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PDB ID	:	8X1C
EMDB ID	:	EMD-37990
Title	:	Structure of nucleosome-bound SRCAP-C in the ADP-bound state
Authors	:	Yu, J.; Wang, Q.; Yu, Z.; Li, W.; Wang, L.; Xu, Y.
Deposited on	:	2023-11-06
Resolution	:	3.20 Å(reported)

This is a 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. dev 70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7(2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f EM} {f structures} \ (\#{f Entries})$
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 >=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 EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain		
1	А	130	8%		17% 11%
1	Е	130	68%	12%	• 19%
2	В	126	5 6% 20%	•	24%
2	F	126	62% 11%	••	25%
3	С	136	53% 15% ••		30%
3	G	136	6 5% 6%	•	29%
4	D	103	• 68%	11%	21%
4	Н	103	73%	5%	22%



Mol	Chain	Length		Quality	y of chain		
5	Ι	3230	20% 6	% •	74%		
6	J	364	28%	7% ••	63%		
7	K	396		73%		24%	
8	L	154	0 %	55%	13%	32%	
9	М	456	.	75%		17%	• 6%
9	0	456	•	81%		139	% • 5%
9	Q	456	•	75%		20%	• •
10	Ν	463	•	77%		12%	10%
10	Р	463	.	72%		19%	• 8%
10	R	463	•	72%		18%	• 8%
11	S	375		97	%		•
11	U	375		61% 72%		22%	•••
12	Т	429		61% 83%		10	% • 6%
13	V	467	33%	9% •	56%	%	
14	W	227		82% 70%		11% •	18%
15	X	147	10%	52%		31%	
16	Y	147	9%	<u>-</u>	50%	259	%



2 Entry composition (i)

There are 18 unique types of molecules in this entry. The entry contains 56519 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 Histone H2A type 1-C.

Mol	Chain	Residues		Ato	ms	AltConf	Trace	
1	А	116	Total 898	C 564	N 179	O 155	0	0
1	Е	105	Total 808	C 510	N 158	O 140	0	0

• Molecule 2 is a protein called Histone H2B type 1-C/E/F/G/I.

Mol	Chain	Residues		At	oms	AltConf	Trace		
2	В	96	Total 755	C 473	N 138	0 142	${ m S} { m 2}$	0	0
2	F	94	Total 736	C 461	N 134	0 139	$\begin{array}{c} \mathrm{S} \\ \mathrm{2} \end{array}$	0	0

• Molecule 3 is a protein called Histone H3.1.

Mol	Chain	Residues		At	oms	AltConf	Trace		
2	C	05	Total	С	Ν	0	S	0	0
		90	779	491	148	136	4	0	0
2	C	07	Total	С	Ν	0	S	0	0
)	G	97	801	505	155	137	4		

• Molecule 4 is a protein called Histone H4.

Mol	Chain	Residues		At	oms	AltConf	Trace		
4	D	81	Total 646	C 407	N 126	0 112	S 1	0	0
4	Н	80	Total 638	C 401	N 125	0 111	S 1	0	0

• Molecule 5 is a protein called Helicase SRCAP.



Mol	Chain	Residues		А	AltConf	Trace			
5	Ι	852	Total 7031	C 4476	N 1299	O 1217	S 39	0	0

• Molecule 6 is a protein called Vacuolar protein sorting-associated protein 72 homolog.

Mol	Chain	Residues		At	oms	AltConf	Trace		
6	J	135	Total 1114	C 708	N 203	O 199	$\frac{S}{4}$	0	0

• Molecule 7 is a protein called Actin-related protein 6.

Mol	Chain	Residues		At	AltConf	Trace			
7	K	394	Total 3209	C 2054	N 526	0 611	S 18	0	0

• Molecule 8 is a protein called Zinc finger HIT domain-containing protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	L	105	Total 823	C 506	N 157	0 152	S 8	0	0

• Molecule 9 is a protein called RuvB-like 1.

Mol	Chain	Residues		At	oms			AltConf	Trace
9	М	428	Total 3293	C 2075	N 567	O 635	S 16	0	0
9	0	435	Total 3339	C 2105	N 571	O 646	S 17	0	0
9	Q	440	Total 3368	C 2121	N 579	0 651	S 17	0	0

• Molecule 10 is a protein called RuvB-like 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	Ν	415	Total 3223	C 2016	N 565	O 627	S 15	0	0
10	Р	427	Total 3287	C 2054	N 576	0 642	S 15	0	0
10	R	424	Total 3293	C 2057	N 578	0 642	S 16	0	0

• Molecule 11 is a protein called Actin, cytoplasmic 1.



Mol	Chain	Residues		At	AltConf	Trace			
11	q	275	Total	С	Ν	0	\mathbf{S}	0	0
	11 5	515	2925	1850	491	561	23	0	
11	T	250	Total	С	Ν	0	S	0	0
	U	009	2802	1775	468	540	19	0	0

• Molecule 12 is a protein called Actin-like protein 6A.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	Т	403	Total 3146	C 1988	N 535	O 599	S 24	0	0

• Molecule 13 is a protein called DNA methyltransferase 1-associated protein 1.

Mol	Chain	Residues		Ate	oms			AltConf	Trace
13	V	204	Total 1757	C 1117	N 327	O 309	$\frac{S}{4}$	0	0

• Molecule 14 is a protein called YEATS domain-containing protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	W	187	Total 1542	C 998	N 255	0 284	${ m S}{ m 5}$	0	0

• Molecule 15 is a DNA chain called DNA (147-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
15	Х	147	Total 3034	C 1435	N 572	O 880	Р 147	0	0

• Molecule 16 is a DNA chain called DNA (147-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Y	147	Total 2990	C 1422	N 540	0 882	Р 146	0	0

• Molecule 17 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues		Ate	oms			AltConf
17	т	1	Total	С	Ν	Ο	Р	0
11	1	T	27	10	5	10	2	0
17	М	1	Total	С	Ν	0	Р	0
11	111	T	27	10	5	10	2	0
17	N	1	Total	С	Ν	Ο	Р	0
11	11	I	27	10	5	10	2	0
17	0	1	Total	\mathbf{C}	Ν	Ο	Р	0
11	U	I	27	10	5	10	2	0
17	Р	1	Total	\mathbf{C}	Ν	Ο	Р	0
11	1	T	27	10	5	10	2	0
17	0	1	Total	\mathbf{C}	Ν	Ο	Р	0
	<u>ل</u>		27	10	5	10	2	0
17	B	1	Total	С	Ν	Ο	Р	0
11	10	1	27	10	5	10	2	U

• Molecule 18 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $\rm C_{10}H_{16}N_5O_{13}P_3).$





Mol	Chain	Residues	Atoms					AltConf
18	K	1	Total	С	Ν	Ο	Р	0
10	Γ	T	31	10	5	13	3	0
19	Т	1	Total	С	Ν	Ο	Р	0
10	1	L	31	10	5	13	3	0
19	T	1	Total	С	Ν	Ο	Р	0
10	U	L	31	10	5	13	3	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.

- Chain A: 72% 17% 11% MET SER GLY GLY GLY GLY GLY GLY ALA • Molecule 1: Histone H2A type 1-C Chain E: 68% 19% 12% MET SER GLY GLY GLY GLY GLY GLY CLYS GLY ALA ALA ALA ALA ALA IIS IIS VLA • Molecule 2: Histone H2B type 1-C/E/F/G/IChain B: 56% 20% 24% • Molecule 2: Histone H2B type 1-C/E/F/G/IChain F: 62% 25% 11%
- Molecule 1: Histone H2A type 1-C



• Molecule 3: Histone H	3.1			
Chain C:	53%	15% ••	30%	
MET ALA ALA ALA ALA THR LLYS SLN SLY CLY CLY CLY CLY ALA ALA ALA ARG ALA	LYS CLN CLN CLN LLEU ALA ALA ALA ALA ALA ALA ALA ALA ALA CLY CLY	VAL VAL LYS LYS FRO FRO HTS ARG 642 P43 P43 C44	145 145 145 148 148 149 151 151 151 151	E59 160 161
162 164 164 166 166 166 168 183 183 169 1109 1100	K115 V117 V117 V120 M120 K122 A135			
• Molecule 3: Histone H	3.1			
Chain G:	65%	6% ·	29%	
MET ALA ALA ALA ARG THR CVN CVN CVN CVN CVN CVN CVN CVN CVN ARG CVN ARG ARC ARC ARC ARC	LYS CLBU CLBU ALB ALA ALA ALA ALA ALA ARG ALA ARG ARG ARG ARG CYY	0 417 1 417 1 418 1 418 1 419 1 419 1 419 1 413 1 41 1 41	V101 V101 D106 R129 R129 R131 R131 ALA	
• Molecule 4: Histone H	4			
Chain D:	68%	11%	21%	
MET SER SER SER SER ARG GLY GLY GLY GLY GLY GLY GLY ALA ARG GLY ARG GLY	HIS ARG LYS VAL L22 L22 R23 R23 R23 R23 R23 R23 R23 R24 R44 R44 R45 R45 R45 R45 R46 R46 R46 R46 R46 R46 R46 R46 R46 R46	H75 R78 K79 T80 V81 C102		
• Molecule 4: Histone H	4			
Chain H:	73%	5%	22%	
MET SER GLY GLY CLYS CLYS GLY CLYS GLY GLY GLY ALA ALA ALA ALA	HIS ARG LYS LEU LEU LEU LEU E63 E63 E63 K79 K79	G102		
• Molecule 5: Helicase S	RCAP			
Chain I: 20% 69	% •	74%		
MET GLN SER SER SER PRO PRO PRO PRO PRO CLN VAL LEU VAL CLN CLN CLN CLN CLN CLN CLN CLN CLN CL	MET VAL SER SER ASP ASP ASP ASP ASP ASP ASN ASN ASN ASN AASN A	SER SER PRO PRO PLA SER SER SER GLY GLY GLY	PRO PRO GLN FILE ALA GLN GLN SER SER SER SER SER SER SER	GLY PRO
PRO GLY PRO PRO PRO ASP ASP VAL THR VAL LEU CLEU CLEU CLEU SER SER SER SER SER	ALA ALA ASP ALA ASP LEU ASN LVS GLY GLY CTRP CLYS GLU CLU CLU CLU CLU CLU	A94 E95 196 A97 E98 A100 K101 H102	E103 A104 E105 E107 T106 R109 A111 A111	L112 L113 R114 E116 E116 F118 V119 S120
L121 K122 R123 F124 F124 F126 F126 F126 F128 F131 F131 F131 F133 F133 F133	G1355 H1355 W137 D138 Y139 L140 C141 E142 E142 E142 E142 E143 G146 W146 W146 U147	S148 D150 F151 A152 A152 A152 A152 K156 W157 K156	R159 6160 V161 A162 R163 R167 R167 H173 E174	E175 Q176 A177 A177 E180 E181 E181 A183 A183 A183 A183 E186 E186
E187 4188 A188 A195 A195 A195 A195 A195 A195 A195 A195	E210 (K226 K226 L229 L233 F241 K242 Y243 Y243 C249 Q249	N252 PRO PRO LEU THR SER SER ALA CLYS SER SER	PRO PRO CYS CYS CYS SER SER ALA ALA SER SER SER	PKU PRO ORG

WORLDWIDE PROTEIN DATA BANK



LEU	ALA SFR	SER	THR	PRO	VAL	VAL	MET	PRO	SER	THR	PRO	GLY	SER.	LEU	ALA	ALA	SER	PRO WAT	V AL PRO	ALA	PRO THD	PRO	VAL	LEU ALA	PRO	SER	THR	GLN	MET	LEU	ALA	PRO VAT	PRO	SER	PRO I FII	PRO	SER PRO	ALA	SER	GLN	THR	
ALA	LEU	PRO	ALA LEU	ALA	PRO THR	TEU	GLY	SER	SER	PRO	GLN	THR	LEU SER	LEU	GLY	GLY	ASN	PRO	GLY	PRO	PHE	THR	GLN	THR	SER	LEU	PRO	ALA	SER	LEU	PRO	THR	ALA	GLN	THR	SER	LEU AI.A	PRO	GLY	PRO	GLY	
PRO	THR	THR	LEU SER	LEU	ALA	ALA	PRO	LEU	ALA	PRO ALA	SER	PRO	VAL GLY	PRO	ALA	ALA	HIS	THR	THR	LEU	ALA	ALA	SER	SER	ALA	SER	TEU	ALA	ALA	SER	GLN	THR	THR	LEU	DRU	ALA	PRO VAL	PRO	THR	GLY	PRO ALA	
ALA	ALA	THR	ALA	LEU	ALA	ALA	SER	GLN	SER	PRO ALA	SER	GLN	ALA SER	SER	LEU	VAL VAL	SER	ALA	GLY	ALA	ALA	LEU	PRO	VAL THR	MET	VAL	ARG	LEU	VAL	SER	ASP	GLU	ASP	THR	THR	TEU	ARG	GLY	PRO Prod	SER	PRO PRO	
															~			<u>~</u>	<u> </u>			~		~	0		4	10								- -		~	<u> </u>		<u> </u>	
SER	THR AL.A	THR	SER	GLY	GLY	ARG	PRO	ARG	CLN	PRO PRO	PRO	PRO	ARG	SER	P188:	L188		R189(R190(1190	L192		T192	Q193(P193		I193(R103(H194(P194(T194	E195		L196	S1970 E197	I197:	1ALT	1197	M198(C199(
1994	015 2015		2029		2055	2061	2062	2064	2065 2065	2066	2068		50.72	2075	2076	2078	2079		2086	2087	2088	2090		2094	2098		1112	2114	2115 2116	2117 2118	2119 2119	2120	2122	2123	2124	2125	2137	2138 2139	2140	2141 2142	2143 2144	
H	5M		A H		3	R			F	He	T W		1	3	<u>日</u>					3	R			R	R	, L	-	E F		50 F		S C		N.	8		^D		5M		E W	
D2145	02149	D2150	K2151	12167	S2168 F2169	R2170	02 FUT	L2177		K2183 R2184	M2185		M2189	E2192		TYR	PHE	LYS	GLN	THR	ILE	GLU	LEU	PHE ASP	MET	PRO 1 EU	GLU	GLU	SER	SER	SER	VAL	SER	ALA	CI II	GLU	GLU GLU	GLU	THR	ALA	SER LYS	
GLN	THR	ILE	CLU	GLN	ALA	CYS	ARG	GLU	ASP	GLU GLU	ASP	ILE	ARG ALA	ALA	THR	GLN	LYS	ALA	GLN	VAL	ALA	TEU	ALA	GLU PHF.	ASN	GLU	ASP	GLY	PRO	ALA	GLU	GL Y	GLU	ALA	GLY	PRO	GL Y AL A	GLU	ASP	GLU	MET SER	
ARG	ALA	GLN	GLU	ALA	ALA	VAL	GLU	LEU	THR	PRO TLE	GLU	ARG	T YR ALA	MET	LYS	LEU	GLU	ALA	LEU	GLU	GLU	SER	ARG	GLU	LEU	LYS	ALA	GLU	GLN	VAL	ALA	ALA	LYS	ASP	LEU	GLN	ALA LVS	GLU	GLU	PHE	ARG LEU	
PRO	GLN	GLU	GLU	GLY	PRO	ALA	GLY	GLU	SER	SER	GLY	THR	GLY	GLY	THR	ARG	ARG	SER	LYS	ALA	LYS	PRO	GLU	ARG PRO	GLY	THR	VAL	SER	ARG	LEU	GLY	ALA	ALA	GLU	THR GI N	GLY	ALA	SIH	THR	VAL	ILE SER	
ALA	HIS	THR	ARG	THR	THR	PRO	PRO	CYS	SER	PRO ALA	ALG	GLU	ARG VAL	PRO	ARG	ALA	PRO	ARG	ARG	PRO	THR	ALA	SER	ALA PRO	ALA	ALA	PRO	ALA	VAL	PRO	PRO	VAL	ALA	PRO	VAL	ILE	SER ALA	PRO	ASN	ILE	THR ILE	
LEU	PRO VAL.	HIS	TLEU	PRO	SER	PRO	PRO	SER	GLN	TLE	PRO	CYS	SER	PRO	ALA	THR	PRO	PRO	ALA	CYS	THR	PRO	PRO	ALA HTS	THR	PRO PPO	PRO	ALA	THR	CYS	VAL	THR	SER	SER	PRO I FII	LEU	LEU GLY	PRO	PR0	VAL	PR0 ILE	
SER	ALA SFR	VAL	ASN	LEU	PRO L'EII	GLY	LEU	PRO	GLU	ALA	LEU	CYS	GLN	ALA	LEU	ALA SER	PRO	GLU	LEU	GLU	LEU	SER	VAL	ALA SFR	SER	GLU	SER	SER 1 EII	SER	LEU	PRO	PRO 1 VC	ASP	LEU	LEU PRO	VAL	ALA VAL	GLU	ILE	PRO	VAL SER	
GLU	LYS	LEU	LEU	THR	PRO SFR	ALA	PRO GED	LEU	THR	LEU GLII	ALA	GLY	SER	PRO	ASN	GLN	GLU	GLN	GLU	PRO	ASP	ALA	GLU	GLY THR	THR	LEU	VAL	LEU	GLU	GLY	GLU	LEU	LEU	CYS	VAL	GLU	SER	GLY	LEU	LEU	PRO PRO	
SER	AL.A AL.A	SER	ASP GLU	PRO	LEU GI N	GLU	PRO TEU	GLU	ALA	ASP ARG	THR	SER	GLU	LEU	THR	GLU ALA	LYS	THR	THR	SER	SER	GLU	LYS	PRO GLN	GLU	LEU	THR	ALA	VAL	ALA	PRO	SER	SER	SER	SER AT A	THR	SER	PRO	GLU GLU	PRO	SER PRO	
VLA	LRG PRD	RO	LRG LRG	IRG	THR	NLA NLA	ISP	aru aru	LE	urg 1.Y	ILN	iLY	TLY	IRG	2R.O	ILN 1	RO	PR.O	RO	YS	/AL EII	LEO LRG	'YS	LEU PRO	TY	LRG ETI	AL	THR	AL	ILU ILU	YS	EU EII	AL	ur.c	LRG LRG	IRG	SLN ST N	IRG	TTA TTA	NLA NLA	SER THR	
EU	AL AL	EV :	ER I	TO T	E o	TA I	ER		ER	ER 1	AL	RG		ER /	LY F		EH	ER P		LE			YS I		TA	RO FP		ER 1		HH		LIN		HE E	LE TA	RG P	RG 0	EE	9	LY EV	AL HR	
Y	V V		U SI	N G	τ v λ	Y Al	A S.		A Si	ні н		ID A	L A M	S	0	10	Y Si	5.0		S II	55	D D	R C	A G	P	A P.	10 10	N N	1 E	E C	L L L	55 61		U D	I I	S AI	R A N H	T J	A G	10	10 >F	
GL	GL GL	SE	HA CT	AS	A GL	10 GL	AL		AL	HL HL	PR	PR	VA VA	I LY	AR AR	r AR	15 CT	AR AR	P.R.	5 LY	LY AG	I AR) SE	J PR	t AS	D AL	I AR	GL	AS	19 CI	T PR	SE		LE	E L	I EY	TH TH	GL	AL AL	PR	t VA	
GL	PRC	HE	E	VAL	ALA	PRC	VAL	GLU	PRC	GLI	H	PRC	PRC	GLN	PRC	A TO	PRC	GLD	VAL	HIS	AR(ASN	PRC	LEU	SEF	PRU	GLU	LYS	ARC	ARC	ARC	PRC	LYS	ALA	ARC	LEU	PR(PRC	GL	EB	SEF	









• Molecule 8: Zinc finger HIT domain-containing protein 1











• Molecule 16: DNA (147-MER)

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	555303	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 $(e^-/\text{\AA}^2)$	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 $(6k \times 4k)$	Depositor
Maximum map value	0.222	Depositor
Minimum map value	-0.080	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.026	Depositor
Map size (Å)	533.6, 533.6, 533.6	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.334, 1.334, 1.334	Depositor

