

May 4, 2025 - 08:30 am BST

PDB ID	:	$9{ m GMA}~/~{ m pdb}\_00009{ m gma}$
EMDB ID	:	EMD-51446
Title	:	MukBEF in a DNA capture state (dimer)
Authors	:	Burmann, F.; Lowe, J.
Deposited on	:	2024-08-28
Resolution	:	9.10  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.dev118
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0rc1
buster-report	:	1.1.7(2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

## 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 9.10 Å.

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



Metric	Whole archive	EM structures
	$(\# { m Entries})$	$(\# { m Entries})$
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	1482	92%	7% •
1	В	1482	85%	13% ••
1	Ο	1482	92%	7% •
1	Р	1482	96%	15% ••
2	С	440	87%	12% ·
2	D	440	87%	12% ·
3	Е	240	• 68% 20%	• 12%
3	F	240	62% 19% ·	18%



Mol	Chain	Length	Quality of chain				
3	Q	240	69%	19%		1	2%
3	R	240	68%	21%		18%	
4	G	78	67%	24%		•	8%
4	Ι	78	78%		13%	•	8%
4	М	78	90%		13%	·	8%
4	S	78	92% 65%	26%		•	8%
5	Κ	2124	97%			_	
6	L	2124	97%		_	_	_

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	4HH	G	36	-	-	Х	-
4	4HH	S	36	-	-	Х	-



## 2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 130919 atoms, of which 64362 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.

Mol	Chain	Residues				AltConf	Trace			
1	Δ	1467	Total	С	Η	Ν	Ο	S	0	0
1	A	1407	23547	7298	11707	2188	2314	40	0	0
1	D	1467	Total	С	Н	Ν	Ο	S	0	0
	D	1407	23546	7298	11706	2188	2314	40	0	0
1	0	1467	Total	С	Н	Ν	Ο	S	0	0
	0	1407	23547	7298	11707	2188	2314	40	0	0
1	D	1467	Total	С	Н	Ν	Ο	S	0	0
1	Г	1407	23546	7298	11706	2188	2314	40	0	0

• Molecule 1 is a protein called Chromosome partition protein MukB.

• Molecule 2 is a protein called Chromosome partition protein MukF.

Mol	Chain	Residues				AltConf	Trace			
9	С	440	Total	С	Н	Ν	0	S	0	0
		440	6982	2218	3451	614	686	13	0	0
0	П	440	Total	С	Η	Ν	0	S	0	0
	D	440	6982	2218	3451	614	686	13	0	0

• Molecule 3 is a protein called Chromosome partition protein MukE.

Mol	Chain	Residues			Atom		AltConf	Trace		
2	F	212	Total	С	Η	Ν	0	S	0	0
J	Ľ	212	3441	1090	1719	301	322	9	0	0
3	F	108	Total	С	Η	Ν	0	S	0	0
5	T,	190	3246	1029	1627	284	298	8	0	0
3	0	919	Total	С	Η	Ν	0	S	0	0
5	Q	212	3441	1090	1719	301	322	9	0	0
2	В	108	Total	С	Н	Ν	Ο	S	0	0
J	п	190	3246	1029	1627	284	298	8	0	0

• Molecule 4 is a protein called Acyl carrier protein.



Mol	Chain	Residues		Atoms							Trace
4	С	79	Total	С	Η	Ν	0	Р	$\mathbf{S}$	0	0
4	G	12	1147	360	564	87	133	1	2	0	0
4	т	79	Total	С	Η	Ν	0	Р	S	0	0
4	1	12	1147	360	564	87	133	1	2	0	0
4	C	79	Total	С	Η	Ν	0	Р	S	0	0
4	G	12	1147	360	564	87	133	1	2	0	0
4	М	79	Total	С	Η	Ν	0	Р	S	0	0
4	111	12	1147	360	564	87	133	1	2	0	0

• Molecule 5 is a DNA chain called pFB526.

Mol	Chain	Residues			Ator	$\mathbf{ns}$		Atoms						
F	K	72	Total	С	Η	Ν	Ο	Р	0	0				
5	Γ	15	2311	708	815	285	430	73	0	0				

• Molecule 6 is a DNA chain called pFB526.

Mol	Chain	Residues			AltConf	Trace				
6	L	73	Total 2320	С 711	Н 823	N 267	0 446	Р 73	0	0

• Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
7	А	1	Total Mg 1 1	0
7	В	1	Total Mg 1 1	0
7	О	1	Total Mg 1 1	0
7	Р	1	Total Mg 1 1	0

• Molecule 8 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues			AltConf				
0	Λ	1	Total	С	Η	Ν	Ο	Р	0
0	A	1	43	10	12	5	13	3	0
8	В	1	Total	С	Η	Ν	Ο	Р	0
0	D	1	43	10	12	5	13	3	0
0	0	1	Total	С	Η	Ν	Ο	Р	0
0	0	1	43	10	12	5	13	3	0
8	P	1	Total	С	Η	Ν	Ο	Р	0
0	1	1	43	10	12	5	13	3	U



