2:C:1275:VAL:HG13	2:C:1287:LEU:HD21	1.96	0.48	
3:D:18:ASP:OD1	3:D:19:ALA:N	2.46	0.48	
3:D:134:ASP:O	3:D:138:VAL:HG22	2.14	0.48	
3:D:650:LYS:HE2	3:D:743:MET:HG3	1.95	0.48	
3:D:788:LEU:HD12	3:D:789:LYS:N	2.29	0.48	
4:E:15:ASN:ND2	4:E:17:PHE:HB2	2.28	0.48	
6:G:19:DC:OP2	6:G:19:DC:H6	1.96	0.48	
7:M:368:ALA:O	7:M:372:GLN:N	2.46	0.48	
2:C:1244:HIS:NE2	2:C:1246:ARG:HB2	2.29	0.48	
2:C:1256:GLN:O	2:C:1301:ARG:NH1	2.46	0.48	
2:C:1269:ARG:CB	5:F:0:DC:OP1	2.62	0.48	
1:B:84:ASN:O	1:B:128:HIS:NE2	2.44	0.48	
1:B:104:LYS:HD3	1:B:110:VAL:HG22	1.96	0.48	
2:C:557:ARG:O	2:C:576:SER:N	2.45	0.48	
6:G:0:DG:H2"	6:G:1:DG:H4'	1.91	0.48	
2:C:521:LEU:HD11	2:C:664:GLY:HA2	1.96	0.48	
2:C:1288:GLN:NE2	3:D:1354:GLY:O	2.44	0.48	
3:D:848:VAL:HG22	3:D:858:VAL:HG22	1.96	0.48	
7:M:279:UNK:HA	7:M:288:UNK:HA	1.95	0.48	
3:D:956:GLY:HA3	3:D:984:LEU:HB3	1.96	0.47	
1:B:210:THR:HG23	1:B:211:ILE:HG13	1.97	0.47	
2:C:1304:MET:HE1	2:C:1315:MET:HA	1.96	0.47	



		Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
5:F:-15:DA:C2	6:G:16:DG:C2	3.02	0.47	
3:D:507:VAL:HB	3:D:730:ALA:HB2	1.96	0.47	
1:B:82:LEU:HD22	1:B:173:VAL:HG22	1.97	0.47	
2:C:565:GLU:O	2:C:569:ILE:HB	2.14	0.47	
3:D:910:ASN:ND2	4:E:15:ASN:O	2.47	0.47	
3:D:1261:LEU:HB3	3:D:1304:ARG:HD3	1.96	0.47	
5:F:-18:DC:O5'	5:F:-18:DC:H2'	2.15	0.47	
7:M:247:LYS:O	7:M:251:ASN:CB	2.63	0.47	
1:B:207:THR:HG22	1:B:209:GLY:H	1.80	0.47	
2:C:670:PHE:HB3	2:C:673:HIS:CD2	2.46	0.47	
2:C:88:ARG:NH1	2:C:1040:ASP:OD1	2.47	0.47	
2:C:159:SER:HB3	2:C:442:VAL:HG21	1.96	0.47	
3:D:546:ALA:HB3	3:D:548:VAL:CG2	2.44	0.47	
3:D:1011:VAL:HG22	3:D:1013:GLY:H	1.79	0.47	
5:F:3:DG:C8	5:F:3:DG:C4'	2.98	0.47	
2:C:200:ARG:CZ	6:G:2:DG:H4'	2.42	0.47	
2:C:321:LEU:HG	2:C:325:LEU:HD23	1.95	0.47	
2:C:1101:LEU:HD21	3:D:508:LEU:HD11	1.97	0.47	
2:C:1292:THR:HG22	2:C:1320:PRO:HG3	1.97	0.47	
2:C:401:GLY:O	2:C:405:PHE:HB2	2.15	0.47	
2:C:401:GLY:O	2:C:405:PHE:CB	2.63	0.47	
2:C:935:THR:HG21	2:C:941:LYS:HG2	1.97	0.47	
3:D:754:ILE:HG22	3:D:755:ILE:N	2.30	0.47	
2:C:1070:HIS:NE2	2:C:1114:GLU:OE1	2.42	0.47	
2:C:709:ALA:HB2	2:C:794:LEU:HB2	1.97	0.47	
2:C:889:PRO:HA	2:C:913:VAL:HG22	1.95	0.47	
6:G:-10:DT:H3'	6:G:-10:DT:OP2	2.15	0.47	
2:C:884:VAL:HG21	2:C:1050:VAL:HG11	1.97	0.46	
3:D:279:LEU:HD11	3:D:296:LYS:HD3	1.96	0.46	
3:D:430:HIS:CE1	3:D:432:LEU:HB2	2.50	0.46	
3:D:723:TYR:O	3:D:727:ASP:HB3	2.14	0.46	
6:G:17:DC:O5'	6:G:17:DC:C2'	2.61	0.46	
2:C:1275:VAL:HG22	2:C:1287:LEU:HD11	1.97	0.46	
3:D:514:THR:HB	3:D:576:ARG:HE	1.79	0.46	
6:G:10:DG:C4	6:G:11:DC:N4	2.84	0.46	
2:C:669:PRO:HD2	2:C:1069:ARG:HE	1.80	0.46	
3:D:137:ARG:HG3	3:D:138:VAL:HG13	1.96	0.46	
3:D:911:LYS:HE3	3:D:1363:TYR:HE2	1.79	0.46	
3:D:1327:GLU:H	3:D:1327:GLU:CD	2.01	0.46	
4:E:2:ALA:HA	4:E:48:VAL:HG11	1.97	0.46	
1:A:18:GLN:HA	1:A:24:ALA:HA	1.97	0.46	