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: ATP, ADP

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	ond lengths	E	Bond angles
	Ullalli	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.23	0/910	0.39	0/1225
1	Е	0.24	0/818	0.38	0/1104
2	В	0.29	0/766	0.41	0/1026
2	F	0.24	0/747	0.37	0/1004
3	С	0.24	0/789	0.39	0/1057
3	G	0.23	0/813	0.39	0/1090
4	D	0.24	0/653	0.41	0/873
4	Н	0.24	0/645	0.42	0/862
5	Ι	0.25	0/7202	0.41	0/9725
6	J	0.29	0/1140	0.42	0/1539
7	Κ	0.24	0/3283	0.42	0/4445
8	L	0.24	0/841	0.41	0/1141
9	М	0.24	0/3335	0.43	0/4495
9	0	0.24	0/3382	0.41	0/4559
9	Q	0.24	0/3413	0.42	0/4603
10	Ν	0.24	0/3257	0.41	0/4381
10	Р	0.24	0/3324	0.43	0/4477
10	R	0.24	0/3329	0.42	0/4479
11	S	0.24	0/2988	0.39	0/4045
11	U	0.25	0/2863	0.43	0/3882
12	Т	0.24	0/3217	0.40	0/4362
13	V	0.24	0/1801	0.39	0/2419
14	W	0.26	0/1578	0.44	0/2128
15	Х	0.96	8/3408~(0.2%)	1.38	$6\overline{2}/5263~(1.2\%)$
16	Y	0.81	$6/\overline{3349}~(0.2\%)$	1.35	42/5162~(0.8%)
All	All	0.38	14/57851~(0.0%)	0.63	$104\overline{/79346}\ (0.1\%)$

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
5	Ι	0	2
6	J	0	2
9	М	0	1
9	Q	0	1
11	U	0	1
All	All	0	7

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	Х	21	DC	C3'-C2'	27.13	1.84	1.52
15	Х	60	DA	O3'-P	-14.98	1.43	1.61
15	Х	130	DG	C1'-N9	-8.87	1.34	1.47
16	Y	-45	DG	C1'-N9	-7.60	1.36	1.47
16	Y	-71	DG	C1'-N9	-7.59	1.36	1.47
15	Х	69	DG	C1'-N9	-7.37	1.36	1.47
16	Y	-122	DG	C1'-N9	-7.34	1.36	1.47
16	Y	-103	DG	C1'-N9	-6.72	1.37	1.47
16	Y	-34	DA	C1'-N9	-6.45	1.38	1.47
15	Х	70	DA	C1'-N9	-6.24	1.38	1.47
15	Х	132	DA	C1'-N9	-6.13	1.38	1.47
16	Y	-78	DA	C1'-N9	-6.12	1.38	1.47
15	Х	35	DA	C1'-N9	-6.04	1.38	1.47
15	Х	43	DA	C1'-N9	-5.89	1.39	1.47

All (104) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
16	Y	-78	DA	O5'-P-OP2	-19.21	87.64	110.70
16	Y	-78	DA	O5'-P-OP1	18.91	133.39	110.70
15	Х	21	DC	C3'-C2'-C1'	-11.27	88.98	102.50
15	Х	141	DC	P-O3'-C3'	-10.40	107.22	119.70
16	Y	-110	DG	P-O3'-C3'	-10.24	107.41	119.70
15	Х	138	DA	P-O3'-C3'	-10.13	107.54	119.70
15	Х	115	DA	P-O3'-C3'	-9.45	108.36	119.70
15	Х	143	DC	P-O3'-C3'	-9.44	108.37	119.70
15	Х	40	DG	P-O3'-C3'	-9.38	108.44	119.70
15	Х	49	DT	P-O3'-C3'	-9.36	108.47	119.70
15	Х	111	DG	P-O3'-C3'	-9.31	108.53	119.70
15	Х	122	DC	P-O3'-C3'	-9.30	108.55	119.70
15	Х	107	DC	P-O3'-C3'	-9.27	108.57	119.70
15	Х	140	DT	P-O3'-C3'	-9.26	108.58	119.70
15	Х	78	DT	P-O3'-C3'	-9.25	108.60	119.70

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
16	Y	-145	DT	P-O3'-C3'	-9.23	108.62	119.70
15	Х	110	DC	P-O3'-C3'	-8.93	108.99	119.70
16	Y	-141	DG	P-O3'-C3'	-8.89	109.04	119.70
15	Х	94	DG	P-O3'-C3'	-8.86	109.06	119.70
15	Х	83	DG	P-O3'-C3'	-8.77	109.18	119.70
15	Х	125	DC	P-O3'-C3'	-8.72	109.24	119.70
15	Х	48	DC	P-O3'-C3'	-8.71	109.25	119.70
15	Х	93	DG	P-O3'-C3'	-8.65	109.32	119.70
16	Y	-30	DT	P-O3'-C3'	-8.63	109.34	119.70
15	Х	136	DG	P-O3'-C3'	-8.59	109.40	119.70
15	Х	77	DG	P-O3'-C3'	-8.58	109.41	119.70
15	Х	144	DC	P-O3'-C3'	-8.53	109.46	119.70
16	Y	-132	DT	P-O3'-C3'	-8.52	109.47	119.70
16	Y	-31	DC	P-O3'-C3'	-8.49	109.52	119.70
15	Х	98	DT	P-O3'-C3'	-8.45	109.56	119.70
16	Y	-94	DC	P-O3'-C3'	-8.38	109.65	119.70
15	Х	101	DA	P-O3'-C3'	-8.33	109.71	119.70
15	Х	118	DT	P-O3'-C3'	-8.29	109.75	119.70
15	Х	21	DC	C4'-C3'-C2'	-8.13	95.78	103.10
15	Х	103	DC	P-O3'-C3'	-8.10	109.98	119.70
16	Y	-37	DC	P-O3'-C3'	-8.09	110.00	119.70
15	Х	135	DG	P-O3'-C3'	-8.03	110.07	119.70
16	Y	-89	DT	P-O3'-C3'	-8.02	110.07	119.70
16	Y	-140	DA	P-O3'-C3'	-8.00	110.10	119.70
16	Y	-146	DC	P-O3'-C3'	-7.99	110.12	119.70
15	Х	145	DA	P-O3'-C3'	-7.97	110.13	119.70
16	Y	-81	DC	P-O3'-C3'	-7.96	110.15	119.70
16	Y	-58	DT	P-O3'-C3'	-7.89	110.23	119.70
16	Y	-105	DC	P-O3'-C3'	-7.88	110.24	119.70
15	Х	117	DT	P-O3'-C3'	-7.85	110.28	119.70
15	Х	124	DG	P-O3'-C3'	-7.77	110.38	119.70
16	Y	-138	DT	P-O3'-C3'	-7.72	110.43	119.70
15	Х	114	DC	P-O3'-C3'	-7.50	110.70	119.70
15	Х	84	DC	P-O3'-C3'	-7.42	110.80	119.70
16	Y	-119	DC	P-O3'-C3'	-7.29	110.95	119.70
16	Y	-142	DA	P-O3'-C3'	-7.20	111.06	119.70
15	Х	119	DG	P-O3'-C3'	-7.17	111.10	119.70
15	Х	47	DC	P-O3'-C3'	-7.08	111.20	119.70
15	Х	67	DG	P-O3'-C3'	-7.00	111.30	119.70
15	X	137	DG	P-O3'-C3'	-6.99	111.31	119.70
16	Y	-117	DA	P-O3'-C3'	-6.84	111.49	119.70
16	Y	-64	DG	P-O3'-C3'	-6.78	111.56	119.70

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
15	Х	128	DC	P-O3'-C3'	-6.78	111.57	119.70
15	Х	105	DG	P-O3'-C3'	-6.73	111.62	119.70
15	Х	109	DA	P-O3'-C3'	-6.72	111.63	119.70
15	Х	63	DG	P-O3'-C3'	-6.63	111.74	119.70
15	Х	38	DG	P-O3'-C3'	-6.48	111.92	119.70
16	Y	-77	DC	P-O3'-C3'	6.48	127.47	119.70
16	Y	-52	DC	P-O3'-C3'	6.46	127.45	119.70
15	Х	37	DG	P-O3'-C3'	-6.43	111.98	119.70
16	Y	-136	DC	P-O3'-C3'	-6.40	112.02	119.70
15	Х	69	DG	O5'-P-OP2	-6.39	99.94	105.70
15	Х	66	DG	P-O3'-C3'	-6.34	112.09	119.70
16	Y	-100	DC	P-O3'-C3'	-6.30	112.14	119.70
15	Х	74	DC	P-O3'-C3'	-6.27	112.17	119.70
15	Х	58	DA	P-O3'-C3'	-6.21	112.25	119.70
15	Х	50	DT	P-O3'-C3'	-6.06	112.43	119.70
16	Y	-93	DC	P-O3'-C3'	-6.03	112.46	119.70
16	Y	-101	DT	P-O3'-C3'	-6.01	112.49	119.70
15	Х	100	DG	P-O3'-C3'	-6.00	112.50	119.70
15	Х	99	DA	P-O3'-C3'	-6.00	112.50	119.70
15	Х	96	DG	P-O3'-C3'	-5.99	112.51	119.70
16	Y	-84	DG	P-O3'-C3'	-5.94	112.58	119.70
16	Y	-106	DA	P-O3'-C3'	-5.92	112.59	119.70
15	Х	102	DG	P-O3'-C3'	-5.91	112.61	119.70
16	Y	-125	DG	P-O3'-C3'	-5.90	112.62	119.70
16	Y	-42	DT	P-O3'-C3'	-5.88	112.64	119.70
15	Х	79	DA	P-O3'-C3'	-5.86	112.67	119.70
16	Y	-43	DT	P-O3'-C3'	-5.83	112.71	119.70
15	Х	87	DT	P-O3'-C3'	-5.78	112.76	119.70
16	Y	-130	DC	O5'-P-OP1	5.78	117.64	110.70
16	Y	-95	DA	P-O3'-C3'	-5.77	112.78	119.70
15	Х	64	DC	P-O3'-C3'	-5.74	112.81	119.70
16	Y	-87	DA	P-O3'-C3'	-5.72	112.84	119.70
16	Y	-97	DG	P-O3'-C3'	-5.69	112.87	119.70
15	Х	62	DC	P-O3'-C3'	-5.67	112.90	119.70
15	Х	21	DC	P-O3'-C3'	-5.64	112.93	119.70
16	Y	-109	DT	P-O3'-C3'	-5.57	113.02	119.70
16	Y	-112	DT	P-O3'-C3'	-5.53	113.07	119.70
16	Y	-135	DC	P-O3'-C3'	-5.51	113.09	119.70
16	Y	-118	DA	P-O3'-C3'	-5.49	113.11	119.70
15	Х	46	DC	P-O3'-C3'	-5.38	113.24	119.70
15	Х	56	DT	P-O3'-C3'	-5.37	113.26	119.70
15	Х	29	DG	P-O3'-C3'	-5.30	113.34	119.70

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
15	Х	95	DT	P-O3'-C3'	-5.29	113.35	119.70
16	Y	-65	DC	P-O3'-C3'	-5.25	113.40	119.70
15	Х	120	DA	P-O3'-C3'	-5.17	113.49	119.70
16	Y	-128	DG	P-O3'-C3'	-5.15	113.52	119.70
15	Х	100	DG	OP1-P-O3'	5.00	116.20	105.20

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	Ι	2029	ARG	Sidechain
5	Ι	860	ARG	Sidechain
6	J	260	ARG	Sidechain
6	J	263	ARG	Sidechain
9	М	263	LEU	Peptide
9	Q	278	GLU	Peptide
11	U	257	CYS	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	898	0	958	35	0
1	Е	808	0	863	22	0
2	В	755	0	782	39	0
2	F	736	0	755	15	0
3	С	779	0	816	63	0
3	G	801	0	839	20	0
4	D	646	0	686	31	0
4	Н	638	0	676	3	0
5	Ι	7031	0	7121	218	0
6	J	1114	0	1136	27	0
7	Κ	3209	0	3132	66	0
8	L	823	0	793	11	0
9	М	3293	0	3397	65	0
9	0	3339	0	3425	41	0
9	Q	3368	0	3453	82	0

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	N	3223	0	3309	41	0
10	Р	3287	0	3335	61	0
10	R	3293	0	3373	58	0
11	S	2925	0	2891	17	0
11	U	2802	0	2760	51	0
12	Т	3146	0	3086	35	0
13	V	1757	0	1736	43	0
14	W	1542	0	1553	53	0
15	Х	3034	0	1648	227	0
16	Y	2990	0	1651	207	0
17	Ι	27	0	12	0	0
17	М	27	0	12	1	0
17	Ν	27	0	12	0	0
17	0	27	0	12	2	0
17	Р	27	0	12	2	0
17	Q	27	0	12	0	0
17	R	27	0	12	2	0
18	Κ	31	0	12	1	0
18	Т	31	0	12	0	0
18	U	31	0	12	1	0
All	All	56519	0	54294	1168	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 11.

All (1168) 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:I:898:ARG:CZ	5:I:2140:TRP:CH2	1.82	1.59
3:C:43:PRO:HG2	16:Y:-78:DA:C4'	1.33	1.54
15:X:21:DC:N4	16:Y:-21:DG:N1	1.63	1.47
15:X:21:DC:C2'	15:X:21:DC:C3'	1.84	1.43
3:C:42:ARG:HH22	15:X:81:DG:C1'	1.33	1.39
15:X:6:DT:N3	16:Y:-6:DA:N1	1.69	1.39
3:C:42:ARG:NH2	15:X:81:DG:C1'	1.84	1.39
3:C:42:ARG:NH2	15:X:81:DG:H1'	1.36	1.36
1:E:14:ALA:N	16:Y:-115:DT:OP1	1.58	1.34
3:C:43:PRO:CG	16:Y:-78:DA:H4'	1.57	1.33
3:C:42:ARG:HD3	3:C:43:PRO:CD	1.59	1.32
5:I:898:ARG:HD2	5:I:2140:TRP:CZ2	1.68	1.28
14:W:38:ARG:CZ	16:Y:-83:DC:OP1	1.82	1.26

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
15:X:21:DC:N4	16:Y:-21:DG:C6	2.01	1.26
1:A:42:ARG:NH2	16:Y:-34:DA:H4'	1.49	1.25
5:I:891:ILE:CD1	16:Y:-49:DA:N3	2.01	1.23
15:X:5:DA:N1	16:Y:-5:DT:N3	1.86	1.22
3:C:42:ARG:CD	3:C:43:PRO:HD3	1.69	1.21
5:I:891:ILE:HD11	16:Y:-49:DA:N3	1.52	1.21
5:I:898:ARG:NH1	5:I:2140:TRP:CH2	2.08	1.21
3:C:42:ARG:HD3	3:C:43:PRO:HD3	1.19	1.19
1:E:14:ALA:N	16:Y:-115:DT:H5"	1.55	1.18
5:I:898:ARG:CD	5:I:2140:TRP:HZ2	1.57	1.18
5:I:99:GLN:CB	14:W:201:LEU:CD2	2.20	1.17
1:A:42:ARG:NH2	16:Y:-34:DA:C4'	2.06	1.17
4:D:45:ARG:HE	15:X:80:DC:C4'	1.56	1.17
3:C:43:PRO:CG	16:Y:-78:DA:C4'	2.18	1.16
3:C:42:ARG:HB3	3:C:43:PRO:HD2	1.17	1.15
5:I:779:GLN:HB3	5:I:2142:PRO:HG2	1.19	1.14
5:I:891:ILE:HD11	16:Y:-49:DA:C4	1.83	1.13
5:I:99:GLN:HB3	14:W:201:LEU:HD23	1.18	1.12
5:I:92:SER:O	14:W:193:GLU:OE2	1.67	1.12
4:D:45:ARG:NE	15:X:80:DC:H4'	1.28	1.11
1:E:77:ARG:NH1	16:Y:-127:DA:H5"	1.65	1.11
5:I:99:GLN:HB2	14:W:201:LEU:HD21	1.23	1.09
1:A:42:ARG:CZ	16:Y:-34:DA:H4'	1.83	1.09
3:C:42:ARG:CB	3:C:43:PRO:HD2	1.84	1.07
5:I:898:ARG:CD	5:I:2140:TRP:CZ2	2.33	1.07
3:C:42:ARG:CD	3:C:43:PRO:CD	2.26	1.07
4:D:79:LYS:HB2	15:X:101:DA:OP1	1.55	1.06
1:E:43:VAL:O	15:X:111:DG:H5'	1.54	1.04
4:D:79:LYS:N	15:X:101:DA:OP2	1.90	1.04
5:I:99:GLN:CB	14:W:201:LEU:HD23	1.87	1.03
3:C:42:ARG:HG3	16:Y:-79:DT:C4'	1.89	1.03
1:E:14:ALA:N	16:Y:-115:DT:C5'	2.20	1.03
5:I:99:GLN:HB2	14:W:201:LEU:CD2	1.82	1.03
5:I:702:GLN:OE1	15:X:58:DA:H5"	1.56	1.02
5:I:898:ARG:HD2	5:I:2140:TRP:HZ2	1.00	1.02
5:I:898:ARG:NE	5:I:2140:TRP:CH2	2.25	1.02
14:W:38:ARG:NE	16:Y:-83:DC:OP1	1.91	1.02
3:C:42:ARG:HG3	16:Y:-79:DT:O4'	1.60	1.01
3:C:42:ARG:NE	3:C:43:PRO:HD3	1.75	0.99
13:V:262:GLU:OE2	14:W:202:LYS:HD3	1.62	0.99
14:W:39:GLU:CB	16:Y:-82:DA:H5"	1.92	0.99

Atom-1	Atom-2	Interatomic	Clash
	1100111 =	distance (Å)	overlap (Å)
3:C:42:ARG:HD3	3:C:43:PRO:HD2	1.45	0.99
15:X:21:DC:C4	16:Y:-21:DG:N1	2.30	0.99
4:D:45:ARG:NE	15:X:80:DC:C4'	2.18	0.98
6:J:261:CYS:HA	10:P:211:ARG:H	1.25	0.98
5:I:891:ILE:HD13	16:Y:-49:DA:N3	1.79	0.97
5:I:898:ARG:CZ	5:I:2140:TRP:HH2	1.41	0.96
15:X:21:DC:N4	16:Y:-21:DG:O6	1.97	0.95
3:C:63:ARG:HD2	15:X:90:DA:H4'	1.48	0.95
5:I:898:ARG:CZ	5:I:2140:TRP:CZ2	2.49	0.95
15:X:21:DC:N3	16:Y:-21:DG:N2	2.13	0.95
3:C:42:ARG:CZ	3:C:43:PRO:HD3	1.96	0.95
5:I:99:GLN:HB3	14:W:201:LEU:CD2	1.88	0.94
5:I:2141:ASN:OD1	5:I:2142:PRO:HD2	1.67	0.94
7:K:138:ASP:OD1	7:K:139:ASN:ND2	1.99	0.94
16:Y:-54:DC:H6	16:Y:-54:DC:H5"	1.33	0.94
3:C:42:ARG:HB3	3:C:43:PRO:CD	1.95	0.93
11:S:324:THR:HG23	15:X:117:DT:P	2.08	0.93
5:I:896:GLN:HA	5:I:899:LYS:HE3	1.50	0.93
15:X:28:DG:H5'	15:X:28:DG:C8	2.03	0.93
1:A:26:PRO:HD3	2:B:37:TYR:CD2	2.03	0.93
5:I:726:LYS:HG2	15:X:56:DT:H4'	1.47	0.92
5:I:891:ILE:CD1	16:Y:-49:DA:C2	2.52	0.92
5:I:705:ARG:NH2	15:X:58:DA:OP1	2.03	0.91
5:I:895:MET:HE1	15:X:51:DG:N3	1.85	0.91
5:I:779:GLN:O	5:I:2142:PRO:HD2	1.70	0.91
15:X:70:DA:H61	16:Y:-70:DT:H3	1.17	0.91
5:I:896:GLN:HA	5:I:899:LYS:CE	2.00	0.91
9:O:106:ILE:HD11	9:O:269:THR:HG23	1.50	0.91
15:X:28:DG:H5'	15:X:28:DG:H8	1.36	0.91
15:X:6:DT:O2	16:Y:-6:DA:H2	1.54	0.90
5:I:891:ILE:HD13	16:Y:-49:DA:C2	2.06	0.90
2:B:28:ARG:NH1	16:Y:-21:DG:OP1	2.04	0.90
5:I:898:ARG:NH1	5:I:2140:TRP:CZ2	2.40	0.88
5:I:726:LYS:HG2	15:X:56:DT:C4'	2.04	0.88
6:J:269:SER:OG	9:Q:150:TYR:CD1	2.26	0.88
5:I:712:TRP:CZ2	15:X:135:DG:OP1	2.27	0.88
4:D:78:ARG:HG2	15:X:101:DA:H5'	1.55	0.87
5:I:898:ARG:NH2	5:I:2140:TRP:CH2	2.42	0.87
9:M:96:MET:SD	9:M:115:ASN:ND2	2.48	0.87
1:A:42:ARG:HH22	16:Y:-34:DA:C4'	1.87	0.87
15:X:5:DA:N6	16:Y:-5:DT:O4	2.08	0.86