### 3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Chromosome partition protein MukB





• Molecule 1: Chromosome partition protein MukB





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L1021 V961 E901	A1022   E962   M902   B	L1024 V964 E904	K1025 🕈 1965 🕈 A905 🕈 E S1026 🔶 B966 🔶 1906 🔶 1	s1027 • R967 • E907 • E	Y1028 ( Y1028 ( Y968 ( A908 ( Li	T1030 • F970 • R910 • R	K1031 🔶 S971 🔶 F911 🔶 E8 01032 🔶 Y972 🔶 L912 🔶 W	D1033 • S973 • Q913 • S	M1034 🕈 D974 💎 Q914 🗬 RE L1035 🔶 S975 🔶 H915 🔶 FS	K1036 🛉 A976 🔶 G916 🔶 E8	E1037 🖤 G977 🖤 S917 🖤 DE L1038 🔶 M978 🔶 A918 🔶 QE	L1039 🔶 L979 🍨 L919 🏺 T	Q1040 ♦ S980 ♦ T920 ♦ Q F1041 ● F981 ● K921 ● D	M1042 • N982 • L922 • Q	K1043 ♦ A983 ♦ E923 ♦ R	11045 • L985 • M925 • Q	G1046 • N986 • V926 • Y		A1049 A L929 A A8 D1050 A R990 Q Q930 K8	A1051		1005 0 H395 0 4935 10 10 10 10 10 10 10 10 10 10 10 10 10	R1056 🕈 A996 👽 H936 👽 L8 A1057 🔶 E997 🔶 E937 🔶 N6	R1058 • 1938 • 1938 • 1938	L1059 P 1939 L339 L339 L339 L339 L339 L339 L339	R1061  S1001  Q941  B8	LU05 H1002 H1002 H2042 H0	L1064      R1004      E944      T8     T8     T9065     T9065     T906     T906     T9075     T9	E1066 • Q1006 • A946 • L	A1067  A1067  K947  Li	s1069 • q1009 • S949 • E6		N1071         Q1011         H951         L8           R1072         A1012         Q952         I8	S1073 • q1013 • A953 • D8	R1074 ♥ Y1014 ♥ K954 ♥ Ri V1075 ♦ S1015 ♦ Q955 ♦ W		L1078 F1016 F1016 B8 V8	E1079 • q1019 • A959 • R8 K1080 • V1020 • L960 • E9
	A1022   E962   M902   B	L1024 V964 E904	K1025 • q965 • A905 • E S1026 • R966 • D906 • 1	s1027	Y1028 • V968 • A908 • L/ E1029 • H969 • A909 • E	T1030 • F970 • R910 • R	K1031 🔶 S971 🔶 F911 🔶 Ek D1032 🔶 Y972 🌩 L912 🔶 W	D1033 • S973 • Q913 • S	M1034 💎 D974 💎 Q914 🗢 RE L1035 🔶 S975 🔶 H915 🄶 FE	K1036 🔶 A976 🍨 G916 🍨 E	E1037 • G977 • S917 • D8 L1038 • M978 • A918 • Q8	L1039 🔶 L979 🄶 L919 🍨 T	q1040		K1043 • A983 • E923 • R		G1046 • N986 • V926 • Y		A1049 L989 L989 A8 D1050 R990 Q Q930 K8	A1051    1991    2931    E8 M1052    Bacop    Bacop    1032    833		L1034 ← E534 ← 4354 ↓ 10 M1055 ← H995 ← 035 ← T8	R1056 🕈 A996 💎 H936 🕈 LE A1057 🔶 E937 🔶 E937 🄶 NG	R1058	E1099 ← D999 ← L939 ← L8 R1060 ← R1000 ← Q940 ← I8	R1061   S1001   1941   F8	R1063 • A1002 • 1942 • 48	L1064 • R1004 • E944 • T8 H1065 • E1005 • T0A5 • T0A5		A1067 ♦ L1007 ♦ K947 ♦ L1 L1068 ● R1008 ● H948 ●	S1069 Q (1009 C S949 E		N1071 ♥ q1011 ♥ H951 ♥ L8 R1072 ♦ A1012 ♦ q952 ● I8	s1073 • q1013 • A953 • D8	RI074         Y1014         K354         N           V1075         ◆         S1015         ◆         q955         ∨		410// H101/ H101/ H90/ H90/ H90/ H90/ H90/ H90/ H90/ H90	E1079 $\blacklozenge$ q1019 $\blacklozenge$ A959 $\blacklozenge$ R8 K1080 $\diamondsuit$ V1020 $\diamondsuit$ L960 $\diamondsuit$ E3
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  | A676  | L677   | E679                              | R680                                | F681<br>Ceon  | 0083<br>G683  | V684                                    | L685                                  | L686<br>S687  
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  | A703                                | L704<br>1705   | 6071<br>G706   | P707                               | A708<br>R709  
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  | V928  | L929                                    | g331   | D932                              | r 934   | <b>q</b> 935<br>H936   | E937  | 1938<br>1939 ♦  | 0940   | 0941  
  | Y943                                | E944   | 1946<br>A946   | K947                               | H948<br>S949  
  | 0360   | H951  | 4952  | K954                              | 0955 ♥<br>0956 ●   | A957                                | F958   
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   | 1020 • L960   | 1021 • V961 • 1022 • E962 • 1963 • 1963  |  | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| V964 🔶 E904 🔶   | q965 🔶 A905 🌪                 |  | V968                                | H969 A A909 F F970 B R910   | 5971 F911                   | Y972 Q913 Q913 Q   |   |   | G977   | L979 C L919                       | S980                                | E981 (1921)   | A983 E923   | D984 P924                               | L985 M925                             | N986 (V926 (V92) (V926 (V92) (V926 ( | K988  | L989 • L929                             |  | R992 <b>•</b> D932                | E994 (1934 (1934 (1934 (1934 (1934 (1935)))))   | H995 • Q935 • A Q936 • A   | E997 🔶 E937   | C 1033 C | R1000 🔶 🖓 🖓  | S1001 (1941)<br>B1002 (1942)   | A1003 Y943                          | R1004 C E944   | L1005 A A946   | L1007 🔶 K947 🄶                     | R1008 		 H948  | q1010 • q950 •   |   | A1012 4 4952  | Y1014 🔶 K954 🔶                    | s1015 ♥ q955 ♥<br>q1016 ♦ q956 ●   | F1017 A A957                        | N1018 • F958 • D1019 • A959 •  | V1020 L960  | L1021 V961<br>A1022 C E962<br>S1023 I 1963   |  |