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
3:D:724:MET:O	3:D:728:SER:CB	2.64	0.46	
3:D:158:GLN:HG2	3:D:160:LEU:HD23	1.97	0.46	
6:G:-9:DC:H2"	6:G:-8:DG:OP1	2.15	0.46	
1:A:23:HIS:HA	1:A:205:MET:O	2.16	0.46	
5:F:-7:DG:C5	5:F:-6:DC:N4	2.84	0.46	
2:C:1069:ARG:NH1	2:C:1231:TYR:HB3	2.27	0.46	
7:M:161:ILE:O	7:M:165:ILE:HG13	2.16	0.46	
1:B:104:LYS:HG2	1:B:105:SER:H	1.81	0.46	
2:C:1244:HIS:CE1	2:C:1265:PHE:HA	2.51	0.46	
3:D:616:PRO:O	3:D:620:PHE:CB	2.64	0.46	
7:M:149:ASP:H	7:M:155:THR:HG22	1.81	0.46	
2:C:707:ALA:O	2:C:711:ASP:HB2	2.16	0.46	
3:D:974:VAL:HG12	3:D:975:ILE:N	2.31	0.46	
6:G:-11:DC:C2'	6:G:-10:DT:C5'	2.93	0.46	
7:M:280:UNK:N	7:M:288:UNK:HA	2.31	0.46	
2:C:720:ARG:HH21	2:C:736:VAL:HG21	1.81	0.45	
2:C:1231:TYR:CE2	2:C:1233:LEU:HD21	2.52	0.45	
6:G:-10:DT:H1'	6:G:-9:DC:H5'	1.98	0.45	
6:G:-6:DC:H2"	6:G:-5:DT:O5'	2.16	0.45	
1:A:186:ASN:OD1	1:A:187:VAL:N	2.49	0.45	
2:C:322:LEU:O	2:C:326:SER:HB2	2.16	0.45	
3:D:161:THR:HG22	3:D:162:GLU:N	2.29	0.45	
2:C:156:PHE:O	2:C:174:ALA:HA	2.16	0.45	
2:C:541:GLU:CG	2:C:542:ARG:HD3	2.42	0.45	
2:C:1254:VAL:O	2:C:1255:THR:OG1	2.29	0.45	
3:D:850:LYS:HB2	3:D:851:PRO:HD2	1.99	0.45	
2:C:200:ARG:NH2	6:G:2:DG:C4'	2.68	0.45	
6:G:19:DC:C1'	6:G:20:DA:H5'	2.45	0.45	
7:M:223:HIS:O	7:M:224:LEU:HG	2.17	0.45	
1:B:26:VAL:HB	1:B:203:ILE:HB	1.98	0.45	
2:C:92:TYR:HE2	2:C:129:LEU:HB3	1.82	0.45	
2:C:361:SER:O	2:C:364:VAL:N	2.50	0.45	
5:F:3:DG:C8	5:F:3:DG:C5'	2.85	0.45	
6:G:16:DG:H2"	6:G:17:DC:H6	1.80	0.45	
1:A:164:ASP:OD1	1:A:164:ASP:N	2.35	0.45	
2:C:838:CYS:HB2	2:C:918:LEU:HD12	1.97	0.45	
2:C:933:VAL:HG22	2:C:1050:VAL:HG13	1.99	0.45	
6:G:-14:DG:OP2	6:G:-14:DG:C8	2.70	0.45	
7:M:193:LYS:C	7:M:195:LEU:H	2.19	0.45	
1:A:108:GLY:H	1:A:133:LEU:HB2	1.82	0.45	
2:C:636:CYS:HB2	2:C:645:PHE:HD2	1.82	0.45	