Atom-1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
4:D:79:LYS:H	15:X:101:DA:P	1.98	0.86
3:C:69:ARG:NH2	15:X:90:DA:OP2	2.08	0.85
4:D:45:ARG:HG3	15:X:81:DG:OP1	1.77	0.85
5:I:898:ARG:NE	5:I:2140:TRP:CZ2	2.42	0.85
13:V:262:GLU:OE2	14:W:202:LYS:CD	2.23	0.85
5:I:895:MET:HG2	15:X:51:DG:O4'	1.76	0.85
15:X:6:DT:O4	16:Y:-6:DA:N6	2.08	0.84
2:B:92:GLN:HE22	13:V:64:ASP:HB2	1.41	0.84
3:C:42:ARG:CD	3:C:43:PRO:HD2	2.02	0.84
5:I:92:SER:OG	14:W:193:GLU:HG2	1.78	0.84
1:A:42:ARG:NH2	16:Y:-34:DA:O4'	2.11	0.84
3:C:42:ARG:HH21	15:X:81:DG:H1'	1.03	0.83
10:R:313:ASN:O	10:R:353:ARG:NH1	2.11	0.83
5:I:895:MET:CE	15:X:51:DG:N3	2.41	0.83
10:N:19:ILE:HD11	9:O:283:VAL:HG11	1.60	0.83
1:A:42:ARG:HB2	16:Y:-33:DG:OP1	1.79	0.83
2:B:30:ARG:HA	16:Y:-22:DC:OP1	1.78	0.83
10:N:435:ASP:OD2	10:N:438:ARG:NH1	2.13	0.82
15:X:41:DT:H2"	15:X:42:DA:H5'	1.60	0.82
5:I:2167:ILE:HD11	5:I:2177:LEU:HG	1.62	0.82
6:J:269:SER:HA	9:Q:150:TYR:HB3	1.62	0.82
5:I:750:ASN:HD21	5:I:758:ARG:NE	1.77	0.81
5:I:779:GLN:HB3	5:I:2142:PRO:CG	2.05	0.81
3:C:43:PRO:HG2	16:Y:-78:DA:C5'	2.09	0.81
15:X:46:DC:H4'	15:X:46:DC:OP1	1.77	0.81
5:I:702:GLN:OE1	15:X:58:DA:C5'	2.28	0.81
16:Y:-130:DC:OP2	16:Y:-130:DC:H6	1.62	0.81
15:X:43:DA:H2"	15:X:44:DT:H5"	1.63	0.81
5:I:779:GLN:CB	5:I:2142:PRO:HG2	2.07	0.80
14:W:39:GLU:HB3	16:Y:-82:DA:H5"	1.61	0.80
15:X:44:DT:H2"	15:X:45:DC:H5"	1.63	0.80
3:C:42:ARG:HG3	16:Y:-79:DT:H4'	1.64	0.80
4:D:78:ARG:CG	15:X:101:DA:H5'	2.11	0.79
2:F:30:ARG:NH2	16:Y:-119:DC:H4'	1.97	0.79
1:A:29:ARG:NH2	2:B:37:TYR:HE2	1.79	0.79
5:I:899:LYS:NZ	5:I:907:PHE:CZ	2.50	0.79
6:J:310:TYR:OH	10:R:169:GLU:O	2.01	0.79
15:X:72:DA:C2	16:Y:-71:DG:C2	2.71	0.79
15:X:136:DG:H2'	15:X:137:DG:C8	2.17	0.79
3:C:42:ARG:CB	3:C:43:PRO:CD	2.54	0.78
5:I:898:ARG:NE	5:I:2140:TRP:HH2	1.71	0.78

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
15:X:20:DA:C2	15:X:21:DC:C5	2.71	0.78
16:Y:-131:DG:H2"	16:Y:-130:DC:C5	2.19	0.78
9:M:322:SER:OG	10:R:21:ARG:O	2.02	0.78
9:O:249:ARG:NH1	9:O:250:PRO:O	2.16	0.78
3:C:69:ARG:HH22	15:X:90:DA:P	2.07	0.78
15:X:6:DT:O2	16:Y:-6:DA:C2	2.37	0.78
16:Y:-76:DG:H1'	16:Y:-75:DC:H5'	1.66	0.77
4:D:79:LYS:CB	15:X:101:DA:OP1	2.31	0.77
1:E:77:ARG:HH11	16:Y:-127:DA:H5"	1.48	0.77
9:Q:336:CYS:HG	10:R:340:TYR:HH	1.31	0.77
2:B:92:GLN:HE22	13:V:64:ASP:CB	1.98	0.77
3:G:41:TYR:HD1	15:X:142:DT:O3'	1.68	0.77
5:I:750:ASN:HD21	5:I:758:ARG:HE	1.32	0.76
16:Y:-51:DC:H2"	16:Y:-50:DA:H5"	1.66	0.76
5:I:192:ARG:O	11:S:169:TYR:OH	2.03	0.76
15:X:6:DT:N3	16:Y:-6:DA:C2	2.46	0.76
7:K:214:GLN:NE2	7:K:331:ASP:OD2	2.19	0.76
7:K:172:ARG:NH1	8:L:101:TYR:O	2.18	0.76
10:P:194:THR:OG1	10:P:203:SER:OG	2.01	0.76
4:D:32:PRO:HG2	16:Y:-86:DA:H2'	1.68	0.76
9:M:210:ALA:O	9:M:211:THR:OG1	2.02	0.76
5:I:750:ASN:ND2	5:I:758:ARG:HE	1.82	0.76
6:J:269:SER:CA	9:Q:150:TYR:HB3	2.16	0.76
14:W:38:ARG:NH1	16:Y:-83:DC:OP1	2.19	0.76
13:V:55:ARG:NH2	15:X:39:DA:H5"	2.01	0.75
3:C:42:ARG:NH2	15:X:81:DG:N9	2.35	0.75
9:Q:254:GLN:O	9:Q:258:SER:OG	2.05	0.75
3:C:42:ARG:NH1	3:C:43:PRO:HD3	2.02	0.75
15:X:72:DA:C2	16:Y:-71:DG:N2	2.55	0.75
11:S:324:THR:HG23	15:X:117:DT:OP2	1.86	0.75
2:B:116:THR:HG22	13:V:57:VAL:CG1	2.17	0.74
2:F:31:LYS:HA	2:F:31:LYS:HZ2	1.50	0.74
7:K:115:GLU:OE2	7:K:117:TYR:OH	2.05	0.74
15:X:6:DT:C2	16:Y:-6:DA:C2	2.75	0.74
10:R:247:ILE:HG12	10:R:272:VAL:HG22	1.68	0.74
1:A:17:ARG:NE	15:X:29:DG:OP2	2.20	0.74
1:A:26:PRO:HG3	2:B:37:TYR:CE2	2.22	0.74
3:C:66:PRO:HG3	15:X:90:DA:H5"	1.69	0.74
5:I:898:ARG:NH2	5:I:2140:TRP:HH2	1.79	0.74
4:D:45:ARG:HE	15:X:80:DC:H4'	0.81	0.74
3:G:41:TYR:CE1	15:X:142:DT:H4'	2.23	0.74

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
6:J:269:SER:OG	9:Q:150:TYR:CG	2.39	0.74
5:I:933:THR:O	10:N:279:LYS:NZ	2.20	0.74
6:J:269:SER:O	9:Q:150:TYR:HB3	1.88	0.74
10:R:248:ASP:O	10:R:251:ASN:ND2	2.21	0.74
5:I:891:ILE:HG23	16:Y:-50:DA:C2	2.23	0.74
3:C:83:ARG:HD2	15:X:100:DG:H5"	1.70	0.74
5:I:712:TRP:HZ2	15:X:135:DG:OP1	1.69	0.74
11:S:324:THR:CG2	15:X:117:DT:P	2.74	0.74
5:I:842:LYS:NZ	5:I:849:MET:SD	2.60	0.73
3:C:59:GLU:OE1	3:C:59:GLU:N	2.22	0.73
15:X:129:DG:H1	16:Y:-129:DC:H42	1.36	0.73
16:Y:-85:DC:H2"	16:Y:-84:DG:C8	2.24	0.73
2:F:35:SER:HA	2:F:56:MET:SD	2.29	0.72
5:I:92:SER:C	14:W:193:GLU:OE2	2.27	0.72
10:P:249:VAL:HG11	10:P:259:ALA:HA	1.71	0.72
5:I:750:ASN:HD21	5:I:758:ARG:CZ	2.01	0.72
5:I:2169:GLU:OE1	5:I:2170:ARG:HG3	1.88	0.72
5:I:1993:CYS:SG	5:I:1994:HIS:N	2.62	0.72
8:L:129:VAL:HA	10:N:171:ILE:HD11	1.71	0.72
10:P:191:ASP:OD1	10:P:207:ARG:NH1	2.23	0.72
15:X:6:DT:C4	16:Y:-6:DA:N1	2.58	0.72
14:W:39:GLU:HB2	16:Y:-82:DA:H5"	1.71	0.72
1:A:26:PRO:HB3	2:B:37:TYR:CZ	2.25	0.72
12:T:334:GLY:O	12:T:341:ARG:NH2	2.23	0.72
16:Y:-107:DG:H1'	16:Y:-106:DA:C8	2.25	0.71
10:N:194:THR:OG1	10:N:203:SER:OG	2.08	0.71
12:T:70:ILE:HD13	12:T:105:HIS:CG	2.26	0.71
1:E:20:ARG:HG2	2:F:121:SER:OG	1.91	0.71
9:M:178:GLU:OE2	10:R:186:LYS:NZ	2.19	0.71
3:C:42:ARG:CG	3:C:43:PRO:HD2	2.19	0.71
12:T:70:ILE:HG22	12:T:70:ILE:O	1.91	0.71
9:O:366:TYR:OH	17:O:501:ADP:N7	2.24	0.71
5:I:842:LYS:NZ	5:I:846:GLU:OE2	2.13	0.71
5:I:750:ASN:HD21	5:I:758:ARG:NH2	1.88	0.70
15:X:35:DA:H2"	15:X:36:DG:H5'	1.72	0.70
7:K:380:GLU:OE1	7:K:380:GLU:N	2.24	0.70
9:O:96:MET:SD	9:O:115:ASN:ND2	2.64	0.70
6:J:269:SER:HA	9:Q:150:TYR:CB	2.22	0.70
6:J:302:ARG:NH1	6:J:307:ASP:OD1	2.24	0.70
10:P:262:SER:OG	9:Q:248:ALA:HB1	1.91	0.70
5:I:784:GLU:N	5:I:784:GLU:OE1	2.24	0.70

	A 4 D	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
16:Y:-54:DC:H6	16:Y:-54:DC:C5'	2.05	0.70
1:A:26:PRO:HB3	2:B:37:TYR:OH	1.91	0.70
1:E:14:ALA:N	16:Y:-115:DT:P	2.64	0.70
9:Q:268:LYS:O	9:Q:269:THR:HG22	1.92	0.70
12:T:69:TYR:OH	12:T:80:GLU:OE2	2.09	0.70
5:I:2167:ILE:CD1	5:I:2177:LEU:HG	2.21	0.70
5:I:899:LYS:NZ	5:I:907:PHE:CE2	2.60	0.69
9:Q:269:THR:HG23	9:Q:269:THR:O	1.91	0.69
1:A:26:PRO:HD3	2:B:37:TYR:CE2	2.26	0.69
3:C:66:PRO:CG	15:X:90:DA:H5"	2.22	0.69
5:I:195:ALA:HB3	11:S:169:TYR:CE1	2.27	0.69
9:Q:362:ARG:NH1	9:Q:364:MET:SD	2.66	0.69
12:T:173:GLY:O	12:T:354:ASN:ND2	2.24	0.69
9:Q:106:ILE:HD12	9:Q:268:LYS:HB2	1.74	0.69
4:H:68:ASP:OD2	4:H:93:GLN:NE2	2.25	0.69
5:I:201:ASP:OD1	11:S:351:THR:OG1	2.11	0.69
7:K:322:GLY:O	7:K:325:LEU:HD22	1.92	0.69
11:U:111:ASN:ND2	11:U:115:ASN:OD1	2.25	0.69
9:O:404:ARG:NH1	17:O:501:ADP:O2A	2.26	0.69
15:X:111:DG:H2'	15:X:112:DA:C8	2.28	0.69
5:I:750:ASN:ND2	5:I:758:ARG:HH21	1.90	0.68
5:I:892:ASN:HD21	15:X:50:DT:H4'	1.58	0.68
5:I:2119:ARG:O	15:X:54:DG:H4'	1.93	0.68
16:Y:-50:DA:H5"	16:Y:-50:DA:C8	2.28	0.68
2:B:87:THR:OG1	2:B:90:GLU:OE1	2.10	0.68
12:T:81:ASN:ND2	12:T:245:GLN:O	2.26	0.68
16:Y:-82:DA:H1'	16:Y:-81:DC:H5'	1.75	0.68
3:G:41:TYR:CD1	15:X:142:DT:O3'	2.45	0.68
15:X:20:DA:C2	15:X:21:DC:C6	2.81	0.68
10:P:55:ALA:O	10:P:59:VAL:HG13	1.93	0.68
3:C:42:ARG:NH2	15:X:81:DG:O4'	2.13	0.68
5:I:726:LYS:HB3	15:X:57:DT:H5'	1.74	0.68
10:N:161:LEU:O	10:N:172:TYR:N	2.27	0.68
4:D:78:ARG:HG2	15:X:101:DA:C5'	2.23	0.68
10:P:253:ARG:NH2	10:P:264:ASP:OD2	2.27	0.68
2:B:90:GLU:OE1	2:B:90:GLU:N	2.27	0.67
7:K:30:PHE:HB3	7:K:54:LEU:HD22	1.76	0.67
11:U:107:GLU:OE1	11:U:108:ALA:N	2.27	0.67
15:X:20:DA:H1'	15:X:21:DC:H5'	1.75	0.67
10:R:139:GLU:OE1	10:R:204:LYS:NZ	2.28	0.67
5:I:2067:GLN:HG2	5:I:2137:ASP:HB3	1.75	0.67

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
9:Q:96:MET:SD	9:Q:115:ASN:ND2	2.68	0.67
16:Y:-139:DA:H2"	16:Y:-138:DT:H5"	1.76	0.67
4:D:45:ARG:HE	15:X:80:DC:C3'	2.08	0.67
2:F:31:LYS:HA	2:F:31:LYS:CE	2.25	0.67
5:I:705:ARG:HD3	5:I:727:LEU:HD21	1.75	0.67
9:O:42:GLN:NE2	9:O:364:MET:O	2.28	0.67
10:P:21:ARG:NH1	9:Q:61:MET:O	2.28	0.67
1:E:88:ARG:NH2	1:E:100:VAL:O	2.28	0.67
5:I:2121:GLY:N	15:X:55:DG:OP1	2.27	0.67
5:I:712:TRP:CE2	15:X:135:DG:OP1	2.48	0.66
11:U:11:ASP:OD1	11:U:137:GLN:NE2	2.27	0.66
3:G:41:TYR:HE1	15:X:142:DT:H4'	1.60	0.66
5:I:898:ARG:NH1	5:I:2140:TRP:CZ3	2.63	0.66
4:D:79:LYS:HB2	15:X:101:DA:P	2.35	0.66
5:I:705:ARG:HH21	15:X:58:DA:P	2.18	0.66
5:I:2140:TRP:HE3	5:I:2140:TRP:H	1.39	0.66
7:K:356:ILE:HD13	7:K:356:ILE:H	1.60	0.66
9:M:135:VAL:HG12	9:M:189:ASP:O	1.94	0.66
15:X:21:DC:N3	16:Y:-21:DG:C2	2.64	0.66
7:K:121:ALA:HB2	7:K:376:VAL:HG12	1.77	0.66
11:U:12:ASN:ND2	11:U:17:CYS:SG	2.68	0.66
13:V:265:SER:HB3	14:W:199:GLU:OE2	1.95	0.66
16:Y:-70:DT:H4'	16:Y:-69:DC:H5'	1.77	0.66
5:I:768:GLN:O	5:I:769:ARG:NH1	2.28	0.66
16:Y:-85:DC:H2"	16:Y:-84:DG:H8	1.60	0.66
10:P:260:LEU:O	10:P:262:SER:N	2.29	0.66
16:Y:-39:DT:H4'	16:Y:-39:DT:OP1	1.95	0.66
2:B:51:ILE:O	15:X:19:DC:OP1	2.14	0.65
2:B:116:THR:HG22	13:V:57:VAL:HG11	1.77	0.65
15:X:35:DA:C2	16:Y:-34:DA:C2	2.85	0.65
3:C:42:ARG:HB3	16:Y:-78:DA:H5"	1.77	0.65
1:E:77:ARG:CZ	16:Y:-127:DA:H4'	2.27	0.65
5:I:898:ARG:CZ	5:I:2140:TRP:CZ3	2.73	0.65
2:B:39:TYR:OH	15:X:19:DC:H3'	1.97	0.65
5:I:898:ARG:HH12	5:I:2067:GLN:HE22	1.43	0.65
15:X:73:DG:H1'	15:X:74:DC:H5'	1.77	0.65
1:E:77:ARG:NH1	16:Y:-127:DA:C5'	2.53	0.65
15:X:5:DA:N1	16:Y:-5:DT:C4	2.64	0.65
3:C:42:ARG:NH2	15:X:81:DG:C4	2.64	0.65
5:I:1932:VAL:HG12	10:R:275:GLN:HG3	1.79	0.65
11:U:138:ALA:HB1	11:U:163:VAL:HG11	1.79	0.65