| L1024 $\blacklozenge$ V964 $\diamondsuit$ E904 $\diamondsuit$ | K1025 🕈 q965 🔶 A905 🔶         | S1026 ♥ R966 ♥ Q906 ♥ S1027 ● E907 ●   | Y1028                               | E1029 • H969 • A909 • T1030 • F970 • R910 •   | K1031 S971 F911             | u1032 ♥ 1972 ♥ L912 ♥<br>D1033 ♥ S973 ♥ q913 ●   | M1034   M1034   D974   Q914   Control to the second  | C1036 • A976 • G916 •   |  | L1039 C L979 L979 L919            | q1040 ♦ \$380 ♦ T920                | E1041 	 E981 	 K921   | M1042 A N902 A L922 A K1043 A A983 A E923   | D1044 • D984 • P924 •                   | 11045 • L985 • M925                   | G1046 ♥ N986 ♥ V926 ♥<br>V1047 ♥ D987 ♥ A927 ●   | Q1048 🔶 K988 🔶 V928 🔶   |   | A1051 • Q991 • S931 •  | N1052 • R992 • D932 •             | E1054 E394 G334   | M1055 		 H995 		 Q935  | A1057 🔶 E997 🔶 E937 🄶                                   | R1058 • S998 • Q938 • L939 • E1059 • D999 • L939 • C938   | R1060 🔶 R1000 🔶 Q940   | R1061  | R1063 A A1003 Y Y943                | L1064 C R1004 E944 E944  | E1066 Q 1006 A 1945  | A1067 🍨 L1007 🍨 K947 🍨             | L1068 🔶 R1008 🔶 H948 🔮<br>S1069 🔶 D1009 🔶 S949 🔶   | V1070 🔶 q1010 🔶 q950 🔶   |   |   | R1074 🌪 Y1014 🌪 K954 🌪            | V1075 ♥ S1015 ♥ Q955 ♥<br>N1076 ♥ Q1016 ♥ Q956 ●   | 01077 🄶 F1017 🔶 A957 🔶              | L1078 • N1018 • F958 •<br>E1079 • D1019 • A959 •   |   | upost ← Li221 ← 9661 ←<br>11082 ← A1022 ← E962 ←<br>A1083 ← S1023 ← 1963 ←   |  |
| ► L1024 	 V964 	 E904   | K1025 🕈 q965 🛉 A905 🛉         | S1026 R R966 Q Q906 S1027 R967 R967  | Y1028                               | E1029 H969 A A909   | K1031 • 5971 • 7911         | 1033 ♦ 8973 ♦ 0913 ♦   |   | K1036 A A976 A G916   | E1037  |                                   | q1040 ♦ S980 ♦ T920 ♦               | E1041 	 E981 	 K921   | M1042 M1043 M1044 | D1044 • D984 • P924 •                   | I1045 L985 M925                       | G1046 ♥ N986 ♥ V926 ♥<br>V1047 ♦ D987 ♦ A927 ●   | q1048 + K988 + V928   | A1049 • L989 • L929 •                   | A1051  A1 | N1052                             | E1054 E394 Q334   | M1055 ↔ H995 ↔ Q335 ↔ R1056 ↔ A996 ↔   | A1057 🔶 E997 🔶 E937 🔶                                   | R1068 	♦ S998 	♦ 1938 	♦<br>E1059 	● D999 	● L939 ●   | R1060 • R1000 • Q940   | R1061 		 S1001 		 9941   | R1063 • A1003 • Y943                | L1064 R1004 E944   | E1066 A Q1006 A 946 A  | A1067 🔶 L1007 🌪 K947 🌪             | L1068 • R1008 • H948 • S949 • S949   | V1070 • q1010 • q950 •   | N1071 Q1011 H951  |   | R1074 🔶 Y1014 🌪 K954 🄶            | V1075 ♥ S1015 ♥ Q955 ♥<br>N1076 ♦ Q1016 ♦ Q956 ●   | q1077 🔶 F1017 🔶 A957                | L1078 		 N1018 	 F958  | K1080 V1020 L960  | 4,061         L1021         V961           11082         A1022         E962           A1083         \$1023         1963  |  |
| F1084 	 E904  | C1085 • K1025 • Q965 • A905   | E1086 S1026 R966 Q906 A1087 S1027 R967 S1027 S10 | E1088 • Y1028 • V968 • A908         | M1089 🔶 E1029 🔶 H969 🔶 A909 <table-cell></table-cell>                                       | NIO91 KI031 S971 F911       | V1082         ↓ 1032         ↓ 1032         ↓ 1032         ↓ 1033 <th abstarbalaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaa<="" th=""><th>K1094 A M1034 D D974 Q Q914</th><th>L1096 • K1036 • A976 • G916 •</th><th>R1097 ♦ E1037 ♦ G977 ♦ S917 ♦</th><th>L1099 C L1039 L979 L919 L919</th><th>E1100 • q1040 • S980 • T920</th><th>R1101 E1041 E981 K921</th><th>V1103 • K1043 • A983 • E923 •</th><th>Y1104 • D1044 • D984 • P924 •</th><th>q1105 • 11045 • L985 • M925</th><th><math display="block">1106 \qquad \qquad 01046 \qquad \qquad 01986 \qquad \qquad 0926 \qquad \qquad \\ 11107 \qquad \qquad 01047 \qquad \qquad 0987 \qquad \qquad 0987 \qquad \qquad 0027 \qquad \qquad \\ 00000000000000000000000000000000</math></th><th>E1108 • q1048 • K988 • V928 •</th><th>q1109 ♦ A1049 ♦ L989 ♦ L929 ♦</th><th></th><th>S1112 		 N1052 		 R992 		 D932</th><th>K1114 E1054 E394 Q334 Q334</th><th>A1115 	M1055 	H995 	9 	Q935<br/>G1116 	R1056 	M996 	H936</th><th>W1117 A A1057 C E997 E937</th><th>C1118</th><th>V1120 • R1060 • R1000 • q940</th><th>M1121 R1061 S1001 Q941</th><th>M1123 M1063 M1003 Y943</th><th>K1125 L1064 R1004 E944 K1125</th><th>D1126 H1005 E1006 A946 A</th><th>1126 A1067 A</th><th>V1129 L1068 R1008 H948 V1129 S1069 S</th><th>E1130 • V1070 • Q1010 • Q950 •</th><th>R1132 N1071 Q1011 H951</th><th>L1133 A A10/2 A1012 A1013 A 4953</th><th>H1134 R1074 Y1014 K954 R1135</th><th>R1136 V1075 V1075 Q955 V1016 Q956 V</th><th>E1137 Q1077 F1017 A957</th><th>A1139 L1078 A N1018 F F968 A A1139 A E1079 A 01019 A A969 A</th><th>Y1140 ♥ K1080 ♦ V1020 ♥ L960 ♦</th><th>E1142         41081         L1021         9561           61143         11082         A1022         E962           61143         A1083         S1023         1963</th></th> | <th>K1094 A M1034 D D974 Q Q914</th> <th>L1096 • K1036 • A976 • G916 •</th> <th>R1097 ♦ E1037 ♦ G977 ♦ S917 ♦</th> <th>L1099 C L1039 L979 L919 L919</th> <th>E1100 • q1040 • S980 • T920</th> <th>R1101 E1041 E981 K921</th> <th>V1103 • K1043 • A983 • E923 •</th> <th>Y1104 • D1044 • D984 • P924 •</th> <th>q1105 • 11045 • L985 • M925</th> <th><math display="block">1106 \qquad \qquad 01046 \qquad \qquad 01986 \qquad \qquad 0926 \qquad \qquad \\ 11107 \qquad \qquad 01047 \qquad \qquad 0987 \qquad \qquad 0987 \qquad \qquad 0027 \qquad \qquad \\ 