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
3:D:370:LYS:HB2	3:D:409:TRP:HZ3	1.81	0.45	
6:G:13:DG:H2"	6:G:14:DT:C5	2.52	0.45	
7:M:280:UNK:O	7:M:287:UNK:O	2.34	0.45	
1:B:104:LYS:HG2	1:B:105:SER:N	2.32	0.45	
2:C:349:GLU:O	2:C:353:VAL:HG23	2.15	0.45	
2:C:542:ARG:CB	6:G:4:DG:O4'	2.63	0.45	
3:D:264:ASP:HB2	3:D:324:LEU:HB2	1.99	0.45	
5:F:3:DG:C8	5:F:3:DG:C3'	2.99	0.45	
6:G:14:DT:C2'	6:G:15:DT:C7	2.88	0.45	
7:M:264:UNK:O	7:M:266:UNK:N	2.49	0.45	
2:C:578:TYR:HD2	2:C:659:GLN:HG2	1.82	0.45	
1:B:41:ASN:OD1	1:B:44:ARG:NH1	2.50	0.45	
3:D:865:HIS:CE1	3:D:867:GLN:HB2	2.52	0.45	
3:D:1140:ARG:HH12	3:D:1236:GLU:HB3	1.81	0.45	
5:F:-19:DG:N2	6:G:20:DA:C2	2.85	0.45	
5:F:6:DT:C2'	5:F:7:DG:OP2	2.65	0.45	
6:G:10:DG:H2"	6:G:11:DC:H5	1.82	0.44	
2:C:322:LEU:O	2:C:326:SER:CB	2.65	0.44	
2:C:1032:LYS:HE2	2:C:1036:ILE:HD11	1.99	0.44	
3:D:1325:PHE:CD1	3:D:1325:PHE:O	2.71	0.44	
5:F:4:DG:H4'	5:F:4:DG:OP1	2.16	0.44	
6:G:-11:DC:C1'	6:G:-10:DT:C5'	2.90	0.44	
7:M:194:ASP:C	7:M:196:ARG:H	2.21	0.44	
2:C:183:TRP:CE2	6:G:1:DG:C6	3.06	0.44	
3:D:517:CYS:HA	3:D:716:GLN:HE21	1.82	0.44	
3:D:848:VAL:HG23	3:D:857:LEU:HB2	1.98	0.44	
3:D:1219:ASP:OD1	3:D:1222:ARG:NH2	2.42	0.44	
6:G:-18:DT:O2	6:G:-17:DT:C2	2.70	0.44	
1:B:46:ILE:HD12	1:B:224:LEU:HD12	1.99	0.44	
3:D:265:LEU:HD13	3:D:330:MET:SD	2.57	0.44	
2:C:551:HIS:HB3	2:C:554:HIS:CE1	2.53	0.44	
2:C:930:ASP:HB3	2:C:1053:TYR:CD2	2.53	0.44	
3:D:353:SER:O	3:D:465:GLN:HA	2.17	0.44	
3:D:609:TYR:HB2	3:D:617:THR:HG21	2.00	0.44	
3:D:811:GLU:OE1	3:D:890:THR:OG1	2.27	0.44	
3:D:1058:SER:HA	3:D:1108:GLN:HA	1.98	0.44	
7:M:277:UNK:O	7:M:391:HIS:N	2.42	0.44	
1:A:158:ARG:HG2	1:A:161:SER:HG	1.81	0.44	
2:C:3:TYR:C	2:C:5:TYR:H	2.20	0.44	
2:C:196:VAL:HG21	2:C:209:ILE:HG21	1.99	0.44	
2:C:302:ILE:HG22	2:C:309:LEU:HB3	2.00	0.44	