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
11:U:241:GLU:OE2	11:U:241:GLU:N	2.30	0.65
2:F:31:LYS:HZ2	2:F:31:LYS:CA	2.09	0.64
12:T:190:GLN:OE1	12:T:190:GLN:N	2.30	0.64
15:X:87:DT:H1'	15:X:88:DT:C6	2.32	0.64
9:M:428:GLU:N	9:M:428:GLU:OE1	2.30	0.64
3:C:43:PRO:CG	16:Y:-78:DA:O4'	2.45	0.64
10:N:134:GLU:O	10:N:235:ARG:NH1	2.30	0.64
14:W:81:VAL:HG11	14:W:86:TYR:HA	1.79	0.64
16:Y:-84:DG:H1'	16:Y:-83:DC:H5'	1.80	0.64
3:C:42:ARG:CG	16:Y:-79:DT:H4'	2.28	0.64
3:C:42:ARG:NE	3:C:43:PRO:CD	2.54	0.64
7:K:59:PRO:O	7:K:66:VAL:N	2.28	0.64
10:N:384:GLU:OE1	10:N:384:GLU:N	2.30	0.63
13:V:49:ARG:NH2	15:X:40:DG:OP1	2.31	0.63
9:M:270:GLU:N	9:M:270:GLU:OE1	2.31	0.63
2:B:37:TYR:O	2:B:41:VAL:HG23	1.98	0.63
5:I:898:ARG:NH1	5:I:2067:GLN:HE22	1.96	0.63
12:T:395:ILE:O	12:T:399:ILE:HG23	1.99	0.63
5:I:712:TRP:NE1	15:X:135:DG:OP1	2.31	0.63
15:X:97:DC:H5"	15:X:97:DC:H6	1.63	0.63
9:Q:279:ILE:HD12	9:Q:279:ILE:H	1.64	0.63
9:Q:339:ARG:HE	10:R:306:ILE:HD11	1.63	0.63
16:Y:-50:DA:H8	16:Y:-50:DA:C5'	2.12	0.62
1:A:29:ARG:HH21	2:B:37:TYR:HE2	1.47	0.62
2:F:31:LYS:HA	2:F:31:LYS:NZ	2.14	0.62
12:T:352:GLY:O	12:T:355:THR:OG1	2.16	0.62
15:X:18:DA:H61	16:Y:-18:DT:H3	1.46	0.62
3:C:69:ARG:NH2	15:X:90:DA:P	2.72	0.62
5:I:1953:GLU:N	9:Q:126:GLU:OE1	2.31	0.62
7:K:113:LEU:O	7:K:113:LEU:HD13	1.99	0.62
7:K:284:PRO:O	7:K:285:SER:OG	2.09	0.62
15:X:112:DA:H61	16:Y:-112:DT:H3	1.47	0.62
15:X:137:DG:H2"	15:X:138:DA:C8	2.34	0.62
16:Y:-83:DC:H1'	16:Y:-82:DA:H5'	1.82	0.62
14:W:38:ARG:CD	16:Y:-83:DC:OP1	2.46	0.62
1:A:25:PHE:CZ	1:A:59:THR:HG21	2.35	0.62
9:Q:450:GLN:OE1	9:Q:450:GLN:N	2.33	0.62
5:I:620:GLU:OE1	5:I:620:GLU:N	2.33	0.62
9:M:103:SER:OG	9:M:105:GLU:OE1	2.17	0.62
5:I:617:GLN:OE1	5:I:617:GLN:N	2.33	0.62
9:Q:129:GLU:OE2	9:Q:195:ALA:N	2.33	0.62

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
9:Q:419:ILE:HD13	10:R:37:LEU:HD13	1.82	0.62
1:A:24:GLN:O	2:B:37:TYR:CD1	2.53	0.61
9:Q:279:ILE:HA	9:Q:282:VAL:HG22	1.82	0.61
5:I:725:TYR:HB3	5:I:758:ARG:HD2	1.80	0.61
16:Y:-47:DG:H8	16:Y:-47:DG:OP2	1.82	0.61
5:I:629:LEU:HD13	5:I:630:VAL:N	2.15	0.61
5:I:750:ASN:CG	5:I:758:ARG:HH21	2.03	0.61
14:W:38:ARG:CZ	16:Y:-83:DC:P	2.88	0.61
15:X:21:DC:O2	15:X:22:DG:O4'	2.18	0.61
5:I:2141:ASN:OD1	5:I:2183:LYS:HD3	2.00	0.61
10:R:435:ASP:N	10:R:435:ASP:OD1	2.34	0.61
1:A:26:PRO:CG	2:B:37:TYR:CE2	2.84	0.61
16:Y:-58:DT:H2"	16:Y:-57:DA:C8	2.36	0.61
3:G:40:ARG:NH2	16:Y:-64:DG:O4'	2.34	0.61
9:M:260:MET:SD	9:M:260:MET:N	2.74	0.61
10:P:349:ASP:O	10:P:353:ARG:NH1	2.33	0.61
7:K:201:VAL:O	7:K:204:GLN:N	2.33	0.61
15:X:36:DG:H1'	15:X:37:DG:C8	2.36	0.61
5:I:2098:ARG:NH2	15:X:55:DG:OP2	2.33	0.61
9:Q:385:ASN:O	9:Q:424:SER:OG	2.10	0.61
15:X:98:DT:H3	16:Y:-98:DA:H61	1.48	0.61
10:R:34:ASP:OD1	10:R:40:ARG:NE	2.31	0.61
13:V:243:GLU:OE1	13:V:243:GLU:N	2.34	0.61
2:F:90:GLU:N	2:F:90:GLU:OE1	2.34	0.60
10:P:393:ILE:O	10:P:397:THR:OG1	2.08	0.60
15:X:60:DA:H1'	15:X:61:DA:H5'	1.83	0.60
16:Y:-50:DA:C8	16:Y:-50:DA:C5'	2.84	0.60
16:Y:-7:DC:H2"	16:Y:-6:DA:H5'	1.82	0.60
10:R:286:GLU:OE1	10:R:286:GLU:N	2.35	0.60
5:I:730:GLN:NE2	5:I:731:ASP:OD1	2.34	0.60
5:I:754:PHE:O	5:I:760:GLN:NE2	2.34	0.60
6:J:188:GLU:OE2	6:J:192:ARG:NH2	2.34	0.60
7:K:29:GLN:NE2	7:K:73:GLN:OE1	2.35	0.60
7:K:270:LEU:HD13	7:K:270:LEU:O	2.02	0.60
9:M:366:TYR:OH	17:M:501:ADP:N7	2.24	0.60
11:S:156:GLY:O	11:S:303:THR:OG1	2.18	0.60
13:V:262:GLU:CD	14:W:202:LYS:HG3	2.22	0.60
5:I:729:LEU:CD2	5:I:757:GLN:O	2.49	0.60
5:I:2141:ASN:OD1	5:I:2142:PRO:CD	2.46	0.60
9:M:357:ARG:O	10:R:404:GLN:NE2	2.34	0.60
10:P:404:GLN:NE2	9:Q:357:ARG:O	2.34	0.60

A + a 1	At any 0	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
3:C:43:PRO:HG2	16:Y:-78:DA:H4'	0.64	0.60
3:C:43:PRO:HG3	16:Y:-78:DA:O4'	2.01	0.60
5:I:92:SER:HG	14:W:193:GLU:HG2	1.64	0.60
5:I:726:LYS:CG	15:X:56:DT:H4'	2.26	0.60
9:O:66:VAL:O	9:O:329:PHE:N	2.34	0.60
14:W:39:GLU:HB2	16:Y:-83:DC:O3'	2.01	0.60
16:Y:-70:DT:C4'	16:Y:-69:DC:H5'	2.32	0.60
16:Y:-6:DA:H2"	16:Y:-5:DT:H71	1.84	0.60
7:K:200:HIS:O	7:K:202:ILE:N	2.35	0.59
15:X:20:DA:N3	15:X:21:DC:C6	2.69	0.59
9:Q:192:TYR:N	9:Q:201:LYS:O	2.35	0.59
5:I:122:LYS:O	13:V:225:ARG:NH2	2.35	0.59
9:O:371:MET:HG3	9:O:403:LEU:HD13	1.85	0.59
11:S:324:THR:CG2	15:X:116:DA:O3'	2.51	0.59
16:Y:-98:DA:H2"	16:Y:-97:DG:H8	1.67	0.59
5:I:709:ARG:NH1	15:X:135:DG:OP2	2.36	0.59
6:J:260:ARG:O	6:J:261:CYS:HB3	2.01	0.59
9:M:27:ASP:OD1	9:M:31:LEU:N	2.34	0.59
13:V:141:GLN:N	13:V:141:GLN:OE1	2.35	0.59
5:I:661:ALA:O	5:I:667:TRP:NE1	2.35	0.59
3:G:42:ARG:N	15:X:143:DC:OP1	2.32	0.59
5:I:96:ILE:HG12	14:W:201:LEU:HD11	1.84	0.59
10:P:381:GLU:N	10:P:381:GLU:OE1	2.35	0.59
9:M:182:LYS:O	9:M:184:ARG:NH1	2.36	0.59
15:X:84:DC:H2"	15:X:85:DG:C8	2.37	0.59
3:C:117:VAL:N	16:Y:-76:DG:OP1	2.33	0.59
9:Q:236:GLN:OE1	9:Q:237:ASP:N	2.35	0.59
10:R:136:GLU:N	10:R:136:GLU:OE1	2.35	0.59
15:X:16:DT:H1'	15:X:17:DG:H5'	1.82	0.59
15:X:140:DT:H3	16:Y:-140:DA:H61	1.51	0.59
16:Y:-146:DC:H2"	16:Y:-145:DT:H5"	1.85	0.59
15:X:70:DA:H1'	15:X:71:DC:H5"	1.85	0.58
5:I:168:MET:SD	11:U:351:THR:HG23	2.43	0.58
5:I:891:ILE:HD11	16:Y:-49:DA:C2	2.28	0.58
11:U:9:VAL:HG13	11:U:104:LEU:HD11	1.84	0.58
13:V:51:GLU:HB3	13:V:58:TYR:CZ	2.39	0.58
16:Y:-2:DT:H2"	16:Y:-1:DG:C8	2.38	0.58
6:J:170:GLU:N	6:J:170:GLU:OE1	2.34	0.58
7:K:56:TYR:OH	7:K:200:HIS:N	2.36	0.58
9:Q:271:ILE:HD13	9:Q:272:THR:H	1.69	0.58
10:R:306:ILE:HD13	10:R:338:THR:CG2	2.34	0.58

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
5:I:895:MET:HE3	15:X:51:DG:N3	2.18	0.58
5:I:629:LEU:HD11	5:I:656:LEU:HG	1.85	0.58
11:U:139:VAL:HG12	11:U:143:TYR:CZ	2.39	0.58
15:X:6:DT:C2	16:Y:-6:DA:N1	2.62	0.58
4:D:36:ARG:NH1	16:Y:-86:DA:OP1	2.34	0.58
4:H:79:LYS:HB2	16:Y:-44:DA:OP1	2.04	0.58
5:I:779:GLN:O	5:I:2141:ASN:OD1	2.21	0.58
10:N:112:GLU:OE2	9:O:269:THR:HG21	2.03	0.58
2:B:112:THR:HG21	13:V:61:LEU:CD2	2.34	0.58
7:K:296:GLU:OE1	7:K:296:GLU:N	2.36	0.57
9:M:173:ASP:OD2	9:M:175:SER:OG	2.22	0.57
9:O:42:GLN:OE1	9:O:364:MET:N	2.37	0.57
10:R:370:ILE:HD11	10:R:399:LEU:HD11	1.86	0.57
2:B:112:THR:CG2	13:V:61:LEU:HD21	2.34	0.57
5:I:899:LYS:HZ1	5:I:907:PHE:HZ	1.49	0.57
9:Q:134:GLU:OE2	9:Q:209:TYR:OH	2.18	0.57
1:A:111:ILE:HG22	1:A:113:ALA:H	1.69	0.57
4:D:79:LYS:C	15:X:101:DA:OP1	2.43	0.57
1:E:14:ALA:CA	16:Y:-115:DT:OP1	2.51	0.57
1:E:92:GLU:OE1	1:E:92:GLU:N	2.38	0.57
16:Y:-130:DC:OP2	16:Y:-130:DC:C6	2.51	0.57
3:C:42:ARG:CG	16:Y:-79:DT:C4'	2.76	0.57
8:L:89:GLU:N	8:L:89:GLU:OE1	2.36	0.57
9:M:115:ASN:OD1	9:M:118:ARG:NH1	2.37	0.57
16:Y:-60:DT:H1'	16:Y:-59:DT:H5'	1.87	0.57
9:O:53:VAL:HG12	9:O:83:ILE:HG23	1.86	0.57
1:A:29:ARG:NH2	2:B:37:TYR:CE2	2.69	0.57
1:E:28:GLY:HA3	16:Y:-117:DA:H3'	1.86	0.57
5:I:895:MET:HE1	15:X:51:DG:C2	2.38	0.57
9:M:426:GLU:N	9:M:426:GLU:OE1	2.38	0.57
11:U:248:ILE:O	11:U:249:THR:OG1	2.18	0.57
3:G:40:ARG:HH22	16:Y:-64:DG:C1'	2.18	0.57
5:I:705:ARG:NH2	15:X:58:DA:P	2.78	0.57
14:W:39:GLU:HB3	16:Y:-82:DA:C5'	2.34	0.57
15:X:111:DG:H2'	15:X:112:DA:H8	1.69	0.57
4:D:79:LYS:CA	15:X:101:DA:OP1	2.53	0.57
10:P:262:SER:CB	9:Q:248:ALA:HB1	2.35	0.57
10:R:205:LEU:HD13	10:R:225:VAL:HB	1.86	0.57
16:Y:-98:DA:H2"	16:Y:-97:DG:C8	2.40	0.57
5:I:629:LEU:HD21	5:I:656:LEU:HG	1.86	0.57
9:Q:247:ASN:ND2	9:Q:279:ILE:HD11	2.19	0.57



Atom-1	Atom-2	Interatomic	Clash
		distance (Å)	overlap (Å)
11:U:222:ASP:OD1	11:U:312:ARG:NH1	2.37	0.57
15:X:110:DC:H2"	15:X:111:DG:C8	2.39	0.57
1:A:17:ARG:NH2	15:X:29:DG:OP2	2.38	0.56
5:I:760:GLN:N	5:I:760:GLN:OE1	2.38	0.56
5:I:2141:ASN:CG	5:I:2142:PRO:HD2	2.26	0.56
11:U:138:ALA:CB	11:U:163:VAL:HG11	2.35	0.56
2:B:89:ARG:NH2	13:V:63:SER:HB3	2.20	0.56
9:Q:117:ARG:NH2	9:Q:280:ASN:OD1	2.37	0.56
9:Q:278:GLU:O	9:Q:280:ASN:N	2.37	0.56
5:I:629:LEU:HD22	5:I:629:LEU:O	2.06	0.56
12:T:414:GLN:N	12:T:414:GLN:OE1	2.38	0.56
1:E:42:ARG:O	2:F:85:THR:OG1	2.18	0.56
5:I:726:LYS:CG	15:X:56:DT:C4'	2.81	0.56
5:I:780:ASN:HA	5:I:2141:ASN:OD1	2.06	0.56
1:A:121:GLU:HG3	3:C:41:TYR:OH	2.06	0.56
7:K:3:THR:HG23	7:K:18:SER:HB3	1.88	0.56
11:S:188:TYR:HB2	11:S:267:LEU:HD21	1.87	0.56
16:Y:-54:DC:H5"	16:Y:-54:DC:C6	2.26	0.56
5:I:2079:LEU:CD1	5:I:2115:ILE:HD11	2.36	0.56
11:U:300:SER:OG	11:U:338:SER:OG	2.20	0.56
11:U:305:MET:O	11:U:335:ARG:NH2	2.37	0.56
9:M:411:THR:HG21	10:N:68:ILE:HG21	1.88	0.55
10:P:63:ILE:HD13	10:P:295:VAL:HG21	1.88	0.55
11:S:324:THR:CG2	15:X:117:DT:O5'	2.54	0.55
11:S:324:THR:HG21	15:X:116:DA:O3'	2.06	0.55
16:Y:-104:DA:H2"	16:Y:-103:DG:O5'	2.06	0.55
1:A:17:ARG:CZ	15:X:29:DG:OP2	2.55	0.55
9:Q:106:ILE:HD11	9:Q:110:GLU:HG3	1.87	0.55
9:M:172:LEU:HD11	9:M:193:ILE:HD13	1.87	0.55
9:M:401:THR:HG22	9:M:402:THR:H	1.72	0.55
15:X:41:DT:C2'	15:X:42:DA:H5'	2.33	0.55
16:Y:-145:DT:H2"	16:Y:-144:DG:H5"	1.88	0.55
15:X:72:DA:H2	16:Y:-71:DG:C2	2.24	0.55
10:R:268:ILE:O	10:R:272:VAL:HG23	2.07	0.55
5:I:780:ASN:HB2	5:I:2141:ASN:HD21	1.72	0.55
10:R:142:VAL:O	10:R:190:GLY:N	2.39	0.55
1:A:54:VAL:HG21	2:B:95:VAL:HG21	1.87	0.55
5:I:729:LEU:HD21	5:I:757:GLN:O	2.07	0.55
9:O:28:GLU:OE1	9:O:28:GLU:N	2.38	0.55
12:T:333:VAL:HG11	12:T:345:TYR:CE2	2.41	0.55
16:Y:-58:DT:H2"	16:Y:-57:DA:N7	2.22	0.55



Atom-1	Atom-2	Interatomic	Clash
	1100111 =	distance (Å)	overlap (Å)
2:F:101:GLY:O	2:F:104:ALA:N	2.39	0.55
13:V:50:PRO:O	13:V:51:GLU:HG3	2.06	0.55
15:X:87:DT:H4'	15:X:88:DT:H5'	1.89	0.55
2:B:112:THR:HG21	13:V:61:LEU:HD21	1.87	0.55
11:U:259:GLU:O	11:U:263:GLN:N	2.38	0.55
13:V:54:HIS:O	13:V:58:TYR:HB3	2.07	0.55
16:Y:-137:DC:H4'	16:Y:-136:DC:OP2	2.07	0.54
8:L:127:THR:O	10:N:171:ILE:HD12	2.07	0.54
8:L:149:CYS:SG	8:L:150:LEU:N	2.80	0.54
9:M:43:GLU:N	9:M:43:GLU:OE1	2.37	0.54
4:D:80:THR:N	15:X:101:DA:OP1	2.40	0.54
10:P:400:ARG:NH2	17:P:501:ADP:O2A	2.41	0.54
9:Q:148:GLY:O	9:Q:150:TYR:N	2.39	0.54
9:M:415:LEU:HD21	10:N:61:GLU:HB2	1.90	0.54
9:M:108:LYS:NZ	9:M:310:GLU:OE2	2.28	0.54
16:Y:-44:DA:H2'	16:Y:-43:DT:H71	1.89	0.54
10:P:264:ASP:OD1	10:P:264:ASP:N	2.41	0.54
10:R:31:LEU:HG	10:R:33:LEU:HD13	1.90	0.54
11:U:270:GLU:OE1	11:U:271:SER:N	2.41	0.54
11:U:316:GLU:N	11:U:316:GLU:OE1	2.41	0.54
16:Y:-87:DA:H2"	16:Y:-86:DA:C8	2.43	0.54
16:Y:-74:DG:H1'	16:Y:-73:DC:H5'	1.88	0.54
1:A:24:GLN:O	2:B:37:TYR:HD1	1.91	0.54
5:I:802:GLU:OE2	5:I:802:GLU:N	2.41	0.54
15:X:5:DA:H2	16:Y:-5:DT:O2	1.91	0.54
9:O:106:ILE:CD1	9:O:269:THR:HG23	2.29	0.54
3:C:66:PRO:HD3	15:X:90:DA:H3'	1.90	0.53
5:I:138:ASP:OD1	5:I:139:TYR:N	2.42	0.53
5:I:902:ASN:ND2	5:I:2137:ASP:OD2	2.41	0.53
9:Q:415:LEU:HD13	10:R:61:GLU:HB3	1.90	0.53
15:X:51:DG:H1	16:Y:-51:DC:H42	1.53	0.53
7:K:253:GLU:N	7:K:253:GLU:OE1	2.40	0.53
1:E:45:ALA:HB2	15:X:111:DG:OP2	2.08	0.53
5:I:151:PHE:CD2	12:T:399:ILE:HG22	2.44	0.53
5:I:229:LEU:O	5:I:233:LEU:HD23	2.08	0.53
14:W:39:GLU:CB	16:Y:-82:DA:C5'	2.79	0.53
5:I:750:ASN:HD21	5:I:758:ARG:HH21	1.49	0.53
9:M:173:ASP:O	9:M:175:SER:N	2.41	0.53
1:A:16:SER:HA	15:X:29:DG:H5"	1.90	0.53
9:Q:275:LEU:O	9:Q:280:ASN:HB3	2.09	0.53
11:S:182:GLY:O	11:S:213:LYS:NZ	2.41	0.53