00000000000000000000000000000000</math></th> <th>E1108 • q1048 • K988 • V928 •</th> <th>q1109 ♦ A1049 ♦ L989 ♦ L929 ♦</th> <th></th> <th>S1112 		 N1052 		 R992 		 D932</th> <th>K1114 E1054 E394 Q334 Q334</th> <th>A1115 	M1055 	H995 	9 	Q935<br/>G1116 	R1056 	M996 	H936</th> <th>W1117 A A1057 C E997 E937</th> <th>C1118</th> <th>V1120 • R1060 • R1000 • q940</th> <th>M1121 R1061 S1001 Q941</th> <th>M1123 M1063 M1003 Y943</th> <th>K1125 L1064 R1004 E944 K1125</th> <th>D1126 H1005 E1006 A946 A</th> <th>1126 A1067 A</th> <th>V1129 L1068 R1008 H948 V1129 S1069 S</th> <th>E1130 • V1070 • Q1010 • Q950 •</th> <th>R1132 N1071 Q1011 H951</th> <th>L1133 A A10/2 A1012 A1013 A 4953</th> <th>H1134 R1074 Y1014 K954 R1135</th> <th>R1136 V1075 V1075 Q955 V1016 Q956 V</th> <th>E1137 Q1077 F1017 A957</th> <th>A1139 L1078 A N1018 F F968 A A1139 A E1079 A 01019 A A969 A</th> <th>Y1140 ♥ K1080 ♦ V1020 ♥ L960 ♦</th> <th>E1142         41081         L1021         9561           61143         11082         A1022         E962           61143         A1083         S1023         1963</th> | K1094 A M1034 D D974 Q Q914   | L1096 • K1036 • A976 • G916 •  | R1097 ♦ E1037 ♦ G977 ♦ S917 ♦     | L1099 C L1039 L979 L919 L919        | E1100 • q1040 • S980 • T920   | R1101 E1041 E981 K921   | V1103 • K1043 • A983 • E923 •           | Y1104 • D1044 • D984 • P924 •         | q1105 • 11045 • L985 • M925  | $1106 \qquad \qquad 01046 \qquad \qquad 01986 \qquad \qquad 0926 \qquad \qquad \\ 11107 \qquad \qquad 01047 \qquad \qquad 0987 \qquad \qquad 0987 \qquad \qquad 0027 \qquad \qquad \\ 00000000000000000000000000000000$ | E1108 • q1048 • K988 • V928 •           | q1109 ♦ A1049 ♦ L989 ♦ L929 ♦  |                                   | S1112 		 N1052 		 R992 		 D932  | K1114 E1054 E394 Q334 Q334   | A1115 	M1055 	H995 	9 	Q935<br>G1116 	R1056 	M996 	H936 | W1117 A A1057 C E997 E937   | C1118  | V1120 • R1060 • R1000 • q940   | M1121 R1061 S1001 Q941              | M1123 M1063 M1003 Y943   | K1125 L1064 R1004 E944 K1125   | D1126 H1005 E1006 A946 A           | 1126 A1067 A   | V1129 L1068 R1008 H948 V1129 S1069 S | E1130 • V1070 • Q1010 • Q950 •                                | R1132 N1071 Q1011 H951  | L1133 A A10/2 A1012 A1013 A 4953  | H1134 R1074 Y1014 K954 R1135   | R1136 V1075 V1075 Q955 V1016 Q956 V | E1137 Q1077 F1017 A957   | A1139 L1078 A N1018 F F968 A A1139 A E1079 A 01019 A A969 A | Y1140 ♥ K1080 ♦ V1020 ♥ L960 ♦   | E1142         41081         L1021         9561           61143         11082         A1022         E962           61143         A1083         S1023         1963 |
| F1084 ♦ L1024 ♦ V964 ♦ E904 ♦                                 | C1085 • K1025 • q965 • A905 • | E1086 S1026 R966 9 9906 9  | E1088 A Y1028 A Y968 A 908          | M1089 C E1029 H969 A 8909 E E1050 E E1050 E E1050 E E1050 E E1050 E E1050 E E10 E           |                             | V1092 V1092 V1092 V1092 V1093 V10913 V109100000 V100000000000000000000000000  | K1094 ♦ M1034 ♦ D974 ♦ Q914 ♦   | L1096 C X1036 A A976 G916 C   | R1097 C E1037 C C977 S917 C 2977 C C977 C C9 | L1099 L1039 L999 L1039 L999       | E1100 • q1040 • S980 • T920         | R1101 	 E981 	 K921   | ◆ Y1103 ◆ K1043 ◆ A983 ◆ E923 ◆   | V1104 ♦ D1044 ♦ D984 ♦ P924 ♦           | q1105 ♦ I1045 ♦ L985 ♦ M925           | III06 	 G1046 	 N986 	 V926 	 100 	 1107 	 1047 	 D987 	 4927 	 107 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1047 	 1  | E1108 • q1048 • K988 • V928 •   | q1109 ♦ A1049 ♦ L989 ♦ L929 ♦           |  | S1112 	 N1052 	 R992 	 D932       | A1113         A1003         L993         F933           K1114         E1054         E994         0934 | A1115 M1055 H1995 Q355 Q1116 H1056 A A996 H1936  | W1117 A A1057 E997 E937                                 | C1118 R1058 S998 Q938 A1119 E1059 D999 L939   | V1120 K1060 K1000 Q Q940   | R1122 C R1061 S1001 Q941 C R1122 R1002 R10002 R1002 R1 | M1123 A R1003 A 11003 A 1403        | K1125 L1064 R1004 E944   | D1126 H1005 E1005 1945 H1005 A1946 A1005 A | 01128 A1067 L1007 K947             | V1129 L1068 R1008 H948 V1129 S1069 D1009 S949  | E1130 V1070 Q1010 Q1050 Q  | R1132 N1071 Q1011 H961  | L1133 A N10/2 A1012 4952  | H1134 K1074 Y1014 K954            | R1136 V1075 S1015 Q955 V<br>R1136 N1076 Q1016 Q956 V   | E1137 q1077 F1017 A957              | A1139 L1078 N1018 F958   | V1140 K1080 V1020 L960                                      | E1142         41081         L1021         V961           G1143         11082         11022         E962           G1143         A1083         \$1023         11963 |  |