	juo puge	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
2:C:700:VAL:HG22	2:C:1117:LEU:HD22	2.00	0.44	
3:D:535:ARG:O	3:D:539:SER:N	2.51	0.44	
3:D:937:ILE:C	3:D:939:GLY:N	2.71	0.44	
2:C:802:VAL:HG21	2:C:1230:MET:HB3	2.00	0.44	
2:C:1042:LEU:HD13	2:C:1046:VAL:HG13	1.99	0.44	
3:D:36:GLY:HA3	3:D:61:ILE:HG21	1.99	0.44	
3:D:810:THR:HG23	3:D:811:GLU:H	1.83	0.44	
1:A:39:LEU:O	1:A:43:LEU:HB3	2.18	0.44	
1:A:165:GLU:CD	1:A:166:ARG:H	2.13	0.44	
2:C:26:TYR:CE2	2:C:28:LEU:HB2	2.53	0.44	
5:F:-5:DG:H8	5:F:-5:DG:H2'	1.68	0.44	
5:F:15:DA:H2	6:G:-15:DT:O2	2.00	0.44	
6:G:8:DA:H2'	6:G:9:DT:H72	1.98	0.44	
2:C:522:SER:O	2:C:526:HIS:HB2	2.18	0.43	
3:D:22:ILE:HG12	3:D:1336:ALA:HA	1.98	0.43	
3:D:646:ILE:HD11	3:D:764:ARG:HD3	1.98	0.43	
3:D:1145:PHE:HB3	3:D:1309:ILE:HD12	1.99	0.43	
6:G:4:DG:N3	6:G:4:DG:H5'	2.32	0.43	
2:C:901:LEU:O	2:C:905:ILE:HD13	2.17	0.43	
3:D:270:ARG:O	3:D:274:ASN:HB2	2.18	0.43	
3:D:355:ILE:HD13	3:D:447:ILE:HB	2.00	0.43	
2:C:59:ILE:HD11	2:C:476:LYS:HG3	2.00	0.43	
2:C:540:ARG:O	2:C:542:ARG:N	2.50	0.43	
2:C:762:ASN:O	2:C:833:ILE:N	2.38	0.43	
2:C:1304:MET:O	2:C:1308:ILE:HG12	2.17	0.43	
3:D:466:MET:HG3	3:D:467:ALA:H	1.83	0.43	
3:D:583:VAL:HG13	3:D:587:LEU:HD22	1.98	0.43	
3:D:1263:LYS:HB2	3:D:1307:LEU:HD11	2.00	0.43	
5:F:12:DT:H2'	5:F:13:DG:H8	1.70	0.43	
7:M:318:PHE:CB	7:M:322:ASN:CB	2.95	0.43	
2:C:538:LEU:HD11	2:C:543:ALA:HB3	2.00	0.43	
2:C:1278:LEU:HD12	2:C:1287:LEU:HD13	2.00	0.43	
3:D:515:ARG:HH12	3:D:724:MET:HG2	1.83	0.43	
3:D:655:SER:O	3:D:658:GLU:HB2	2.19	0.43	
3:D:657:ALA:O	3:D:660:GLU:HB2	2.19	0.43	
3:D:1260:MET:O	3:D:1307:LEU:HB2	2.18	0.43	
1:B:40:GLY:O	1:B:44:ARG:HB2	2.18	0.43	
2:C:470:ARG:HD2	2:C:497:PRO:HB3	2.00	0.43	
2:C:653:MET:HG3	2:C:655:VAL:H	1.82	0.43	
2:C:1122:LYS:HD3	2:C:1229:TYR:CZ	2.54	0.43	
3:D:194:LEU:HD23	3:D:228:VAL:HG22	1.99	0.43	