Atom-1	Atom-2	Interatomic	Clash
1100III-1	1100111-2	distance (Å)	overlap (Å)
15:X:141:DC:H5"	15:X:141:DC:H6	1.73	0.53
1:A:42:ARG:CB	16:Y:-33:DG:OP1	2.54	0.53
5:I:2063:LEU:HD23	5:I:2114:PHE:HB3	1.90	0.53
15:X:72:DA:C2	16:Y:-71:DG:N1	2.76	0.53
1:A:26:PRO:CD	2:B:37:TYR:CE2	2.91	0.53
4:D:45:ARG:CG	15:X:81:DG:OP1	2.52	0.53
11:U:116:ARG:NH1	11:U:371:HIS:O	2.41	0.53
13:V:50:PRO:C	13:V:51:GLU:HG3	2.28	0.53
13:V:190:ASP:OD1	13:V:191:LEU:N	2.42	0.53
13:V:262:GLU:OE2	14:W:202:LYS:CE	2.57	0.53
14:W:38:ARG:NH1	16:Y:-83:DC:P	2.82	0.53
5:I:157:TRP:O	5:I:161:VAL:HG23	2.07	0.53
10:R:97:ASP:OD1	10:R:98:THR:HG23	2.08	0.53
14:W:39:GLU:HB2	16:Y:-82:DA:P	2.49	0.53
16:Y:-103:DG:H4'	16:Y:-103:DG:OP1	2.09	0.53
2:B:116:THR:HG22	13:V:57:VAL:HG13	1.91	0.53
9:Q:396:GLU:O	9:Q:399:THR:OG1	2.27	0.53
14:W:131:LYS:NZ	14:W:173:ALA:O	2.40	0.53
5:I:92:SER:O	14:W:193:GLU:CD	2.44	0.52
7:K:97:GLU:OE1	7:K:124:ARG:NH1	2.39	0.52
9:Q:293:GLU:OE1	9:Q:293:GLU:N	2.42	0.52
15:X:70:DA:N6	16:Y:-70:DT:H3	1.97	0.52
10:N:196:ASP:O	10:N:200:GLY:N	2.38	0.52
10:R:117:GLU:OE2	10:R:269:LYS:NZ	2.42	0.52
15:X:28:DG:C8	15:X:28:DG:C5'	2.85	0.52
5:I:779:GLN:O	5:I:2142:PRO:CD	2.51	0.52
12:T:70:ILE:N	12:T:70:ILE:HD12	2.24	0.52
6:J:218:THR:OG1	10:P:189:ALA:HB1	2.09	0.52
10:P:68:ILE:HD13	10:P:68:ILE:H	1.73	0.52
11:U:59:GLN:O	11:U:62:ARG:NE	2.37	0.52
15:X:129:DG:H2"	15:X:130:DG:C8	2.44	0.52
14:W:29:ASN:OD1	14:W:116:HIS:NE2	2.41	0.52
16:Y:-54:DC:C5'	16:Y:-54:DC:C6	2.91	0.52
3:C:42:ARG:NH2	15:X:81:DG:N3	2.57	0.52
4:D:75:HIS:O	2:F:89:ARG:NH1	2.36	0.52
9:O:106:ILE:HD13	9:O:267:LYS:O	2.09	0.52
14:W:39:GLU:CB	16:Y:-82:DA:OP1	2.58	0.52
15:X:67:DG:H2"	15:X:68:DG:C8	2.45	0.52
16:Y:-94:DC:H2'	16:Y:-93:DC:C6	2.45	0.52
12:T:37:PHE:CE2	12:T:70:ILE:HG23	2.45	0.52
13:V:262:GLU:OE1	14:W:202:LYS:HG3	2.10	0.52



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
15:X:5:DA:C2	16:Y:-5:DT:N3	2.60	0.52
5:I:2079:LEU:HD12	5:I:2115:ILE:HD11	1.92	0.51
9:M:283:VAL:HG11	10:R:19:ILE:HD11	1.92	0.51
9:O:21:VAL:HG12	9:O:39:LEU:HD21	1.92	0.51
9:Q:132:GLU:OE2	9:Q:230:LYS:NZ	2.30	0.51
10:R:366:ASP:O	10:R:370:ILE:HG23	2.10	0.51
12:T:317:LEU:HD13	12:T:317:LEU:O	2.09	0.51
15:X:45:DC:H2"	15:X:46:DC:H5"	1.92	0.51
15:X:120:DA:H5"	15:X:120:DA:H8	1.75	0.51
16:Y:-132:DT:H2"	16:Y:-131:DG:C8	2.44	0.51
3:C:43:PRO:HD2	16:Y:-78:DA:H5"	1.92	0.51
4:D:32:PRO:HG2	16:Y:-86:DA:C2'	2.40	0.51
3:G:40:ARG:NH1	16:Y:-63:DC:C5'	2.73	0.51
5:I:705:ARG:HD3	5:I:727:LEU:CD2	2.40	0.51
9:O:43:GLU:N	9:O:43:GLU:OE1	2.40	0.51
15:X:20:DA:C2	15:X:21:DC:C4	2.98	0.51
15:X:26:DC:H2"	15:X:27:DT:C6	2.45	0.51
6:J:269:SER:C	9:Q:150:TYR:HB3	2.30	0.51
16:Y:-1:DG:H1'	16:Y:0:DT:H5'	1.91	0.51
5:I:2066:THR:OG1	5:I:2072:LEU:HD21	2.11	0.51
9:Q:71:PRO:HD2	9:Q:74:THR:HG21	1.92	0.51
16:Y:-73:DC:H1'	16:Y:-72:DT:H5'	1.92	0.51
5:I:2185:MET:O	5:I:2189:MET:HG2	2.11	0.51
9:Q:71:PRO:O	9:Q:76:LYS:NZ	2.41	0.51
9:Q:255:ASP:O	9:Q:257:LEU:N	2.44	0.51
9:Q:303:GLU:OE1	9:Q:305:HIS:NE2	2.44	0.51
5:I:750:ASN:ND2	5:I:758:ARG:NH2	2.53	0.51
15:X:141:DC:H2'	15:X:142:DT:H71	1.91	0.51
3:G:40:ARG:HA	16:Y:-63:DC:OP1	2.11	0.51
10:P:182:LEU:O	10:P:186:LYS:N	2.44	0.51
10:R:40:ARG:O	10:R:53:ARG:NH2	2.44	0.51
10:R:74:LEU:HD11	10:R:328:THR:HG22	1.92	0.51
12:T:363:ARG:NE	12:T:367:GLU:OE2	2.43	0.51
5:I:896:GLN:CA	5:I:899:LYS:HE3	2.31	0.51
5:I:941:ILE:HD12	5:I:941:ILE:H	1.76	0.51
10:P:430:TYR:O	10:P:438:ARG:NH2	2.41	0.51
7:K:69:ASP:OD1	7:K:70:VAL:N	2.44	0.51
9:O:69:ALA:O	9:O:363:THR:OG1	2.28	0.51
15:X:33:DC:H2'	15:X:34:DT:H71	1.92	0.51
1:E:32:ARG:HE	16:Y:-117:DA:P	2.34	0.50
9:M:323:ILE:O	10:R:21:ARG:NH2	2.44	0.50



A + a 1		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
12:T:383:ASN:ND2	12:T:383:ASN:O	2.44	0.50
14:W:140:ASP:OD1	14:W:141:GLU:N	2.43	0.50
16:Y:-47:DG:H2"	16:Y:-46:DG:N7	2.26	0.50
10:R:141:GLU:N	10:R:164:LYS:O	2.41	0.50
15:X:35:DA:H4'	15:X:35:DA:OP1	2.12	0.50
1:E:44:GLY:HA2	15:X:111:DG:O5'	2.10	0.50
5:I:137:TRP:NE1	12:T:184:ASP:O	2.43	0.50
12:T:79:ARG:NH2	12:T:80:GLU:OE1	2.44	0.50
5:I:629:LEU:HD11	5:I:656:LEU:CG	2.41	0.50
5:I:899:LYS:NZ	5:I:899:LYS:CB	2.75	0.50
10:R:306:ILE:HD13	10:R:338:THR:HG21	1.93	0.50
11:U:282:ILE:HD11	11:U:294:TYR:CZ	2.47	0.50
15:X:79:DA:H2"	15:X:80:DC:C5	2.46	0.50
15:X:112:DA:N6	16:Y:-112:DT:H3	2.09	0.50
9:M:308:ASP:OD1	9:M:309:ILE:N	2.42	0.50
7:K:15:ILE:C	7:K:15:ILE:HD12	2.32	0.50
7:K:58:LEU:H	7:K:58:LEU:HD23	1.76	0.50
7:K:114:PHE:O	7:K:118:GLN:NE2	2.42	0.50
1:E:20:ARG:CG	2:F:121:SER:OG	2.59	0.50
5:I:890:VAL:HG13	5:I:891:ILE:HD12	1.93	0.50
6:J:302:ARG:NH1	6:J:307:ASP:O	2.45	0.50
11:U:303:THR:HG22	11:U:303:THR:O	2.11	0.50
7:K:32:SER:HB2	7:K:54:LEU:HD23	1.94	0.49
14:W:50:TYR:HB3	14:W:87:GLU:HB3	1.94	0.49
15:X:123:DG:H2"	15:X:124:DG:H8	1.77	0.49
16:Y:-48:DG:H2"	16:Y:-47:DG:C8	2.47	0.49
9:Q:28:GLU:OE1	9:Q:28:GLU:N	2.44	0.49
9:Q:52:ILE:HD11	9:Q:83:ILE:HD13	1.94	0.49
9:Q:279:ILE:HG22	9:Q:283:VAL:HG23	1.94	0.49
4:D:79:LYS:N	15:X:101:DA:P	2.76	0.49
3:G:40:ARG:HH22	16:Y:-64:DG:H1'	1.77	0.49
5:I:1980:MET:SD	5:I:2030:THR:HA	2.51	0.49
10:N:33:LEU:HD21	10:N:53:ARG:HG2	1.94	0.49
9:Q:405:TYR:OH	9:Q:437:PHE:O	2.30	0.49
11:U:193:LEU:O	11:U:194:THR:HB	2.11	0.49
3:C:43:PRO:HD2	16:Y:-78:DA:C5'	2.42	0.49
5:I:129:GLU:OE1	5:I:129:GLU:N	2.41	0.49
7:K:105:ILE:HG23	7:K:106:GLN:N	2.27	0.49
7:K:266:GLN:OE1	7:K:266:GLN:N	2.44	0.49
9:M:172:LEU:HD23	9:M:180:LEU:HD11	1.94	0.49
15:X:98:DT:H2"	15:X:99:DA:C8	2.47	0.49



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
4:D:79:LYS:HB2	15:X:100:DG:H3'	1.94	0.49
11:U:306:TYR:HB3	11:U:309:ILE:HG23	1.95	0.49
5:I:895:MET:O	5:I:899:LYS:HE3	2.12	0.49
10:P:378:GLU:OE1	10:P:407:THR:OG1	2.29	0.49
11:U:108:ALA:HB1	11:U:109:PRO:HD2	1.92	0.49
16:Y:-101:DT:H2"	16:Y:-100:DC:C6	2.48	0.49
5:I:733:GLN:HE21	15:X:133:DC:H4'	1.78	0.49
10:P:249:VAL:HG13	10:P:261:PHE:HE2	1.77	0.49
5:I:725:TYR:HB3	5:I:758:ARG:CD	2.42	0.49
5:I:949:ILE:HD13	5:I:949:ILE:O	2.12	0.49
10:N:19:ILE:HD11	9:O:283:VAL:CG1	2.36	0.49
1:A:92:GLU:OE2	2:B:102:GLU:N	2.46	0.49
5:I:96:ILE:CG1	14:W:197:LEU:HD11	2.42	0.49
10:N:47:VAL:CG2	10:N:373:ILE:HD12	2.43	0.49
9:O:339:ARG:NH2	10:P:307:GLU:OE2	2.45	0.49
15:X:4:DG:H2"	15:X:5:DA:C8	2.47	0.49
3:C:43:PRO:CG	16:Y:-78:DA:C5'	2.81	0.49
5:I:795:HIS:O	5:I:798:GLN:NE2	2.44	0.49
10:R:74:LEU:O	10:R:357:VAL:N	2.39	0.49
11:U:362:TYR:O	11:U:366:GLY:N	2.46	0.49
5:I:615:ARG:NH2	5:I:687:LYS:O	2.46	0.48
10:P:449:ALA:O	9:Q:333:ARG:NH2	2.45	0.48
15:X:129:DG:N2	16:Y:-128:DG:N2	2.61	0.48
10:P:196:ASP:O	10:P:200:GLY:N	2.45	0.48
9:M:405:TYR:CE2	9:M:409:LEU:HD11	2.49	0.48
9:0:311:CYS:O	9:O:315:LEU:HD23	2.13	0.48
12:T:69:TYR:C	12:T:70:ILE:HD12	2.34	0.48
11:U:252:ASN:O	11:U:256:ARG:N	2.45	0.48
13:V:213:LEU:HD22	13:V:213:LEU:H	1.77	0.48
3:C:82:LEU:HD22	4:D:81:VAL:HG23	1.93	0.48
2:F:102:GLU:OE1	2:F:102:GLU:N	2.42	0.48
9:M:386:ILE:HG22	9:M:425:ILE:HB	1.94	0.48
10:R:362:TYR:OH	17:R:501:ADP:N7	2.27	0.48
15:X:57:DT:H2"	15:X:58:DA:C8	2.48	0.48
15:X:101:DA:H61	16:Y:-101:DT:H3	1.62	0.48
16:Y:-130:DC:OP2	16:Y:-130:DC:H2'	2.14	0.48
3:C:42:ARG:HE	3:C:42:ARG:HA	1.78	0.48
6:J:219:VAL:HG11	6:J:263:ARG:CZ	2.43	0.48
7:K:67:ASN:O	7:K:69:ASP:N	2.47	0.48
15:X:98:DT:H3	16:Y:-98:DA:N6	2.11	0.48
16:Y:-43:DT:H1'	16:Y:-42:DT:H5'	1.94	0.48



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
10:P:31:LEU:O	10:P:44:GLN:NE2	2.47	0.48
10:P:276:ILE:O	10:P:280:VAL:HG23	2.13	0.48
9:Q:110:GLU:HG2	9:Q:269:THR:HA	1.94	0.48
15:X:43:DA:H2'	15:X:44:DT:H72	1.95	0.48
3:C:51:ILE:HD11	4:D:43:VAL:O	2.13	0.48
6:J:282:ARG:N	6:J:283:PRO:HD3	2.28	0.48
9:Q:279:ILE:HD12	9:Q:279:ILE:N	2.29	0.48
9:M:105:GLU:OE1	9:M:105:GLU:N	2.47	0.48
10:N:22:ILE:HD12	10:N:22:ILE:N	2.29	0.48
9:O:180:LEU:HD21	9:O:200:VAL:HG11	1.96	0.48
15:X:138:DA:H2"	15:X:139:DT:H5"	1.96	0.48
16:Y:-116:DT:H5'	16:Y:-116:DT:H6	1.77	0.48
5:I:2141:ASN:OD1	5:I:2183:LYS:CD	2.62	0.48
7:K:31:ARG:O	7:K:55:PHE:N	2.36	0.48
14:W:42:GLY:O	14:W:93:TRP:HB3	2.13	0.48
15:X:112:DA:H2"	15:X:113:DC:C6	2.49	0.48
9:O:302:ASP:OD1	9:O:303:GLU:N	2.47	0.48
5:I:202:VAL:HG11	11:S:143:TYR:CD1	2.49	0.47
5:I:899:LYS:NZ	5:I:899:LYS:HB2	2.27	0.47
5:I:1936:ILE:HD13	5:I:1936:ILE:H	1.78	0.47
5:I:891:ILE:CG2	16:Y:-50:DA:C2	2.95	0.47
7:K:186:GLU:OE2	8:L:41:GLN:NE2	2.48	0.47
9:O:303:GLU:OE1	9:O:305:HIS:NE2	2.47	0.47
9:Q:105:GLU:OE1	9:Q:105:GLU:N	2.47	0.47
11:U:163:VAL:O	11:U:163:VAL:HG13	2.14	0.47
15:X:43:DA:H61	16:Y:-43:DT:H3	1.62	0.47
15:X:49:DT:C6	15:X:50:DT:H72	2.49	0.47
7:K:237:VAL:HG12	7:K:267:ILE:HD11	1.96	0.47
9:M:316:HIS:HB3	9:M:354:LEU:HD13	1.95	0.47
10:N:40:ARG:O	10:N:53:ARG:NH2	2.48	0.47
8:L:42:ASP:OD1	8:L:43:ASP:N	2.48	0.47
10:P:362:TYR:OH	17:P:501:ADP:N7	2.32	0.47
11:U:159:VAL:HG22	18:U:401:ATP:O1G	2.14	0.47
10:N:115:LYS:NZ	10:N:305:ASP:OD2	2.24	0.47
11:U:6:ALA:HB2	11:U:100:GLU:OE1	2.15	0.47
15:X:140:DT:H3	16:Y:-140:DA:N6	2.12	0.47
4:D:46:ILE:N	15:X:81:DG:OP1	2.39	0.47
5:I:859:CYS:SG	5:I:860:ARG:N	2.88	0.47
11:U:248:ILE:O	11:U:248:ILE:HG22	2.14	0.47
16:Y:-136:DC:H6	16:Y:-136:DC:H5"	1.80	0.47
16:Y:-46:DG:C6	16:Y:-45:DG:C6	3.03	0.47



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
5:I:726:LYS:HG2	15:X:56:DT:O4'	2.13	0.47
5:I:727:LEU:HD12	5:I:730:GLN:OE1	2.14	0.47
6:J:209:GLY:O	6:J:211:ILE:N	2.47	0.47
7:K:12:ASN:CG	7:K:24:VAL:HG22	2.35	0.47
10:N:205:LEU:HD22	10:N:205:LEU:N	2.30	0.47
12:T:21:TYR:CD2	12:T:22:THR:HG23	2.49	0.47
3:C:42:ARG:CG	16:Y:-79:DT:O4'	2.48	0.47
9:M:74:THR:HB	9:M:363:THR:HG22	1.97	0.47
9:M:123:ARG:O	9:M:293:GLU:N	2.48	0.47
9:Q:401:THR:OG1	9:Q:402:THR:N	2.48	0.47
11:U:273:GLY:O	11:U:277:THR:N	2.36	0.47
15:X:5:DA:C2	16:Y:-5:DT:C2	3.03	0.47
6:J:261:CYS:H	10:P:210:THR:HA	1.80	0.47
7:K:6:LEU:HD12	7:K:79:PHE:CZ	2.50	0.47
9:M:316:HIS:CB	9:M:354:LEU:HD13	2.45	0.47
9:M:415:LEU:HD23	10:N:58:VAL:HG13	1.96	0.47
13:V:59:ALA:O	13:V:63:SER:HB2	2.15	0.47
16:Y:-109:DT:H2"	16:Y:-108:DA:C8	2.50	0.47
5:I:918:THR:HG23	5:I:918:THR:O	2.15	0.47
10:P:244:LEU:HD11	10:P:280:VAL:HG21	1.97	0.47
9:Q:54:GLU:N	9:Q:54:GLU:OE1	2.48	0.47
7:K:6:LEU:HG	7:K:15:ILE:HG22	1.97	0.46
9:Q:129:GLU:OE2	9:Q:196:ASN:N	2.40	0.46
1:A:26:PRO:HD3	2:B:37:TYR:CG	2.49	0.46
7:K:57:ILE:HG22	7:K:70:VAL:CG2	2.45	0.46
9:M:218:GLU:OE1	9:M:219:GLU:N	2.42	0.46
10:N:346:ILE:HB	10:N:351:LEU:HD23	1.97	0.46
10:N:424:ASP:OD1	10:N:425:ASP:N	2.48	0.46
15:X:37:DG:H2"	15:X:38:DG:C8	2.51	0.46
7:K:24:VAL:O	7:K:24:VAL:HG13	2.15	0.46
9:M:33:LYS:O	9:M:46:ARG:NH1	2.49	0.46
10:P:262:SER:HB2	9:Q:248:ALA:HB1	1.97	0.46
5:I:206:TRP:HE1	11:S:148:THR:HG23	1.79	0.46
5:I:815:ILE:HD12	5:I:815:ILE:N	2.31	0.46
14:W:38:ARG:HG2	14:W:41:ASP:HB3	1.97	0.46
16:Y:-42:DT:H1'	16:Y:-41:DA:H5'	1.97	0.46
3:C:109:LEU:HD13	3:G:129:ARG:HG2	1.97	0.46
2:F:60:ASN:O	2:F:64:ASN:ND2	2.44	0.46
7:K:13:ALA:N	7:K:25:ILE:O	2.46	0.46
7:K:331:ASP:OD1	7:K:331:ASP:N	2.48	0.46
9:Q:129:GLU:OE1	9:Q:129:GLU:N	2.41	0.46