| G1144 ♦ F1084 ♦ L1024 ♦ V964 ♦ E904 ♦                         | A1145 C1085 A K1025 Q Q965 A  | L1146 C E1086 S S1026 R966 Q Q906 P  | s1148 • E1088 • Y1028 • V968 • A908 | M149 M1089 E1029 H969 A009 S1150 E70 R910 8910  | DILL NIOI KIO3I S971 F911   | ALIEZ V VIOSZ V 1092 V 1092 V 1972 V 1912 V 1153 V 0913 V  | L1154 K1094 M1034 D974 Q914 Q914 Q914 C014 C014 C014 C014 C014 C014 C014 C0   | A1156 C L1096 K1036 A A976 G916 A   | L157 	 R1097 	 E1037 	 6977 	 5917   | L1159 L1099 L1039 L1039 L979 L919 | A1160 E1100 • Q1040 • S980 • T920 • | Viloi Riloi 🔶 Elo4i 🔶 E98i 🔶 K92i 🄶                                     | MI164         D1102         M1042         M1052         L922           E1165         Y1103         K1043         A983         E923  | H1166 Y1104 Y1104 P924                  | L1167 Q1105 Q1105 M925 M925 W         | R1168 🔶 I1106 💎 G1046 👻 N986 👻 V926 🕈<br>D1169 🔶 R1107 🔶 V1047 🔶 D987 🔶 A927 🔶   | E1108 • Q1048 • V928 • V928   | R1172  Q1109  A1049  L989  L929         |  | D11/6 S1112 W1052 R992 D932       | K1178 A1113 A1000 L935 F935 F935  | n11/5 A1115 M1055 ↔ H995 ↔ Q935 ↔ P1180 ↔ G1116 ↔ R1055 ↔ A996 ↔ H936 ↔  | E1181 W1117 A1057 E997 E997 E937                        | A1102 C1118 R1068 € S998 € Q938 € K1183 € A1119 € E1059 € D999 € L939 €   | V1184 V1120 V1120 V1120 V1120 V11300 V1135 V11300 V113000 V1130000 V1130000 V1130000 V1130000000000 | F1186 M1121 R1061 S1001 Q941 Q941 P1186 R1122 P1165 P11002 P1002 P | F1187 M1123 A R1063 A A1003 Y 943   | A1189<br>K1125<br>K1125<br>K125<br>K125<br>K1064<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004<br>K1004 | V1190 D1126 A1005 A1005 A1005 A946 A1191 A1006 A1946   | Q1192 Q1192 A1126 A1067 A1067 K947 | L106 H108 H1008 H948 H1008 H1008 H948 H1008 H1008 H1048 H1008 H1048 H104   | R1195 E1130 V1070 Q1010 Q950 Q   | R1197 H1132 N1071 Q1011 H951<br>11198 R1132 N1075 N1077 N1075 | L100 L133 A1012 4952 4953 401013 401013 4953 4  | U2200 H134 R1074 Y1014 K854       | $11202 \qquad \qquad 111302 \qquad \qquad 11136 \qquad \qquad 11075 \qquad \qquad 11075 \qquad \qquad 11075 \qquad \qquad 11075 \qquad \qquad 11076 \qquad \qquad 11016 \qquad \qquad 11056 \qquad \qquad 11076 \qquad \qquad 11016 \qquad \qquad 110$ | R1204 E1137 Q1077 C1017 A957 A      | T1205 T1205 L1078 N1018 F958 D1206 A1139 E1079 D1019 A959  | V140 V1080 V1020 L960                                       | E1142         41041         L1021         V961           G1143         A1022         E962         E163           A1083         A1083         E1083         E1083   |  |
| ♦ G1144 ♦ F1084 ♦ L1024 ♦ V964 ♦ E904 ♦                       | A1145 C1085 K1025 Q965 A905   | <ul> <li>L1146 € E1086 € S1026 € R966 € Q906 €</li> <li>R1147 € A1087 € S1027 € R967 € E907 €</li> </ul>   | S1148 E1088 Y1028 Y1028 A908        | M1149     M1089     E1029     H969     S1150     E1060     T1030     F370     R910     S115 | DI151 N1091 K1031 S971 F911 | VI152     VI022     V1022     V1022     V1032     V1033     V103     V103     V103     V103     V103     V103     V10  | LIJE4 K1094 M1034 D974 Q914 Q   | 4125         41096         10036         4036         4036         4036         4036           A1156         11096         K1036         40376         6916         40316 | LIJE7 RID97 EJ037 G977 S917  |                                   | ♦ A1160 E1100 Q Q1040 S980 Q T920   | N.101     E1041     E981     Kg21       N100     N100     N100     1000 | ● E1165 ● Y1103 ● K1043 ● A983 ● E923 ●   | ♦ H1166 ♦ Y1104 ♦ D1044 ♦ D984 ♦ P924 ● | L1167 Q Q1105 Q 11045 Q L985 Q M926 Q | H1168      H1106      G1046      G1046      H1986      V226      V226      V1047      D987      A27             | E1108 • 41048 • K988 • V928   | ♦ R1172 ♥ Q1109 ♦ A1049 ♦ L929 ♦ L929 ♦ | Elife villi Alobi elige desi elige   | P1177 S1112 N NJO52 S R992 D932 P | K1178 K1114 E1054 E994 Q934   | H115 A H105 ← H995 ← 1935 ←     F1160 ← 1116 ← R1056 ← A996 ← H936 ←   | ♦ E1181 ♦ W1117 ♦ A1057 ♦ E997 ♦ E937 ♦                 | KI183     K1183     A1119     E1059     D999     L933   | ♦ <sup>V1184</sup><br>q1185 ♦ v1120 ♦ R1060 ♦ R1000 ♦ q940 ♦   | M121         R1061         S1001         Q941           F1186         R1122         N1062         B1002         D642   | F1187 M1123 M123 N1063 M11003 Y1430 | A1189 A V124 LIO64 A R1004 B B944 A V1400 K1125 A V1400 A V1400A V1400A V1400A V1400A V1400A V1400A V1400A V1400A V1400A V1400   | V1190 D1126 H1005 H1005 A1190 A1191  | ♦ q1192 M112/ A1067 A L1007 K947 K | Initial         Initial <t< th=""><th>R1196         E1130         V1070         q1010         q950</th><th>R1197 11196 11132 N1071 Q1011 H961 Q1011 P1196</th><th>R1199         L1133         N10/2         N1012         N952           01013         01013         01013         A953         01013</th><th>♦ 41201 H134 K1074 ♦ Y1014 ¥ K964</th><th>I1202 ♦ R1136 ♦ V1075 ♥ S1015 ♥ 9955 ♥<br/>11203 ♦ R1136 ♦ N1076 ♦ 01016 ♦ 0956 ●</th><th>► 11204 E1137 Q1077 E1017 A957</th><th>L1205 	 L1078 	 N1018 	 F958 	 11205 	 L1078 	 01019 	 13959 	 13959 	 11206 	 1139 	 11206 	 1139 	 11206 	 11206 	 1139 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 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Q1077 E1017 A957      | L1205 	 L1078 	 N1018 	 F958 	 11205 	 L1078 	 01019 	 13959 	 13959 	 11206 	 1139 	 11206 	 1139 	 11206 	 11206 	 1139 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 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11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 11206 	 1120 | V1140 K1080 V1020 L980                                      | Bil42     q1081     L1021     V961       61143     11082     A1022     E982       61143     A1083     \$1023     1963  |  |