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
2:C:660:VAL:HG23	2:C:661:VAL:HG23	2.00	0.43	
3:D:810:THR:HG23	3:D:811:GLU:N	2.34	0.43	
6:G:0:DG:C2'	6:G:1:DG:O4'	2.67	0.43	
2:C:594:VAL:HG22	2:C:599:VAL:HG13	2.01	0.43	
7:M:406:UNK:CB	7:M:416:SER:HA	2.49	0.43	
1:A:234:LEU:HD23	1:B:214:GLU:HB2	2.00	0.43	
2:C:975:ILE:HA	2:C:978:VAL:HG12	2.00	0.43	
6:G:13:DG:H2"	6:G:14:DT:C6	2.54	0.43	
7:M:279:UNK:HA	7:M:288:UNK:CA	2.48	0.43	
3:D:81:ARG:HA	3:D:92:VAL:HG21	2.01	0.43	
3:D:705:THR:OG1	3:D:718:SER:HA	2.19	0.43	
3:D:850:LYS:HB3	3:D:857:LEU:HD11	2.00	0.43	
3:D:1146:GLU:HA	3:D:1308:GLY:O	2.19	0.43	
6:G:14:DT:H2"	6:G:15:DT:C5	2.53	0.43	
2:C:257:ALA:HA	2:C:285:ILE:HG21	2.01	0.43	
2:C:669:PRO:HG3	2:C:1069:ARG:HH21	1.83	0.43	
2:C:1293:VAL:HA	2:C:1297:ASP:HB2	2.01	0.43	
2:C:1339:LEU:HD23	3:D:20:ILE:HG12	2.01	0.43	
3:D:119:SER:O	3:D:120:LEU:HB2	2.19	0.43	
3:D:1372:ARG:O	3:D:1376:GLY:N	2.52	0.43	
1:A:38:THR:HG21	1:B:46:ILE:HG13	2.01	0.42	
1:B:104:LYS:NZ	1:B:110:VAL:HA	2.34	0.42	
2:C:591:TYR:O	2:C:603:ILE:HA	2.19	0.42	
2:C:1020:GLU:O	2:C:1024:GLU:HB2	2.19	0.42	
6:G:-17:DT:P	7:M:367:LEU:CD2	3.07	0.42	
6:G:12:DT:C2'	6:G:13:DG:C8	3.00	0.42	
7:M:319:ILE:CD1	7:M:319:ILE:C	2.85	0.42	
7:M:443:THR:CB	7:M:455:ARG:HA	2.49	0.42	
1:B:40:GLY:O	1:B:44:ARG:CB	2.67	0.42	
3:D:600:ALA:O	3:D:604:MET:CB	2.67	0.42	
6:G:19:DC:OP2	6:G:19:DC:C6	2.72	0.42	
2:C:1244:HIS:HE1	2:C:1265:PHE:CD1	2.37	0.42	
2:C:1324:ASN:HA	2:C:1327:LEU:HD12	2.01	0.42	
3:D:211:GLU:OE2	5:F:-14:DA:P	2.77	0.42	
2:C:548:ARG:HD3	2:C:569:ILE:HG23	2.01	0.42	
3:D:482:ALA:O	3:D:488:ASN:ND2	2.52	0.42	
4:E:7:GLN:O	4:E:11:GLU:HB2	2.18	0.42	
6:G:12:DT:H1'	6:G:13:DG:C8	2.54	0.42	
2:C:859:GLU:HA	2:C:862:LEU:HB2	2.01	0.42	
3:D:620:PHE:CE2	3:D:624:ILE:HD11	2.54	0.42	
3:D:918:ILE:HG22	3:D:1252:HIS:CE1	2.54	0.42	