Atom-1	Atom-2	Interatomic	Clash
		distance (A)	overlap (A)
9:Q:269:THR:O	9:Q:269:THR:CG2	2.59	0.46
16:Y:-68:DC:H2"	16:Y:-67:DC:C6	2.50	0.46
4:D:45:ARG:HG3	15:X:81:DG:P	2.55	0.46
5:I:2145:ASP:OD1	5:I:2149:GLN:NE2	2.46	0.46
7:K:22:VAL:HG12	7:K:360:TRP:CE3	2.51	0.46
9:O:55:LEU:O	9:O:58:SER:OG	2.26	0.46
9:Q:53:VAL:HG22	9:Q:83:ILE:HG23	1.97	0.46
13:V:56:GLU:H	13:V:56:GLU:CD	2.19	0.46
15:X:46:DC:H2'	15:X:47:DC:C6	2.51	0.46
16:Y:-108:DA:C5	16:Y:-107:DG:C6	3.03	0.46
3:C:85:GLN:HA	16:Y:-97:DG:OP1	2.15	0.46
6:J:219:VAL:HG21	6:J:263:ARG:NH2	2.30	0.46
8:L:26:ARG:NH2	15:X:73:DG:H5"	2.31	0.46
9:Q:21:VAL:HG23	9:Q:21:VAL:O	2.16	0.46
9:Q:27:ASP:OD1	9:Q:31:LEU:N	2.45	0.46
15:X:19:DC:H2"	15:X:20:DA:H8	1.80	0.46
5:I:629:LEU:HD22	5:I:629:LEU:C	2.36	0.46
5:I:191:LEU:C	5:I:191:LEU:HD23	2.36	0.46
7:K:195:VAL:HG22	7:K:195:VAL:O	2.16	0.46
9:M:135:VAL:HG21	9:M:138:LEU:HD11	1.97	0.46
10:P:258:LEU:O	10:P:259:ALA:HB3	2.16	0.46
10:R:192:VAL:HB	10:R:205:LEU:HD12	1.97	0.46
12:T:81:ASN:OD1	12:T:247:THR:HG23	2.16	0.46
12:T:350:VAL:O	12:T:389:ARG:NH1	2.48	0.46
11:U:278:THR:O	11:U:282:ILE:HG23	2.16	0.46
1:E:42:ARG:HD2	16:Y:-108:DA:H4'	1.98	0.46
10:P:147:ILE:HD13	10:P:179:ILE:HG21	1.98	0.46
14:W:122:GLN:NE2	14:W:131:LYS:O	2.46	0.46
15:X:52:DG:H1'	15:X:53:DC:H5'	1.97	0.46
9:M:74:THR:O	9:M:366:TYR:OH	2.34	0.45
10:P:147:ILE:HD12	10:P:148:ASP:N	2.31	0.45
16:Y:-136:DC:H1'	16:Y:-135:DC:H5'	1.98	0.45
3:G:41:TYR:HE1	15:X:142:DT:C4'	2.26	0.45
5:I:979:THR:HG22	5:I:980:ALA:N	2.31	0.45
7:K:135:TYR:O	7:K:139:ASN:N	2.49	0.45
10:P:291:ILE:O	10:P:292:ILE:HG23	2.15	0.45
11:U:97:ALA:O	11:U:101:HIS:ND1	2.50	0.45
11:U:222:ASP:O	11:U:312:ARG:NH2	2.48	0.45
13:V:208:VAL:N	13:V:209:PRO:CD	2.79	0.45
15:X:87:DT:C4'	15:X:88:DT:H5'	2.45	0.45
3:C:42:ARG:NE	3:C:42:ARG:HA	2.31	0.45



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
7:K:57:ILE:HG22	7:K:70:VAL:HG22	1.98	0.45
9:Q:415:LEU:HD11	10:R:62:MET:HB3	1.97	0.45
15:X:24:DG:H2"	15:X:25:DC:C5	2.52	0.45
3:C:62:ILE:O	3:C:93:GLN:NE2	2.50	0.45
15:X:21:DC:H1'	15:X:22:DG:H5'	1.97	0.45
15:X:109:DA:H2"	15:X:110:DC:C6	2.51	0.45
1:E:73:ASN:O	1:E:73:ASN:ND2	2.44	0.45
5:I:2067:GLN:HG3	5:I:2068:MET:HG3	1.97	0.45
6:J:180:GLU:O	6:J:184:LEU:HD23	2.16	0.45
9:M:61:MET:CE	10:R:22:ILE:HD11	2.45	0.45
9:M:320:GLU:OE2	9:M:357:ARG:NH1	2.49	0.45
10:N:191:ASP:OD1	10:N:207:ARG:NE	2.44	0.45
14:W:39:GLU:CB	16:Y:-82:DA:P	3.05	0.45
16:Y:-113:DG:H2"	16:Y:-112:DT:OP2	2.16	0.45
3:G:40:ARG:NH1	16:Y:-63:DC:H5'	2.32	0.45
5:I:859:CYS:SG	5:I:860:ARG:NH1	2.90	0.45
10:P:205:LEU:H	10:P:205:LEU:HD22	1.80	0.45
9:Q:378:ARG:HG3	9:Q:407:VAL:HG21	1.99	0.45
11:U:37:ARG:NH2	11:U:81:ASP:OD1	2.45	0.45
13:V:56:GLU:N	13:V:56:GLU:OE1	2.49	0.45
2:B:96:ARG:NH2	13:V:64:ASP:HB3	2.31	0.45
5:I:121:LEU:O	13:V:225:ARG:NH2	2.50	0.45
9:Q:171:LYS:C	9:Q:172:LEU:HD22	2.37	0.45
9:Q:217:ALA:CB	10:R:199:THR:HG23	2.47	0.45
9:Q:255:ASP:O	9:Q:258:SER:N	2.40	0.45
10:R:351:LEU:HD13	10:R:354:LEU:HD12	1.97	0.45
11:U:80:ASP:OD1	11:U:81:ASP:N	2.49	0.45
15:X:63:DG:H1'	15:X:64:DC:H5'	1.99	0.45
2:B:89:ARG:CZ	13:V:63:SER:HB3	2.47	0.45
3:G:43:PRO:HG2	15:X:68:DG:C5'	2.45	0.45
7:K:86:VAL:HG21	7:K:116:GLU:HB3	1.99	0.45
7:K:325:LEU:HD21	18:K:401:ATP:C6	2.51	0.45
9:M:189:ASP:OD1	9:M:205:ARG:NH1	2.50	0.45
16:Y:-139:DA:C2'	16:Y:-138:DT:H5"	2.46	0.45
3:G:40:ARG:NH2	16:Y:-64:DG:C1'	2.80	0.45
4:H:62:LEU:O	4:H:63:GLU:C	2.56	0.45
11:U:71:ILE:N	11:U:71:ILE:HD12	2.31	0.45
5:I:1923:LEU:HD22	5:I:1923:LEU:H	1.82	0.45
15:X:101:DA:N6	16:Y:-101:DT:H3	2.15	0.45
16:Y:-47:DG:H2"	16:Y:-46:DG:C8	2.52	0.45
3:G:43:PRO:HG2	15:X:68:DG:H5'	1.98	0.44



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
9:M:271:ILE:HD13	9:M:271:ILE:H	1.81	0.44
12:T:42:GLY:H	12:T:75:LEU:HD13	1.81	0.44
15:X:99:DA:C2	16:Y:-98:DA:C2	3.05	0.44
16:Y:-100:DC:H2"	16:Y:-99:DT:H71	1.99	0.44
9:M:313:THR:HG21	10:R:303:MET:HG3	1.99	0.44
9:O:316:HIS:NE2	9:O:353:ASP:OD2	2.44	0.44
9:Q:130:VAL:HG13	9:Q:192:TYR:CE2	2.52	0.44
11:S:324:THR:HG23	15:X:117:DT:O5'	2.14	0.44
5:I:896:GLN:HA	5:I:899:LYS:NZ	2.32	0.44
9:Q:15:ILE:HD12	9:Q:15:ILE:H	1.83	0.44
11:U:101:HIS:CG	11:U:101:HIS:O	2.69	0.44
13:V:236:ARG:O	13:V:241:VAL:HG12	2.17	0.44
7:K:182:ASN:ND2	8:L:35:LEU:O	2.43	0.44
9:M:369:GLN:OE1	9:M:369:GLN:N	2.47	0.44
10:N:356:ILE:N	10:N:356:ILE:HD12	2.32	0.44
10:P:166:THR:HG22	10:P:229:ASP:HA	1.99	0.44
11:U:101:HIS:NE2	11:U:130:PRO:HD2	2.32	0.44
11:U:149:THR:HG21	11:U:293:LEU:CD2	2.47	0.44
15:X:51:DG:H1	16:Y:-51:DC:N4	2.14	0.44
1:A:116:LEU:HB3	1:A:117:PRO:HD3	1.98	0.44
4:D:32:PRO:CB	16:Y:-86:DA:OP2	2.66	0.44
5:I:726:LYS:HA	5:I:726:LYS:HD2	1.39	0.44
5:I:729:LEU:HD23	5:I:757:GLN:O	2.16	0.44
6:J:214:TYR:HB3	10:P:147:ILE:HG23	1.99	0.44
10:N:94:LEU:HD21	10:N:98:THR:CG2	2.48	0.44
12:T:80:GLU:O	12:T:81:ASN:C	2.55	0.44
15:X:50:DT:H1'	15:X:51:DG:H5'	1.98	0.44
15:X:90:DA:C6	15:X:91:DG:C6	3.06	0.44
1:A:121:GLU:N	3:C:41:TYR:OH	2.51	0.44
5:I:640:ILE:HG13	5:I:792:LEU:HD22	2.00	0.44
9:M:319:LEU:C	9:M:319:LEU:HD12	2.37	0.44
10:N:166:THR:HG22	10:N:229:ASP:HA	2.00	0.44
9:O:447:LEU:HD13	10:P:331:GLY:HA2	1.98	0.44
15:X:132:DA:H61	16:Y:-132:DT:H3	1.66	0.44
5:I:96:ILE:HG12	14:W:197:LEU:HD11	1.98	0.44
5:I:178:GLN:O	5:I:178:GLN:NE2	2.50	0.44
5:I:1971:GLU:OE1	5:I:1971:GLU:N	2.45	0.44
5:I:2125:VAL:HG21	5:I:2151:ARG:HG2	2.00	0.44
9:O:326:ILE:N	9:O:326:ILE:HD12	2.32	0.44
9:O:353:ASP:O	9:O:357:ARG:NH1	2.51	0.44
10:P:112:GLU:OE2	9:Q:269:THR:HG21	2.17	0.44



A + a 1		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
9:Q:135:VAL:HG13	9:Q:135:VAL:O	2.18	0.44
9:Q:353:ASP:OD1	9:Q:357:ARG:NH1	2.47	0.44
10:R:435:ASP:OD1	10:R:438:ARG:NH1	2.51	0.44
15:X:36:DG:H2"	15:X:37:DG:OP2	2.16	0.44
15:X:72:DA:H2"	15:X:73:DG:H5'	2.00	0.44
5:I:92:SER:CA	14:W:193:GLU:HG2	2.47	0.44
5:I:751:ILE:HG22	5:I:751:ILE:O	2.18	0.44
10:R:166:THR:HG22	10:R:229:ASP:HA	1.99	0.44
15:X:3:DG:H2"	15:X:4:DG:C8	2.53	0.44
16:Y:-138:DT:H2"	16:Y:-137:DC:C6	2.53	0.44
16:Y:-118:DA:H2"	16:Y:-117:DA:C8	2.53	0.44
16:Y:-64:DG:H1'	16:Y:-63:DC:H5'	2.00	0.44
4:D:78:ARG:CD	15:X:101:DA:H5'	2.48	0.44
9:M:206:CYS:SG	9:M:207:ASP:N	2.90	0.44
10:R:178:MET:O	10:R:182:LEU:HD23	2.18	0.44
12:T:77:VAL:HG12	12:T:78:PRO:HD2	2.00	0.44
11:U:157:ASP:HA	11:U:182:GLY:HA3	2.00	0.44
10:R:378:GLU:HG2	10:R:380:VAL:HG23	2.00	0.43
11:U:306:TYR:O	11:U:308:GLY:N	2.50	0.43
2:B:120:SER:O	2:B:121:SER:OG	2.32	0.43
3:C:61:LEU:HD12	4:D:37:LEU:HD23	2.00	0.43
5:I:678:VAL:CG2	5:I:2123:VAL:HG11	2.48	0.43
10:P:374:ARG:HG2	10:P:403:ILE:HG23	2.01	0.43
11:U:149:THR:HG23	11:U:166:TYR:HA	2.00	0.43
15:X:141:DC:H5"	15:X:141:DC:C6	2.53	0.43
5:I:861:LEU:CD2	5:I:2168:SER:HB2	2.49	0.43
5:I:899:LYS:HE3	5:I:899:LYS:HB2	1.66	0.43
5:I:2088:ARG:NH1	5:I:2090:ASP:OD2	2.51	0.43
8:L:87:LEU:N	8:L:87:LEU:HD22	2.33	0.43
9:M:176:ILE:C	9:M:176:ILE:HD12	2.38	0.43
2:F:31:LYS:HD3	2:F:32:GLU:HG3	1.99	0.43
7:K:115:GLU:O	7:K:117:TYR:N	2.52	0.43
9:O:376:LYS:HG2	9:O:391:LEU:HD11	2.00	0.43
10:P:355:LEU:HD12	10:P:355:LEU:O	2.19	0.43
11:U:70:PRO:HG3	11:U:81:ASP:HB3	2.01	0.43
15:X:78:DT:C2'	15:X:79:DA:C8	3.01	0.43
16:Y:-106:DA:H2"	16:Y:-105:DC:C6	2.53	0.43
16:Y:-11:DT:H2"	16:Y:-10:DA:N7	2.33	0.43
7:K:173:ILE:HG21	7:K:292:MET:O	2.19	0.43
7:K:180:LEU:HD11	7:K:281:LEU:HD21	2.01	0.43
8:L:135:TYR:OH	10:N:169:GLU:O	2.34	0.43



Atom-1	Atom-2	Interatomic	Clash
		distance (A)	overlap (A)
10:R:420:GLU:O	10:R:422:GLN:NE2	2.52	0.43
15:X:72:DA:N3	16:Y:-71:DG:N2	2.66	0.43
5:I:1923:LEU:O	5:I:1927:THR:N	2.48	0.43
7:K:213:SER:OG	7:K:219:ASP:OD2	2.35	0.43
7:K:294:ILE:HG23	7:K:295:PRO:HD3	2.00	0.43
5:I:99:GLN:CG	14:W:201:LEU:CD2	2.92	0.43
5:I:618:LEU:HD22	5:I:618:LEU:N	2.34	0.43
6:J:219:VAL:HG11	6:J:263:ARG:NH1	2.34	0.43
9:Q:143:THR:N	9:Q:153:THR:O	2.51	0.43
10:R:60:LEU:HA	10:R:63:ILE:HD12	2.00	0.43
13:V:245:GLU:OE2	13:V:246:TYR:N	2.50	0.43
1:E:14:ALA:C	16:Y:-115:DT:OP1	2.56	0.43
5:I:2066:THR:O	5:I:2118:THR:N	2.44	0.43
10:N:447:GLN:NE2	9:O:332:ASN:O	2.52	0.43
10:P:130:ARG:HH12	10:P:292:ILE:HG21	1.83	0.43
9:Q:271:ILE:HD13	9:Q:272:THR:N	2.32	0.43
16:Y:-30:DT:H3'	16:Y:-29:DC:C6	2.52	0.43
2:B:28:ARG:NH1	16:Y:-21:DG:P	2.91	0.43
5:I:243:TYR:O	5:I:635:LYS:NZ	2.52	0.43
5:I:682:TRP:NE1	5:I:746:ASP:OD2	2.48	0.43
6:J:170:GLU:O	6:J:174:ARG:NH2	2.52	0.43
10:P:247:ILE:HG22	10:P:276:ILE:HD12	2.00	0.43
10:R:63:ILE:HD13	10:R:295:VAL:HG21	2.01	0.43
16:Y:-116:DT:H5'	16:Y:-116:DT:C6	2.54	0.43
9:M:310:GLU:O	9:M:313:THR:HG22	2.19	0.43
10:P:212:ALA:HB2	10:P:215:TYR:CD1	2.54	0.43
6:J:211:ILE:HG23	6:J:269:SER:HB3	2.01	0.42
7:K:325:LEU:C	7:K:325:LEU:HD23	2.39	0.42
9:M:173:ASP:HB2	10:R:217:ALA:O	2.19	0.42
10:N:166:THR:HG23	10:N:167:GLU:HG3	2.00	0.42
12:T:22:THR:HG22	12:T:38:PRO:HA	2.01	0.42
11:U:2:ASP:OD1	11:U:2:ASP:N	2.52	0.42
13:V:65:LYS:O	13:V:65:LYS:HG2	2.17	0.42
1:A:121:GLU:CG	3:C:41:TYR:OH	2.66	0.42
5:I:2055:LEU:HD23	5:I:2062:VAL:HG12	2.01	0.42
9:O:245:VAL:HG11	10:P:271:GLU:OE2	2.19	0.42
10:P:351:LEU:HD11	10:P:356:ILE:HD11	2.01	0.42
12:T:80:GLU:O	12:T:82:MET:N	2.52	0.42
1:A:54:VAL:HG22	2:B:107:ALA:HB1	2.01	0.42
5:I:697:THR:HG22	5:I:699:TYR:CD1	2.54	0.42
9:M:50:GLY:O	9:M:53:VAL:HG12	2.20	0.42