Chain E: 68% 20% · 12%















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<ul> <li>Molecule 6: pFB526</li> </ul>	
Molecule 6: pFB526 Chain L:	
<ul> <li>Molecule 6: pFB526</li> <li>Chain L:</li> </ul>	00000444606000
Molecule 6: pFB526 Chain L: 97%      A & & & & & & & & & & & & & & & &	DC DC DG DG DG DG DG DG DC DC DC
Molecule 6: pFB526 Chain L: 97%      A & & & & & & & & & & & & & & & &	DC D
Molecule 6: pFB526 Chain L: 97%      A & & & & & & & & & & & & & & & &	DA         DC         DC           DT         DG         DC           DT         DG         DG           DA         DG         DA           DA         DG         DA           DA         DG         DT           DA         DG         DT           DA         DG         DT           DT         DG         DG           DT         DG         DG           DT         DG         DG           DT         DG         DG           DC         DG         DG
Molecule 6: pFB526 Chain L: ·· 97%      A & & & & & & & & & & & & & & & &	DT         DA         DC         DC           DT         DT         DT         DG         DC           DG         DT         DT         DG         DG           DC         DT         DT         DG         DG           DC         DT         DT         DG         DG           DT         DT         DT         DG         DG           DC         DA         DT         DG         DG           DC         DA         DG         DA         DA           DC         DA         DG         DA         DA           DC         DA         DG         DG         DG           DC         DA         DG         DG         DG           DA         DT         DA         DG         DG           DA         DC         DA         DG         DG           DA         DC         DA         DG         DG           DA         DC         DA         DG         DG
Molecule 6: pFB526 Chain L: 97%     *********************************	DG         DT         DA         DC         DC           DT         DT         DT         DT         DT         DG           DG         DT         DT         DG         DC         DC           DG         DG         DT         DT         DG         DG           DT         DT         DT         DT         DT         DG           DT         DT         DT         DT         DG         DG           DT         DT         DT         DT         DG         DG           DA         DC         DC         DA         DA         DG           DA         DC         DC         DA         DA         DA           DA         DC         DA         DA         DC         DA           DA         DC         DA         DC         DA         <
Molecule 6: pFB526 Chain L: 97%      A & & & & & & & & & & & & & & & &	Did         Did <thdid< th=""> <thdid< th=""> <thdid< th=""></thdid<></thdid<></thdid<>
Molecule 6: pFB526 Chain L: 97%      A & & & & & & & & & & & & & & & &	DA         DG         DT         DA         DC         DT           DT         DA         DT         DA         DC         DC         DC           DT         DA         DG         DT         DT         DG         DT         DG           DG         DC         DG         DG         DG         DG         DG         DG           DG         DT         DT         DT         DG         DT         DG         DG           DG         DT         DT         DT         DT         DG         DG         DG           DG         DT         DT         DT         DT         DG         DG         DG           DG         DT         DT         DT         DT         DG         DA         DG           DG         DT         DT         DT         DG         DA         DG         DG           DG         DC         DT         DC         DA         DG         DG           DG         DC         DT         DG         DG         DG         DG           DA         DG         DT         DG         DG         DG         DG
Molecule 6: pFB526 Chain L:	Did         Did <thdid< th=""> <thdid< th=""> <thdid< th=""></thdid<></thdid<></thdid<>