	juo puge	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
2:C:678:ARG:HG2	2:C:1108:ASN:HD21	1.84	0.42	
2:C:1124:ILE:O	2:C:1128:ILE:HD12	2.18	0.42	
3:D:342:LEU:HD21	3:D:1348:LYS:HZ1	1.83	0.42	
3:D:517:CYS:HA	3:D:716:GLN:NE2	2.35	0.42	
3:D:975:ILE:HG22	3:D:977:SER:H	1.84	0.42	
2:C:1032:LYS:O	2:C:1036:ILE:HG12	2.18	0.42	
7:M:167:ASP:HB3	7:M:169:GLU:O	2.20	0.42	
2:C:96:LEU:HD13	2:C:127:ILE:HD12	2.02	0.42	
2:C:200:ARG:CD	6:G:2:DG:H5"	2.44	0.42	
2:C:524:ILE:HD12	2:C:708:VAL:HG13	2.01	0.42	
2:C:1287:LEU:HD23	3:D:1357:ILE:HD11	2.02	0.42	
3:D:649:LYS:O	3:D:653:ILE:HD12	2.20	0.42	
6:G:0:DG:C2'	6:G:1:DG:C4'	2.94	0.42	
2:C:164:THR:HG23	2:C:165:HIS:N	2.34	0.42	
2:C:496:LYS:HB2	2:C:497:PRO:HD3	2.02	0.42	
2:C:799:ASN:HD22	2:C:1231:TYR:HA	1.84	0.42	
3:D:450:HIS:CD2	3:D:453:VAL:HG23	2.53	0.42	
7:M:147:ALA:HB1	7:M:156:ILE:HG12	2.02	0.42	
1:B:74:VAL:HA	1:B:134:THR:HB	2.01	0.42	
2:C:30:ILE:O	2:C:33:ASP:HB2	2.20	0.42	
2:C:540:ARG:HE	2:C:540:ARG:HB2	1.70	0.42	
2:C:1244:HIS:CD2	2:C:1246:ARG:HB2	2.55	0.42	
3:D:319:SER:HB3	5:F:7:DG:H5"	2.02	0.42	
3:D:347:VAL:HG12	3:D:348:ASP:N	2.35	0.42	
1:A:219:ARG:HH12	1:B:6:THR:HG23	1.85	0.41	
1:B:96:ASP:OD1	1:B:97:GLU:N	2.53	0.41	
2:C:188:PHE:CE1	2:C:194:LEU:HG	2.55	0.41	
3:D:422:LEU:HD23	3:D:471:PRO:HG3	2.02	0.41	
3:D:466:MET:HG3	3:D:467:ALA:N	2.36	0.41	
3:D:681:LYS:O	3:D:685:ILE:HG12	2.20	0.41	
6:G:-11:DC:H1'	6:G:-10:DT:H5"	2.01	0.41	
1:A:160:HIS:CD2	1:A:160:HIS:O	2.73	0.41	
2:C:138:ILE:HG12	2:C:139:ASN:HD22	1.86	0.41	
2:C:788:SER:HB2	2:C:796:LEU:HA	2.01	0.41	
3:D:323:PRO:O	3:D:324:LEU:HG	2.20	0.41	
2:C:241:LEU:HD11	2:C:285:ILE:HG12	2.02	0.41	
2:C:373:GLY:CA	7:M:319:ILE:HG21	2.46	0.41	
2:C:1067:ALA:HB2	2:C:1235:LEU:HD11	2.02	0.41	
3:D:159:ILE:HG22	3:D:159:ILE:O	2.20	0.41	
6:G:16:DG:C2'	6:G:17:DC:C6	3.01	0.41	
1:A:227:GLN:HG3	1:B:39:LEU:HD21	2.01	0.41	



		Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
2:C:844:LYS:HE3	7:M:389:TYR:HE2	1.85	0.41	
3:D:1177:ILE:N	3:D:1188:GLU:O	2.47	0.41	
2:C:702:THR:O	2:C:1183:ALA:HB1	2.20	0.41	
3:D:919:ALA:O	3:D:920:ALA:HB3	2.20	0.41	
5:F:-19:DG:H2"	5:F:-18:DC:H6	1.82	0.41	
2:C:1323:PHE:O	2:C:1327:LEU:HG	2.20	0.41	
4:E:19:LEU:O	4:E:23:ALA:HB3	2.20	0.41	
5:F:12:DT:C7	7:M:380:THR:HG21	2.47	0.41	
7:M:191:ALA:C	7:M:193:LYS:H	2.23	0.41	
6:G:-17:DT:P	7:M:367:LEU:HD21	2.61	0.41	
6:G:-7:DA:H5"	6:G:-7:DA:H8	1.85	0.41	
2:C:178:PRO:HD2	2:C:183:TRP:CD1	2.56	0.41	
2:C:798:GLN:HB2	2:C:828:PHE:CE1	2.56	0.41	
3:D:422:LEU:HD11	3:D:469:HIS:HB2	2.03	0.41	
3:D:632:ALA:O	3:D:635:SER:OG	2.31	0.41	
5:F:11:DG:H2"	5:F:12:DT:C7	2.51	0.41	
1:A:218:ARG:NE	1:B:231:PHE:O	2.51	0.41	
2:C:15:PHE:O	2:C:1155:VAL:HA	2.20	0.41	
2:C:662:SER:O	2:C:666:SER:OG	2.27	0.41	
2:C:933:VAL:HG22	2:C:1050:VAL:HA	2.03	0.41	
3:D:41:PRO:HD3	3:D:277:ASN:ND2	2.35	0.41	
3:D:186:GLN:O	3:D:190:LYS:CB	2.68	0.41	
3:D:369:PRO:HG3	3:D:446:ALA:O	2.21	0.41	
5:F:24:DG:H1	6:G:-24:DC:H42	1.69	0.41	
6:G:-10:DT:P	6:G:-10:DT:C3'	3.04	0.41	
6:G:-10:DT:C3'	6:G:-9:DC:H5'	2.51	0.41	
6:G:-3:DA:H4'	6:G:-2:DA:OP1	2.20	0.41	
7:M:280:UNK:O	7:M:287:UNK:C	2.69	0.41	
2:C:10:ARG:HH11	2:C:793:GLU:CD	2.23	0.41	
2:C:92:TYR:CE2	2:C:129:LEU:HB3	2.56	0.40	
2:C:99:LYS:HA	2:C:121:GLU:HB3	2.02	0.40	
3:D:1314:LEU:HD13	3:D:1330:ARG:NH2	2.36	0.40	
6:G:-10:DT:OP2	6:G:-10:DT:H2'	2.20	0.40	
6:G:2:DG:OP2	6:G:2:DG:C8	2.71	0.40	
3:D:576:ARG:HD3	3:D:593:ASN:HA	2.04	0.40	
3:D:625:MET:HG3	3:D:629:PHE:HE2	1.85	0.40	
2:C:526:HIS:HA	2:C:529:ARG:HH22	1.85	0.40	
3:D:813:ASP:HB2	3:D:897:HIS:HD2	1.86	0.40	
3:D:885:VAL:C	3:D:887:SER:H	2.23	0.40	
4:E:6:VAL:HG12	4:E:10:VAL:HG23	2.04	0.40	
7:M:295:PRO:O	7:M:296:ARG:CB	2.68	0.40	



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A + a 1	A + a	Interatomic	Clash		
Atom-1	Atom-2	distance (Å)	overlap (Å)		
1:A:118:ASP:HB3	1:A:121:VAL:HG23	2.04	0.40		
2:C:510:GLN:HG3	2:C:511:LEU:HD12	2.04	0.40		
2:C:636:CYS:HB2	2:C:645:PHE:CD2	2.56	0.40		
2:C:667:LEU:HA	2:C:702:THR:HG21	2.02	0.40		
2:C:806:PRO:HA	2:C:811:ASN:ND2	2.33	0.40		
2:C:874:GLY:H	2:C:928:VAL:HG23	1.87	0.40		
3:D:901:ARG:C	3:D:903:LEU:H	2.24	0.40		
3:D:1263:LYS:HE2	3:D:1315:ALA:HB1	2.03	0.40		
5:F:-4:DC:C4	6:G:4:DG:O6	2.75	0.40		
7:M:249:ALA:O	7:M:253:ILE:HG12	2.21	0.40		
1:A:192:VAL:HB	1:A:198:LEU:HD12	2.02	0.40		
2:C:209:ILE:HD11	2:C:389:PHE:CZ	2.57	0.40		
2:C:227:LYS:HA	2:C:336:LEU:HA	2.03	0.40		
2:C:904:ALA:HB3	2:C:905:ILE:HD12	2.04	0.40		
3:D:162:GLU:HA	3:D:165:TYR:HB3	2.04	0.40		
3:D:1159:ILE:HG22	3:D:1160:SER:N	2.36	0.40		
5:F:-7:DG:H2"	5:F:-6:DC:C6	2.57	0.40		
5:F:-2:DC:N4	5:F:-1:DC:N4	2.69	0.40		
5:F:6:DT:H2"	5:F:7:DG:OP2	2.21	0.40		
6:G:0:DG:C2'	6:G:0:DG:N3	2.84	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 PDB entries followed by that with respect to all EM entries.