Atom_1	Atom_2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
10:P:161:LEU:HB2	10:P:174:LEU:HD11	2.00	0.42
12:T:132:LYS:O	12:T:133:ARG:C	2.58	0.42
10:N:68:ILE:HG23	10:N:68:ILE:O	2.19	0.42
10:R:313:ASN:ND2	10:R:349:ASP:OD2	2.52	0.42
3:G:40:ARG:HH12	16:Y:-63:DC:C5'	2.32	0.42
5:I:99:GLN:CB	14:W:201:LEU:HD21	1.99	0.42
5:I:615:ARG:NE	5:I:688:ARG:O	2.53	0.42
10:P:60:LEU:HA	10:P:63:ILE:HD12	2.01	0.42
10:R:375:CYS:SG	10:R:406:ILE:HD13	2.59	0.42
11:U:149:THR:HG22	11:U:150:GLY:N	2.35	0.42
15:X:125:DC:H2"	15:X:126:DC:H5'	2.01	0.42
5:I:902:ASN:HD21	5:I:2137:ASP:CG	2.22	0.42
7:K:277:VAL:HB	7:K:278:PRO:HD3	2.02	0.42
9:O:40:VAL:HG21	9:O:373:GLN:CD	2.40	0.42
9:O:256:ILE:N	9:O:256:ILE:HD12	2.34	0.42
10:P:63:ILE:HD13	10:P:295:VAL:CG2	2.49	0.42
9:Q:192:TYR:O	9:Q:201:LYS:N	2.51	0.42
12:T:124:GLU:OE2	12:T:133:ARG:NH1	2.53	0.42
15:X:86:DT:H2"	15:X:87:DT:O5'	2.18	0.42
15:X:90:DA:H2"	15:X:91:DG:O5'	2.20	0.42
15:X:140:DT:H2"	15:X:141:DC:C5	2.53	0.42
16:Y:-119:DC:H2"	16:Y:-118:DA:C8	2.55	0.42
2:B:116:THR:CG2	13:V:57:VAL:HG13	2.48	0.42
5:I:159:ARG:O	5:I:163:ARG:NH1	2.52	0.42
5:I:928:LEU:HD22	5:I:928:LEU:C	2.39	0.42
9:Q:157:VAL:HG13	9:Q:157:VAL:O	2.20	0.42
11:S:62:ARG:NH2	11:S:207:GLU:OE2	2.53	0.42
5:I:941:ILE:HD11	9:M:236:GLN:HB3	2.02	0.42
10:N:47:VAL:HG11	10:N:369:GLN:HB3	2.02	0.42
10:R:389:VAL:HG21	10:R:423:VAL:HG23	2.02	0.42
3:C:85:GLN:CB	16:Y:-97:DG:OP1	2.68	0.42
5:I:726:LYS:CB	15:X:56:DT:O3'	2.68	0.42
5:I:2141:ASN:HB3	16:Y:-51:DC:H5"	2.02	0.42
7:K:366:ILE:HG23	7:K:371:ASP:OD2	2.20	0.42
10:N:33:LEU:HD23	10:N:39:PRO:HA	2.01	0.42
10:P:147:ILE:HD11	10:P:157:LYS:HB2	2.02	0.42
12:T:79:ARG:HG2	12:T:80:GLU:HB2	2.01	0.42
15:X:92:DC:H42	16:Y:-92:DG:H1	1.67	0.42
15:X:97:DC:H5"	15:X:97:DC:C6	2.49	0.42
5:I:147:LEU:HD11	5:I:151:PHE:CE1	2.55	0.41
7:K:212:VAL:HG11	7:K:282:PHE:CE1	2.54	0.41



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
13:V:57:VAL:O	13:V:61:LEU:HG	2.19	0.41
13:V:222:HIS:O	13:V:225:ARG:HG3	2.20	0.41
14:W:157:THR:HG22	14:W:157:THR:O	2.21	0.41
16:Y:-120:DT:H1'	16:Y:-119:DC:O4'	2.20	0.41
5:I:818:SER:O	5:I:819:GLN:C	2.58	0.41
9:M:262:GLN:O	9:M:263:LEU:O	2.38	0.41
9:M:319:LEU:HD11	9:M:357:ARG:CD	2.50	0.41
10:N:56:ALA:HA	10:N:59:VAL:HG12	2.02	0.41
9:Q:298:VAL:HG13	9:Q:326:ILE:CG2	2.50	0.41
12:T:266:VAL:O	12:T:301:ARG:NH1	2.53	0.41
11:U:185:LEU:HD13	11:U:185:LEU:O	2.20	0.41
13:V:143:TYR:HA	13:V:147:LEU:HD23	2.01	0.41
15:X:25:DC:H1'	15:X:26:DC:C6	2.55	0.41
15:X:103:DC:C6	15:X:104:DT:H72	2.55	0.41
15:X:134:DC:H5'	15:X:134:DC:C6	2.55	0.41
5:I:895:MET:HE1	15:X:51:DG:N2	2.35	0.41
5:I:988:LYS:N	5:I:989:PRO:HD3	2.35	0.41
5:I:2111:ILE:HD12	5:I:2111:ILE:H	1.85	0.41
7:K:3:THR:HG23	7:K:18:SER:CB	2.49	0.41
12:T:205:GLN:CB	12:T:304:ILE:HG23	2.50	0.41
11:U:247:VAL:O	11:U:249:THR:N	2.53	0.41
14:W:38:ARG:NE	14:W:43:HIS:HB2	2.36	0.41
15:X:145:DA:H1'	15:X:146:DG:O4'	2.20	0.41
16:Y:-18:DT:H2'	16:Y:-17:DC:C5	2.55	0.41
5:I:233:LEU:HD22	5:I:803:PHE:CZ	2.56	0.41
5:I:612:LEU:HD13	5:I:613:LEU:H	1.85	0.41
5:I:898:ARG:NH2	5:I:2140:TRP:CZ3	2.87	0.41
5:I:2065:PHE:CE1	5:I:2116:LEU:HD21	2.55	0.41
6:J:267:THR:HG22	9:Q:153:THR:CB	2.51	0.41
9:O:265:LYS:O	9:O:265:LYS:HG2	2.19	0.41
10:R:47:VAL:H	17:R:501:ADP:HN62	1.69	0.41
11:U:305:MET:O	11:U:306:TYR:C	2.58	0.41
16:Y:-9:DT:H2"	16:Y:-8:DA:N7	2.35	0.41
5:I:99:GLN:HG3	14:W:201:LEU:HD22	2.01	0.41
5:I:1930:GLN:HB3	5:I:1931:PRO:HD3	2.02	0.41
5:I:1973:ILE:HG23	5:I:1977:ILE:HD12	2.01	0.41
7:K:70:VAL:O	7:K:74:VAL:HG23	2.21	0.41
9:M:106:ILE:HG23	9:M:269:THR:HG23	2.03	0.41
10:N:59:VAL:HG23	10:N:62:MET:CE	2.51	0.41
9:O:106:ILE:HD12	9:O:106:ILE:HA	1.96	0.41
10:P:305:ASP:OD1	10:P:306:ILE:N	2.47	0.41



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
9:Q:319:LEU:HD21	9:Q:327:VAL:HG21	2.02	0.41
15:X:20:DA:N1	15:X:21:DC:C4	2.88	0.41
15:X:59:DA:H2"	15:X:60:DA:H5"	2.02	0.41
1:A:123:HIS:HB3	7:K:238:LEU:HD12	2.03	0.41
7:K:69:ASP:OD1	7:K:70:VAL:HG23	2.21	0.41
9:M:408:GLN:OE1	10:N:71:ARG:NH1	2.54	0.41
10:P:137:ILE:HG22	10:P:196:ASP:HA	2.02	0.41
10:R:197:LYS:O	10:R:198:ALA:HB3	2.21	0.41
10:R:335:ILE:HD11	10:R:342:SER:OG	2.20	0.41
11:U:6:ALA:O	11:U:102:PRO:HD2	2.21	0.41
15:X:110:DC:H2"	15:X:111:DG:H8	1.85	0.41
15:X:123:DG:H2"	15:X:124:DG:C8	2.55	0.41
5:I:1900:ARG:O	5:I:1904:ILE:HG23	2.20	0.41
7:K:41:THR:HG22	7:K:42:ALA:H	1.86	0.41
10:N:415:LYS:NZ	9:O:54:GLU:OE2	2.53	0.41
13:V:92:VAL:HG22	13:V:92:VAL:O	2.20	0.41
15:X:43:DA:C8	15:X:44:DT:H72	2.56	0.41
16:Y:-85:DC:C2'	16:Y:-84:DG:C8	2.99	0.41
3:C:66:PRO:HG3	15:X:90:DA:C5'	2.45	0.41
3:G:41:TYR:HA	15:X:143:DC:OP1	2.20	0.41
5:I:95:GLU:HB3	14:W:197:LEU:CD2	2.51	0.41
6:J:209:GLY:O	6:J:211:ILE:HG22	2.20	0.41
10:P:249:VAL:HG11	10:P:259:ALA:CA	2.47	0.41
10:P:261:PHE:CZ	10:P:264:ASP:O	2.74	0.41
14:W:39:GLU:HB2	16:Y:-82:DA:C5'	2.45	0.41
16:Y:-110:DG:H2"	16:Y:-109:DT:C6	2.56	0.41
16:Y:-15:DC:H2"	16:Y:-14:DA:H8	1.85	0.41
7:K:225:LEU:HD23	7:K:225:LEU:H	1.85	0.41
7:K:310:GLN:N	7:K:311:PRO:HD2	2.36	0.41
9:M:263:LEU:O	9:M:263:LEU:HD12	2.21	0.41
9:M:396:GLU:O	9:M:399:THR:OG1	2.27	0.41
10:N:59:VAL:HG23	10:N:62:MET:HE3	2.02	0.41
10:N:331:GLY:O	10:N:344:HIS:N	2.50	0.41
9:O:180:LEU:CD2	9:O:200:VAL:HG11	2.51	0.41
10:P:47:VAL:CG2	10:P:373:ILE:HD12	2.51	0.41
10:P:121:GLN:NE2	10:P:265:THR:OG1	2.51	0.41
10:P:260:LEU:O	10:P:261:PHE:CD1	2.74	0.41
9:Q:247:ASN:CG	9:Q:279:ILE:HD11	2.41	0.41
10:R:52:ALA:HB2	10:R:358:SER:O	2.21	0.41
14:W:30:VAL:HG12	14:W:135:VAL:HG22	2.03	0.41
15:X:78:DT:H2"	15:X:79:DA:C8	2.56	0.41



Atom-1	Atom-2	Interatomic	Clash
	Atom-2	distance (Å)	overlap (Å)
16:Y:-120:DT:H2"	16:Y:-119:DC:OP2	2.20	0.41
16:Y:-32:DT:H1'	16:Y:-31:DC:H5'	2.03	0.41
3:G:97:GLU:O	3:G:101:VAL:HG23	2.21	0.41
5:I:1969:LEU:O	5:I:1970:SER:C	2.60	0.41
5:I:2142:PRO:C	5:I:2144:MET:H	2.24	0.41
9:0:175:SER:O	9:O:254:GLN:NE2	2.50	0.41
9:O:270:GLU:HG3	9:O:275:LEU:HD12	2.02	0.41
10:P:144:GLU:N	10:P:162:THR:OG1	2.54	0.41
12:T:412:SER:OG	13:V:107:ASP:OD2	2.29	0.41
11:U:216:LEU:HD22	11:U:216:LEU:N	2.35	0.41
15:X:43:DA:H2'	15:X:44:DT:C7	2.51	0.41
15:X:120:DA:H5"	15:X:120:DA:C8	2.56	0.41
15:X:139:DT:H2"	15:X:140:DT:C6	2.56	0.41
3:G:106:ASP:OD2	3:G:131:ARG:NE	2.54	0.40
7:K:6:LEU:HD13	7:K:93:ILE:HD11	2.03	0.40
9:M:170:LEU:HD12	10:R:216:ASP:CG	2.42	0.40
9:M:170:LEU:N	9:M:170:LEU:HD22	2.36	0.40
9:Q:276:ARG:HA	9:Q:276:ARG:NE	2.36	0.40
15:X:52:DG:C2'	15:X:53:DC:H5'	2.52	0.40
16:Y:-141:DG:H2"	16:Y:-140:DA:C8	2.56	0.40
16:Y:-61:DT:H2"	16:Y:-60:DT:C6	2.56	0.40
1:A:47:ALA:N	1:A:48:PRO:HD2	2.37	0.40
2:B:74:ALA:HB2	2:B:91:ILE:HD13	2.03	0.40
5:I:92:SER:OG	14:W:193:GLU:CG	2.58	0.40
5:I:1893:ARG:NH2	7:K:344:ASP:OD2	2.52	0.40
5:I:2061:ARG:NH1	5:I:2111:ILE:O	2.54	0.40
9:M:55:LEU:HD21	9:M:61:MET:HB3	2.03	0.40
9:M:61:MET:HE1	10:R:22:ILE:HD11	2.03	0.40
9:O:450:GLN:OE1	10:P:78:GLN:NE2	2.54	0.40
11:S:324:THR:HG21	15:X:116:DA:C3'	2.51	0.40
16:Y:-50:DA:C4'	16:Y:-50:DA:OP1	2.69	0.40
2:B:91:ILE:O	2:B:95:VAL:HG23	2.21	0.40
7:K:151:GLY:O	7:K:323:ASN:ND2	2.54	0.40
9:M:415:LEU:HD21	10:N:61:GLU:CB	2.50	0.40
12:T:70:ILE:HD13	12:T:105:HIS:CD2	2.56	0.40
13:V:266:GLN:O	13:V:270:LYS:HG2	2.21	0.40
7:K:240:ASP:OD1	7:K:242:SER:OG	2.24	0.40
9:M:106:ILE:HG23	9:M:269:THR:CG2	2.51	0.40
10:N:99:PRO:O	10:N:295:VAL:N	2.52	0.40
9:Q:323:ILE:HD12	9:Q:323:ILE:N	2.37	0.40
15:X:39:DA:H2"	15:X:40:DG:H8	1.86	0.40



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:723:THR:OG1	5:I:724:SER:N	2.55	0.40
5:I:780:ASN:O	5:I:2183:LYS:NZ	2.51	0.40
5:I:2076:GLU:OE1	5:I:2086:TYR:OH	2.40	0.40
9:M:24:LEU:HA	9:M:39:LEU:HD12	2.02	0.40
9:Q:159:ILE:HD11	9:Q:191:ILE:HD11	2.02	0.40
10:R:378:GLU:CG	10:R:380:VAL:HG23	2.52	0.40
15:X:3:DG:H2"	15:X:4:DG:H8	1.86	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	entiles
1	А	114/130~(88%)	110 (96%)	4 (4%)	0	100	100
1	Е	103/130~(79%)	102 (99%)	1 (1%)	0	100	100
2	В	94/126~(75%)	93 (99%)	1 (1%)	0	100	100
2	F	92/126~(73%)	86 (94%)	4 (4%)	2(2%)	6	35
3	С	93/136~(68%)	88 (95%)	2 (2%)	3 (3%)	4	26
3	G	95/136~(70%)	93~(98%)	2 (2%)	0	100	100
4	D	79/103~(77%)	78~(99%)	1 (1%)	0	100	100
4	Н	78/103~(76%)	75~(96%)	3 (4%)	0	100	100
5	Ι	844/3230~(26%)	808 (96%)	32 (4%)	4 (0%)	29	67
6	J	129/364~(35%)	120 (93%)	8 (6%)	1 (1%)	19	58
7	Κ	392/396~(99%)	353 (90%)	36 (9%)	3 (1%)	19	58
8	L	101/154~(66%)	95~(94%)	5 (5%)	1 (1%)	15	54
9	М	424/456~(93%)	406 (96%)	17 (4%)	1 (0%)	47	79
9	0	431/456 (94%)	417 (97%)	14 (3%)	0	100	100



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
9	Q	438/456~(96%)	409 (93%)	26~(6%)	3~(1%)	22	61
10	Ν	409/463~(88%)	394 (96%)	15 (4%)	0	100	100
10	Р	423/463~(91%)	401 (95%)	20~(5%)	2~(0%)	29	67
10	R	420/463~(91%)	406 (97%)	14 (3%)	0	100	100
11	S	373/375~(100%)	370~(99%)	3(1%)	0	100	100
11	U	355/375~(95%)	311 (88%)	44 (12%)	0	100	100
12	Т	399/429~(93%)	387~(97%)	11 (3%)	1 (0%)	41	74
13	V	200/467~(43%)	190 (95%)	10 (5%)	0	100	100
14	W	185/227~(82%)	177 (96%)	6 (3%)	2(1%)	14	51
All	All	6271/9764~(64%)	5969 (95%)	279 (4%)	23(0%)	38	69

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	Р	261	PHE
9	Q	278	GLU
9	Q	279	ILE
7	К	201	VAL
9	М	263	LEU
2	F	29	SER
5	Ι	757	GLN
5	Ι	758	ARG
5	Ι	2143	THR
7	Κ	194	HIS
8	L	46	ALA
14	W	85	PRO
2	F	30	ARG
5	Ι	2142	PRO
7	Κ	200	HIS
9	Q	269	THR
3	С	42	ARG
10	Р	263	GLY
12	Т	81	ASN
14	W	86	TYR
6	J	208	PRO
3	С	44	GLY
3	С	43	PRO



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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
1	А	91/99~(92%)	87~(96%)	4 (4%)	28	64
1	Ε	82/99~(83%)	77~(94%)	5~(6%)	18	54
2	В	83/106~(78%)	76~(92%)	7 (8%)	11	39
2	F	81/106~(76%)	78~(96%)	3~(4%)	34	68
3	С	82/111~(74%)	74 (90%)	8 (10%)	8	31
3	G	85/111 (77%)	84 (99%)	1 (1%)	71	88
4	D	66/79~(84%)	66 (100%)	0	100	100
4	Н	65/79~(82%)	65~(100%)	0	100	100
5	Ι	765/2721~(28%)	691~(90%)	74 (10%)	8	31
6	J	123/312~(39%)	105~(85%)	18 (15%)	3	15
7	Κ	359/361~(99%)	336~(94%)	23~(6%)	17	52
8	L	89/133~(67%)	83~(93%)	6 (7%)	16	50
9	М	361/387~(93%)	342 (95%)	19 (5%)	22	58
9	Ο	364/387~(94%)	342 (94%)	22~(6%)	19	54
9	Q	366/387~(95%)	349~(95%)	17 (5%)	27	63
10	Ν	351/390~(90%)	343~(98%)	8 (2%)	50	78
10	Р	352/390~(90%)	334 (95%)	18 (5%)	24	60
10	R	358/390~(92%)	339~(95%)	19 (5%)	22	58
11	S	318/318~(100%)	318 (100%)	0	100	100
11	U	305/318~(96%)	281 (92%)	24 (8%)	12	43
12	Т	346/364~(95%)	336~(97%)	10 (3%)	42	74
13	V	$18\overline{3}/400~(46\%)$	162 (88%)	21 (12%)	5	24
14	W	168/203~(83%)	163~(97%)	5(3%)	41	73
All	All	5443/8251 (66%)	5131 (94%)	312 (6%)	24	56

All (312) residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	А	20	ARG
1	А	36	LYS
1	А	50	TYR
1	А	84	GLN
2	В	36	VAL
2	В	44	GLN
2	В	46	HIS
2	В	60	ASN
2	В	77	LEU
2	В	89	ARG
2	В	113	LYS
3	С	42	ARG
3	С	53	ARG
3	С	64	LYS
3	С	79	LYS
3	С	82	LEU
3	С	115	LYS
3	С	120	MET
3	С	122	LYS
1	Е	68	ASN
1	Е	73	ASN
1	Е	76	THR
1	Е	81	ARG
1	Е	118	LYS
2	F	28	ARG
2	F	30	ARG
2	F	31	LYS
3	G	129	ARG
5	Ι	109	ARG
5	Ι	118	PHE
5	Ι	120	SER
5	Ι	132	ARG
5	Ι	138	ASP
5	Ι	142	GLU
5	Ι	144	MET
5	Ι	145	GLN
5	Ι	163	ARG
5	Ι	167	ARG
5	Ι	177	ARG
5	Ι	178	GLN
5	Ι	182	ARG
5	Ι	190	LYS
5	Ι	193	ARG