DA DG	DG	DG DA DT	DA DA	DA	DC	DC	DA DA	DT DT	DT	DC DT DG	DA DC	DC	DA TU	DG DG	DG DG	DC DC	DG DA DA	DG	DC	DA
DC DC	DC	DT DT DT	DT DT	DA	DA DA	DC DT	DG	DG DA Tr	DC DA DT	DG DT DA	DA DC DT	DG	DC	DG	DC	DT DG DG	DG DG DA	DC	DG DG DA	DG
DC DG	DA DT	DG DA DA	DC	DA DT A	DC	DA DA DA	DC DA	DG DA	DG	DG DC	DA DC DC	DC DC	DA TU	DC	DG DT	DG DC	DA DA DT	50 50	DA DA DC	DA
DG DG	D D	DC DC	DA DA DA	DC	TD TD	DA DC	F 2 2 2	DQ DQ DQ	DA DA	DC DT	DA DC DT	DT	a d d f	DC DC	DC DC	DC DA	DA DC DA	DA DT TT	DA DA TU	DA
DG DCA	DG DG	DA DT DG	DG DA	202	DG	DT DA DA	DG DT	10 DG	DG DG	DC DC	DC DT	DC	2022	2 E D	DC DC	DC DC	DC DC	DG		DC
DT DG TG	DT TO	DA DT DT	DG DC	DG	DA DA	DA DT DC	10 00 00	DG DC	DG DG	DG DA DG	DC DG	50 00	2 T D T	DC	DG DG	DA DA DT	DC DA DT	DG DG	DG DC	DA
DG FG B	bg bg	DC DA	DG DA	D D D	DA	DC DC	2 5 2 2	2 2 2 5	DA DT	DG DT DA	DG TU	DA DT	N P P S	DC DC	DG DC	DG DG	DG DG	DT DC	5 D D D	DA
DA DT	DG DG	DG DA DT	DG DA		DA DA	DA DG	DA DA	DA DA PA	2 2 2 2	DG DG	DA DT DA	DG DG	2 2 2 2	2 5 2 3	DC DT	DG DA DT	DT DA DA	DG DC		DG
DT DA DA	DG DG	DT DC DA	DG DA DC	DC	DG DT	DT DT DA	DC DC	DT DA DA	DA DA DA	DC DT DT	DT DA DG	DA DT TC	DG DA	TO TO	DA DA DA	DA DC DT	DT DC DA	DT TC TC	TD TD	DA
DT DT TU	DA DA	DG DG	DA DT DC	DA	DD	DG DA DA	DG DA DT	DU DC LC	DT D	DG DA DT	DA DA DT	DC	DA	DA	DC DA DA	DA DA DT	DC	DT DT	DC DC	DT
DG DG	DT TO	DC DC	DT DC	DC	2 T D	DG DC	D T D	DG DA	2222	DG DT DA	DG DA DA	DA DA	DA DT	DA DA	DG DG	DA DT DC	DT DC	TD TD	DG DG	DT
DC DT TC	DT	DT DT TU	DC	DC	DG	DA DA DT	D T D	DI DI DI	T T T D D D D D D D D D D D D D D D D D	DC DA DA	DA DC	DA DA	DA DA	DC	DC DC	DC DT	DA DC	DG	DG DG	DG
DG TU TU	DG	DT DT DG	DC DC	DG	DC DA	DA DG DA	DC DT	DC DC	DA DC DT	DC DT DT	DT DT TU		DA DA	DG	DA DA DC	DG DG	DC DT DT	DC DA	DG DG	DA
2222	DG DG	DA DT DA	DC DC	DA DA	DA	DT DT	2 2 5 5		2 2 2 2	DA DG	DC DC	DA DA	8668	DG DG	DC DA	DC DA	DT DT	DC DA	DA DA	BC
FU DE FU	DA	DG DC DA	DC		DA	DA DT DA	2 2 5		2 2 La 9	DC DT DA	DA DT DC	DC	8 T T 2	DC DC	DG DG	DC DC	DG DG	DG DG	DG DG	DT
DG DG	DA DT	DA DA DG	DT DC	DG DG	DT	DT DA DC	D0 00		DG DC	DT DC DA	DA DG DA	DC	DA DA	DT TU	DC DC	DG DA	DT DA DA	90 90	DC	DG
DC DC	DC	DG	DT DG	DC	DG	DG DG	DT DC	DU DU DU	DA DC DA	DC DA DG	DC	DG	2 T T Z	DG	DG C B	DA DA DC	DG DC	DC DT	DA DC	DC
DG DA DA	DG DG	DA DG DA	DA DC	DC	DC DA	DC DC	DG DA		DG DA	DG DA DA	DG DC	DC DC	DC DC	DI	DC DC	DC DG	DG DG	DG DA	DA DA DA	DG
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DC DC	DA	DA DG DG	DA DA TC		DD	DA DA DG		DG DG	D D D D	DG DG DA	DA DC	50 00	DA DA	DC	DC DC	DG A18 A18	619 G20 G21	A22 G23	C24 T25 T76	C27 C27 C28 A29
G30 G31 G32	G33 G34	A35 A36	A37 C38 G39	G43 G44	T45 A46 T17	14/ T49 TE0	150 T51 A52 T53	A54 G55 T56	T59	T66 T67 T68	T76	G79 T83	G84 A85	G86 C87	189 189	DG	TU TU TU	DT DG	DT DG DA	DC DC DC
DG TO TO	50 Dd	DG DG	DG DC	DA	200	DA DA DT	DG DA	DA DA Ad	8 2 2 2	DC DA	DC DA	DG DG	2 2 2 2	2 2 E	DT TU TU	DT DC	DG DG DT	T D D	2 4 9 9 1	BC
DT TT TT	DG DG	DC DC	DC	TO	DG DG	DC F D	DA DA		2255	DC DC	DT DG	DT TT	D P D	2222	DT D	DA DT DT	DC DC	DG DG	AD TD	DA



DA DT DG DG DT DT



# 4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	3754	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE	Depositor
	CORRECTION	
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{\AA}^2)$	40	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.346	Depositor
Minimum map value	-0.086	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.014	Depositor
Recommended contour level	0.07	Depositor
Map size (Å)	720.7206, 720.7206, 720.7206	wwPDB
Map dimensions	166, 166, 166	wwPDB
Map angles $(^{\circ})$	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	4.34169, 4.34169, 4.34169	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: 4HH, ATP, MG