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	231/329~(70%)	210 (91%)	21 (9%)	0	100	100
1	В	233/329~(71%)	218 (94%)	15~(6%)	0	100	100
2	С	1339/1342~(100%)	1234 (92%)	101 (8%)	4 (0%)	41	74
3	D	1335/1407~(95%)	1184 (89%)	138 (10%)	13 (1%)	15	51



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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	entiles
4	Е	72/91~(79%)	67~(93%)	5 (7%)	0	100	100
7	М	311/497~(63%)	260 (84%)	47 (15%)	4 (1%)	12	47
All	All	3521/3995~(88%)	3173 (90%)	327~(9%)	21 (1%)	29	62

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	С	347	ILE
2	С	1155	VAL
3	D	500	ILE
3	D	886	VAL
3	D	938	GLY
3	D	1134	ILE
3	D	1309	ILE
7	М	188	VAL
2	С	1264	GLN
3	D	546	ALA
7	М	156	ILE
2	С	655	VAL
3	D	347	VAL
3	D	915	ILE
3	D	1159	ILE
3	D	331	ILE
3	D	531	LYS
7	М	109	LEU
3	D	83	VAL
3	D	809	VAL
7	М	170	ILE

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
1	А	190/286~(66%)	185 (97%)	5(3%)	46	69
1	В	183/286~(64%)	183 (100%)	0	100	100



Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
2	С	1021/1157~(88%)	1016 (100%)	5~(0%)	88	94
3	D	938/1168~(80%)	933 (100%)	5~(0%)	88	94
4	Ε	53/75~(71%)	53~(100%)	0	100	100
7	М	100/396~(25%)	100 (100%)	0	100	100
All	All	2485/3368~(74%)	2470 (99%)	15 (1%)	86	93

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	\mathbf{Res}	Type
1	А	158	ARG
1	А	159	ILE
1	А	160	HIS
1	А	161	SER
1	А	166	ARG
2	С	100	LEU
2	С	540	ARG
2	С	541	GLU
2	С	542	ARG
2	С	545	PHE
3	D	107	LEU
3	D	109	SER
3	D	311	ARG
3	D	547	ARG
3	D	934	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	66	HIS
1	А	160	HIS
2	С	139	ASN
2	С	518	ASN
2	С	604	HIS
2	С	808	ASN
2	С	811	ASN
2	С	1072	ASN
2	С	1237	HIS
2	С	1264	GLN
3	D	469	HIS
3	D	702	GLN



Continued from previous page...

Mol	Chain	Res	Type
3	D	1218	HIS
3	D	1279	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
8	R	3/4~(75%)	0	0

There are no RNA backbone outliers to report.

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)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-4397. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

Orthogonal projections (i) 6.1

6.1.1Primary map



The images above show the map projected in three orthogonal directions.

6.2Central slices (i)

6.2.1Primary map



X Index: 128



Y Index: 128



Z Index: 128

The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 141

Y Index: 124

Z Index: 106

The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.035. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.



6.5 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.



7 Map analysis (i)

This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.



7.2 Volume estimate (i)



The volume at the recommended contour level is 207 $\rm nm^3;$ this corresponds to an approximate mass of 187 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.



7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.270 ${\rm \AA^{-1}}$



8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.



9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-4397 and PDB model 6GFW. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay (i)



The images above show the 3D surface view of the map at the recommended contour level 0.035 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.



9.2 Q-score mapped to coordinate model (i)



The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model (i)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.035).



9.4 Atom inclusion (i)



At the recommended contour level, 82% of all backbone atoms, 71% of all non-hydrogen atoms, are inside the map.



Map-model fit summary (i) 9.5

The table lists the average atom inclusion at the recommended contour level (0.035) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score	1.0
All	0.7098	0.3720	
А	0.7877	0.4350	
В	0.7063	0.3690	
С	0.7499	0.3990	
D	0.6994	0.3750	
E	0.6898	0.3870	
F	0.6660	0.2650	
G	0.5634	0.2190	
М	0.6010	0.2990	0.0 <
R	0.8488	0.4520	