Mol	Chain	Res	Type
5	Ι	200	LYS
5	Ι	201	ASP
5	Ι	226	LYS
5	Ι	241	GLU
5	Ι	246	LEU
5	Ι	249	GLN
5	Ι	612	LEU
5	Ι	629	LEU
5	Ι	649	LYS
5	Ι	663	GLU
5	Ι	703	LYS
5	Ι	712	TRP
5	Ι	726	LYS
5	Ι	730	GLN
5	Ι	732	HIS
5	Ι	742	TYR
5	Ι	756	SER
5	Ι	758	ARG
5	Ι	784	GLU
5	Ι	785	LEU
5	Ι	798	GLN
5	Ι	800	HIS
5	Ι	801	ARG
5	Ι	807	PHE
5	Ι	820	GLU
5	Ι	821	TYR
5	Ι	847	LYS
5	Ι	852	LYS
5	Ι	857	ILE
5	Ι	860	ARG
5	Ι	864	ARG
5	Ι	899	LYS
5	Ι	928	LEU
5	Ι	936	HIS
5	Ι	938	LEU
5	Ι	949	ILE
5	Ι	958	TYR
5	Ι	966	ARG
5	Ι	1886	LEU
5	Ι	1936	ILE
5	Ι	1945	HIS
5	Ι	1947	THR



Mol	Chain	Res Type	
5	Ι	2015	TRP
5	Ι	2029	ARG
5	Ι	2075	LEU
5	Ι	2078	PHE
5	Ι	2085	LEU
5	Ι	2088	ARG
5	Ι	2090	ASP
5	Ι	2094	ARG
5	Ι	2116	LEU
5	Ι	2120	SER
5	Ι	2138	SER
5	Ι	2139	ASP
5	Ι	2140	TRP
5	Ι	2143	THR
5	Ι	2176	ILE
5	Ι	2177	LEU
5	Ι	2192	GLU
6	J	130	ARG
6	J	131	LYS
6	J	134	ARG
6	J	177	LYS
6	J	181	GLU
6	J	188	GLU
6	J	192	ARG
6	J	206	LYS
6	J	216	SER
6	J	217	VAL
6	J	219	VAL
6	J	260	ARG
6	J	261	CYS
6	J	262	SER
6	J	263	ARG
6	J	267	THR
6	J	306	THR
6	J	323	TYR
7	K	36	ARG
7	K	41	THR
7	K	71	GLN
7	Κ	72	ARG
7	K	85	GLN
7	K	88	PHE
7	Κ	113	LEU



Mol	Chain	Chain Res Type	
7	K	118	GLN
7	К	124	ARG
7	K	168	GLU
7	K	172	ARG
7	K	190	TYR
7	K	202	ILE
7	K	206	LYS
7	K	255	MET
7	K	268	LEU
7	K	273	GLU
7	K	274	ARG
7	K	289	ILE
7	K	294	ILE
7	K	325	LEU
7	K	330	ARG
7	K	356	ILE
8	L	19	LEU
8	L	21	ARG
8	L	40	PHE
8	L	88	LEU
8	L	91	GLN
8	L	148	ARG
9	М	53	VAL
9	М	170	LEU
9	М	182	LYS
9	М	186	GLU
9	М	215	LEU
9	М	218	GLU
9	М	235	ILE
9	М	256	ILE
9	М	260	MET
9	М	263	LEU
9	М	267	LYS
9	М	271	ILE
9	М	274	LYS
9	М	313	THR
9	М	317	ARG
9	М	357	ARG
9	М	362	ARG
9	М	378	ARG
9	М	433	ILE
10	Ν	149	ARG



Mol	Chain	Res	Type
10	Ν	201	LYS
10	N	205	LEU
10	N	209	PHE
10	N	325	ILE
10	N	351	LEU
10	N	381	GLU
10	Ν	444	LYS
9	0	18	HIS
9	0	34	GLN
9	0	55	LEU
9	0	60	LYS
9	0	184	ARG
9	0	221	VAL
9	0	263	LEU
9	0	265	LYS
9	0	268	LYS
9	0	269	THR
9	0	273	ASP
9	0	274	LYS
9	0	275	LEU
9	0	285	LYS
9	0	342	GLU
9	0	353	ASP
9	0	362	ARG
9	0	363	THR
9	0	364	MET
9	0	378	ARG
9	0	391	LEU
9	0	415	LEU
10	Р	21	ARG
10	Р	28	ILE
10	Р	68	ILE
10	Р	147	ILE
10	Р	178	MET
10	Р	209	PHE
10	Р	236	LYS
10	Р	255	GLN
10	Р	261	PHE
10	Р	267	GLU
10	Р	286	GLU
10	Р	330	ARG
10	Р	348	ILE



Mol	Chain	Res	Type
10	Р	354	LEU
10	Р	376	GLU
10	Р	428	ARG
10	Р	429	VAL
10	Р	448	ASP
9	Q	13	GLN
9	Q	177	PHE
9	Q	180	LEU
9	Q	182	LYS
9	Q	196	ASN
9	Q	209	TYR
9	Q	215	LEU
9	Q	236	GLN
9	Q	260	MET
9	Q	271	ILE
9	Q	276	ARG
9	Q	317	ARG
9	Q	389	GLU
9	Q	391	LEU
9	Q	404	ARG
9	Q	427	LYS
9	Q	431	GLU
10	R	21	ARG
10	R	22	ILE
10	R	67	LYS
10	R	68	ILE
10	R	205	LEU
10	R	207	ARG
10	R	211	ARG
10	R	221	GLN
10	R	223	LYS
10	R	246	GLU
10	R	250	ILE
10	R	251	ASN
10	R	258	LEU
10	R	374	ARG
10	R	392	ARG
10	R	422	GLN
10	R	434	LEU
10	R	435	ASP
10	R	444	LYS
12	Т	10	GLU



Mol	Chain	Res	Type	
12	Т	24	ARG	
12	Т	79	ARG	
12	Т	103	LEU	
12	Т	107	TYR	
12	Т	110	HIS	
12	Т	247	THR	
12	Т	317	LEU	
12	Т	383	ASN	
12	Т	399	ILE	
11	U	28	ARG	
11	U	62	ARG	
11	U	78	ASN	
11	U	107	GLU	
11	U	121	GLN	
11	U	123	MET	
11	U	147	ARG	
11	U	161	HIS	
11	U	165	ILE	
11	U	192	ILE	
11	U	194	THR	
11	U	U 196 AF		
11	U	198	TYR	
11	U	210	ARG	
11	U	227	MET	
11	U	270	GLU	
11	U	282	ILE	
11	U	312	ARG	
11	U	326	LYS	
11	U	330	ILE	
11	U	334	GLU	
11	U	353	GLN	
11	U	359	LYS	
11	U	369	ILE	
13	V	51	GLU	
13	V	53	MET	
13	V	56	GLU	
13	V	65	LYS	
13	V	91	LYS	
13	V	96	LYS	
13	V	119	GLU	
13	V	145	LEU	
13	V	222	2 HIS	



Mol	Chain	Res	Type
13	V	224	ARG
13	V	229	GLN
13	V	230	LEU
13	V	237	THR
13	V	244	GLU
13	V	245	GLU
13	V	247	LEU
13	V	249	GLN
13	V	252	ARG
13	V	255	GLU
13	V	261	ARG
13	V	262	GLU
14	W	38	ARG
14	W	83	LYS
14	W	87	GLU
14	W	166	TYR
14	W	170	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain Res		Type
2	В	44	GLN
2	В	92	GLN
4	D	75	HIS
2	F	46	HIS
3	G	76	GLN
5	Ι	136	HIS
5	Ι	145	GLN
5	Ι	178	GLN
5	Ι	249	GLN
5	Ι	252	ASN
5	Ι	652	GLN
5	Ι	733	GLN
5	Ι	750	ASN
5	Ι	892	ASN
5	Ι	936	HIS
5	Ι	2067	GLN
6	J	202	HIS
7	К	139	ASN
7	К	214	GLN
7	K	304	ASN
7	K	310	GLN



Mol	Chain	Res	Type
9	М	203	GLN
9	М	236	GLN
10	N	240	HIS
10	N	245	HIS
10	N	302	HIS
9	0	156	HIS
9	0	241	HIS
9	0	408	GLN
9	0	451	GLN
10	Р	25	HIS
10	Р	44	GLN
10	Р	121	GLN
10	Р	275	GLN
10	R	422	GLN
12	Т	143	HIS
12	Т	327	HIS
12	Т	383	ASN
12	Т	408	GLN
11	U	12	ASN
11	U	78	ASN
11	U	111	ASN
11	U	280	ASN
11	U	371	HIS
13	V	235	ASN
13	V	249	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.



5.6 Ligand geometry (i)

10 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with |Z| > 2 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mal	Tuno	Chain	Dog	Tink	Bo	Bond lengths			ond ang	gles
WIOI	Type	Ullalli	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
18	ATP	K	401	-	26,33,33	0.92	1 (3%)	31,52,52	1.59	6 (19%)
17	ADP	N	501	-	24,29,29	0.95	1 (4%)	29,45,45	1.55	4 (13%)
17	ADP	М	501	-	24,29,29	0.95	1 (4%)	29,45,45	1.53	5 (17%)
18	ATP	U	401	-	26,33,33	0.93	1 (3%)	31,52,52	1.61	6 (19%)
17	ADP	0	501	-	24,29,29	0.94	1 (4%)	29,45,45	1.54	5 (17%)
17	ADP	Ι	3301	-	24,29,29	0.96	1 (4%)	29,45,45	1.45	4 (13%)
17	ADP	Q	501	-	24,29,29	0.96	1 (4%)	29,45,45	1.46	5 (17%)
17	ADP	R	501	-	24,29,29	0.95	1 (4%)	29,45,45	1.49	4 (13%)
18	ATP	Т	501	-	26,33,33	0.93	1 (3%)	31,52,52	1.62	6 (19%)
17	ADP	Р	501	-	24,29,29	0.95	1 (4%)	29,45,45	1.56	5 (17%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	ATP	K	401	-	-	4/18/38/38	0/3/3/3
17	ADP	Ν	501	-	-	4/12/32/32	0/3/3/3
17	ADP	М	501	-	-	3/12/32/32	0/3/3/3
18	ATP	U	401	-	-	4/18/38/38	0/3/3/3
17	ADP	0	501	-	-	5/12/32/32	0/3/3/3
17	ADP	Ι	3301	-	-	6/12/32/32	0/3/3/3
17	ADP	Q	501	-	-	5/12/32/32	0/3/3/3
17	ADP	R	501	-	-	1/12/32/32	0/3/3/3
18	ATP	Т	501	-	-	3/18/38/38	0/3/3/3
17	ADP	Р	501	-	-	4/12/32/32	0/3/3/3



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	R	501	ADP	C5-C4	2.47	1.47	1.40
17	Ι	3301	ADP	C5-C4	2.45	1.47	1.40
17	Q	501	ADP	C5-C4	2.45	1.47	1.40
18	Т	501	ATP	C5-C4	2.44	1.47	1.40
18	U	401	ATP	C5-C4	2.44	1.47	1.40
18	Κ	401	ATP	C5-C4	2.43	1.47	1.40
17	Ν	501	ADP	C5-C4	2.42	1.47	1.40
17	М	501	ADP	C5-C4	2.40	1.47	1.40
17	Р	501	ADP	C5-C4	2.39	1.47	1.40
17	Ō	501	ADP	C5-C4	2.34	1.47	1.40

All (10) bond length outliers are listed below:

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
17	Р	501	ADP	PA-O3A-PB	-3.85	119.60	132.83
18	U	401	ATP	PB-O3B-PG	-3.73	120.03	132.83
17	Ν	501	ADP	PA-O3A-PB	-3.70	120.13	132.83
17	Р	501	ADP	N3-C2-N1	-3.70	122.90	128.68
17	0	501	ADP	PA-O3A-PB	-3.69	120.15	132.83
18	Κ	401	ATP	N3-C2-N1	-3.69	122.91	128.68
17	0	501	ADP	N3-C2-N1	-3.69	122.92	128.68
17	М	501	ADP	N3-C2-N1	-3.67	122.94	128.68
18	Т	501	ATP	N3-C2-N1	-3.66	122.95	128.68
17	Q	501	ADP	N3-C2-N1	-3.65	122.97	128.68
17	Ν	501	ADP	N3-C2-N1	-3.64	122.99	128.68
17	Ι	3301	ADP	N3-C2-N1	-3.63	123.00	128.68
18	U	401	ATP	N3-C2-N1	-3.63	123.01	128.68
17	R	501	ADP	PA-O3A-PB	-3.61	120.42	132.83
18	Т	501	ATP	PA-O3A-PB	-3.54	120.68	132.83
17	Ν	501	ADP	C3'-C2'-C1'	3.54	106.30	100.98
18	Т	501	ATP	PB-O3B-PG	-3.52	120.74	132.83
17	М	501	ADP	C3'-C2'-C1'	3.51	106.27	100.98
18	Κ	401	ATP	PB-O3B-PG	-3.49	120.85	132.83
17	Р	501	ADP	C3'-C2'-C1'	3.44	106.16	100.98
17	R	501	ADP	C3'-C2'-C1'	3.42	106.13	100.98
17	М	501	ADP	PA-O3A-PB	-3.36	121.29	132.83
17	0	501	ADP	C3'-C2'-C1'	3.36	106.04	100.98
17	Q	501	ADP	C3'-C2'-C1'	3.36	106.03	100.98
18	Κ	401	ATP	PA-O3A-PB	-3.34	121.37	132.83
18	Т	501	ATP	C3'-C2'-C1'	3.29	105.92	100.98
18	U	401	ATP	C3'-C2'-C1'	3.24	105.86	100.98
17	Ι	3301	ADP	PA-O3A-PB	-3.22	121.77	132.83



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
18	К	401	ATP	C3'-C2'-C1'	3.20	105.79	100.98
18	U	401	ATP	PA-O3A-PB	-3.18	121.90	132.83
17	Ι	3301	ADP	C3'-C2'-C1'	3.17	105.75	100.98
17	R	501	ADP	N3-C2-N1	-3.15	123.75	128.68
17	Q	501	ADP	PA-O3A-PB	-3.01	122.50	132.83
18	K	401	ATP	C4-C5-N7	-2.79	106.50	109.40
17	Р	501	ADP	C4-C5-N7	-2.77	106.51	109.40
17	Ι	3301	ADP	C4-C5-N7	-2.76	106.52	109.40
18	Т	501	ATP	C4-C5-N7	-2.75	106.53	109.40
17	0	501	ADP	C4-C5-N7	-2.69	106.60	109.40
17	R	501	ADP	C4-C5-N7	-2.68	106.61	109.40
17	Q	501	ADP	C4-C5-N7	-2.67	106.61	109.40
17	М	501	ADP	C4-C5-N7	-2.65	106.64	109.40
18	U	401	ATP	C4-C5-N7	-2.59	106.70	109.40
17	Ν	501	ADP	C4-C5-N7	-2.58	106.71	109.40
17	М	501	ADP	C2-N1-C6	2.07	122.30	118.75
18	U	401	ATP	C2-N1-C6	2.04	122.25	118.75
18	Т	501	ATP	C2-N1-C6	2.04	122.25	118.75
18	K	401	ATP	C2-N1-C6	2.04	122.24	118.75
17	Q	501	ADP	C2-N1-C6	2.03	122.23	118.75
17	0	501	ADP	C2-N1-C6	2.03	122.22	118.75
17	Р	501	ADP	C2-N1-C6	2.02	122.20	118.75

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	Ι	3301	ADP	C5'-O5'-PA-O3A
17	М	501	ADP	PA-O3A-PB-O2B
17	М	501	ADP	PA-O3A-PB-O3B
17	Ν	501	ADP	C5'-O5'-PA-O1A
17	Ν	501	ADP	C5'-O5'-PA-O2A
17	0	501	ADP	C5'-O5'-PA-O1A
17	0	501	ADP	C5'-O5'-PA-O2A
17	Р	501	ADP	C5'-O5'-PA-O3A
17	Q	501	ADP	C5'-O5'-PA-O2A
18	Κ	401	ATP	C5'-O5'-PA-O2A
18	Κ	401	ATP	C5'-O5'-PA-O3A
18	Κ	401	ATP	C3'-C4'-C5'-O5'
18	Т	501	ATP	C5'-O5'-PA-O2A
18	Т	501	ATP	C5'-O5'-PA-O3A
18	U	401	ATP	C5'-O5'-PA-O3A



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Mol	Chain	Res	Type	Atoms
18	U	401	ATP	C3'-C4'-C5'-O5'
17	Р	501	ADP	O4'-C4'-C5'-O5'
17	Р	501	ADP	C3'-C4'-C5'-O5'
17	Ι	3301	ADP	O4'-C4'-C5'-O5'
17	Ι	3301	ADP	C3'-C4'-C5'-O5'
18	U	401	ATP	O4'-C4'-C5'-O5'
18	K	401	ATP	O4'-C4'-C5'-O5'
17	0	501	ADP	O4'-C4'-C5'-O5'
17	Q	501	ADP	PA-O3A-PB-O3B
17	Ν	501	ADP	C5'-O5'-PA-O3A
17	Q	501	ADP	C5'-O5'-PA-O3A
17	Ι	3301	ADP	C5'-O5'-PA-O1A
17	Ι	3301	ADP	C5'-O5'-PA-O2A
17	Р	501	ADP	C5'-O5'-PA-O1A
17	Q	501	ADP	C5'-O5'-PA-O1A
18	U	401	ATP	C5'-O5'-PA-O2A
18	Т	501	ATP	C3'-C4'-C5'-O5'
17	0	501	ADP	C3'-C4'-C5'-O5'
17	Q	501	ADP	PA-O3A-PB-O2B
17	0	501	ADP	C5'-O5'-PA-O3A
17	Ι	3301	ADP	PB-O3A-PA-O2A
17	М	501	ADP	O4'-C4'-C5'-O5'
17	N	501	ADP	O4'-C4'-C5'-O5'
17	R	501	ADP	O4'-C4'-C5'-O5'

Continued from previous page...

There are no ring outliers.

6 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	K	401	ATP	1	0
17	М	501	ADP	1	0
18	U	401	ATP	1	0
17	0	501	ADP	2	0
17	R	501	ADP	2	0
17	Р	501	ADP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be



highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.






















5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-37990. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

6.1.1 Primary map



6.1.2 Raw map



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



6.2 Central slices (i)

6.2.1 Primary map



X Index: 200



Y Index: 200



Z Index: 200

6.2.2 Raw map



X Index: 200

Y Index: 200

Z Index: 200

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: 218



Y Index: 206



Z Index: 226

6.3.2 Raw map



X Index: 217

Y Index: 205



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



6.4 Orthogonal standard-deviation projections (False-color) (i)

6.4.1 Primary map



6.4.2 Raw map



The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.



6.5 Orthogonal surface views (i)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.026. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

6.6 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 528 $\rm nm^3;$ this corresponds to an approximate mass of 477 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 0.312 $\rm \AA^{-1}$



8 Fourier-Shell correlation (i)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.312 ${\rm \AA^{-1}}$



8.2 Resolution estimates (i)

$\mathbf{B}_{\mathrm{assolution ostimato}}(\mathbf{\hat{\lambda}})$	Estimation criterion (FSC cut-off)		
Resolution estimate (A)	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.91	4.76	3.99

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.91 differs from the reported value 3.2 by more than 10 %



9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-37990 and PDB model 8X1C. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay (i)



The images above show the 3D surface view of the map at the recommended contour level 0.026 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 (0.026).



9.4 Atom inclusion (i)



At the recommended contour level, 79% of all backbone atoms, 71% of all non-hydrogen atoms, are inside the map.



1.0

0.0 <0.0

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.026) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7110	0.2970
А	0.7730	0.2670
В	0.8080	0.3070
С	0.7840	0.3120
D	0.8610	0.3610
Е	0.8790	0.4280
F	0.8790	0.4090
G	0.8930	0.4450
Н	0.8840	0.4420
Ι	0.7900	0.3700
J	0.6860	0.2640
К	0.7880	0.2910
L	0.7790	0.2790
М	0.8560	0.4210
Ν	0.8710	0.4260
0	0.8390	0.3980
Р	0.8630	0.4380
Q	0.8590	0.4330
R	0.8660	0.4580
S	0.4050	0.0600
Т	0.3090	0.0010
U	0.3030	0.0140
V	0.0750	0.0230
W	0.0190	-0.0010
Х	0.8550	0.2750
Y	0.8720	0.2790