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	B	ond lengths	E	Bond angles
	Unam	RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	А	0.53	2/11999~(0.0%)	0.98	5/16166~(0.0%)
1	В	1.09	64/11999~(0.5%)	1.35	147/16166~(0.9%)
1	0	0.53	2/11999~(0.0%)	0.98	5/16166~(0.0%)
1	Р	1.14	63/11999~(0.5%)	1.39	165/16166~(1.0%)
2	С	0.83	2/3592~(0.1%)	1.31	23/4862~(0.5%)
2	D	0.84	2/3592~(0.1%)	1.31	22/4862~(0.5%)
3	Е	1.50	19/1753~(1.1%)	1.71	45/2361~(1.9%)
3	F	1.64	24/1648~(1.5%)	1.68	50/2218~(2.3%)
3	Q	1.50	19/1753~(1.1%)	1.70	43/2361~(1.8%)
3	R	1.63	23/1648~(1.4%)	1.68	57/2218~(2.6%)
4	G	0.13	0/558	0.28	0/754
4	Ι	0.13	0/558	0.27	0/754
4	М	0.14	0/558	0.27	0/754
4	S	0.13	0/558	0.28	0/754
5	К	0.69	0/1680	1.66	16/2589~(0.6%)
6	L	0.70	0/1676	1.60	11/2586~(0.4%)
All	All	0.94	220/67570~(0.3%)	1.27	589/91737~(0.6%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	А	0	3
1	В	0	2
1	0	0	3
1	Р	0	3
2	С	0	6
2	D	0	6
3	Е	0	4



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Continued	from	previous	page

Mol	Chain	#Chirality outliers	<b>#Planarity outliers</b>
3	Q	0	2
5	Κ	0	19
6	L	0	17
All	All	0	65

All (220) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	С	295	ARG	C-N	-24.37	1.03	1.33
2	D	295	ARG	C-N	-24.30	1.03	1.33
1	А	589	GLN	C-N	13.59	1.51	1.33
1	0	589	GLN	C-N	13.52	1.51	1.33
3	Е	44	HIS	CE1-NE2	-8.96	1.23	1.32
3	Q	44	HIS	CE1-NE2	-8.90	1.23	1.32
1	В	1166	HIS	CE1-NE2	-8.86	1.23	1.32
1	В	1193	HIS	CE1-NE2	-8.86	1.23	1.32
1	Р	1193	HIS	CE1-NE2	-8.84	1.23	1.32
1	Р	1166	HIS	CE1-NE2	-8.82	1.23	1.32
1	В	175	HIS	CE1-NE2	-8.79	1.23	1.32
1	В	1193	HIS	CD2-NE2	-8.02	1.29	1.37
3	Q	44	HIS	CD2-NE2	-8.00	1.29	1.37
1	Р	1166	HIS	CD2-NE2	-7.97	1.29	1.37
1	Р	1193	HIS	CD2-NE2	-7.95	1.29	1.37
1	В	175	HIS	CD2-NE2	-7.93	1.29	1.37
1	В	1166	HIS	CD2-NE2	-7.93	1.29	1.37
3	Е	44	HIS	CD2-NE2	-7.85	1.29	1.37
3	R	85	ARG	CZ-NH2	-7.79	1.23	1.33
1	Р	1341	ARG	CZ-NH2	-7.77	1.23	1.33
1	Р	1250	ARG	CZ-NH2	-7.74	1.23	1.33
1	Р	1393	ARG	CZ-NH2	-7.72	1.23	1.33
1	Р	1245	ARG	CZ-NH2	-7.72	1.23	1.33
3	Q	203	ARG	CZ-NH2	-7.71	1.23	1.33
1	В	1131	ARG	CZ-NH2	-7.71	1.23	1.33
1	Р	96	ARG	CZ-NH2	-7.71	1.23	1.33
3	R	34	ARG	CZ-NH2	-7.69	1.23	1.33
1	Р	1131	ARG	CZ-NH2	-7.68	1.23	1.33
3	R	161	ARG	CZ-NH2	-7.68	1.23	1.33
1	Р	199	ARG	CZ-NH2	-7.67	1.23	1.33
3	Е	206	ARG	CZ-NH2	-7.67	1.23	1.33
3	R	156	ARG	CZ-NH2	-7.67	1.23	1.33
1	Р	1328	ARG	CZ-NH2	-7.66	1.23	1.33
3	F	31	ARG	CZ-NH2	-7.64	1.23	1.33



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	Q	206	ARG	CZ-NH2	-7.63	1.23	1.33
1	P	1093	GLN	C-N	7.63	1.44	1.33
1	В	1221	ARG	CZ-NH2	-7.62	1.23	1.33
3	Е	31	ARG	CZ-NH2	-7.62	1.23	1.33
1	Р	1132	ARG	CZ-NH2	-7.61	1.23	1.33
1	Р	1254	ARG	CZ-NH2	-7.61	1.23	1.33
1	В	1197	ARG	CZ-NH2	-7.58	1.23	1.33
3	R	31	ARG	CZ-NH2	-7.56	1.23	1.33
1	В	1199	ARG	CZ-NH2	-7.55	1.23	1.33
1	В	240	ARG	CZ-NH2	-7.55	1.23	1.33
1	Р	1221	ARG	CZ-NH2	-7.55	1.23	1.33
1	Р	1197	ARG	CZ-NH2	-7.54	1.23	1.33
3	Q	31	ARG	CZ-NH2	-7.54	1.23	1.33
1	В	1093	GLN	C-N	7.53	1.44	1.33
3	Е	203	ARG	CZ-NH2	-7.53	1.23	1.33
1	В	1132	ARG	CZ-NH2	-7.53	1.23	1.33
1	В	250	ARG	CZ-NH2	-7.49	1.23	1.33
1	Р	1199	ARG	CZ-NH2	-7.48	1.23	1.33
3	F	164	ARG	CZ-NH2	-7.48	1.23	1.33
1	Р	240	ARG	CZ-NH2	-7.47	1.23	1.33
3	Е	67	ARG	CZ-NH2	-7.45	1.23	1.33
3	Q	67	ARG	CZ-NH2	-7.45	1.23	1.33
1	В	199	ARG	CZ-NH2	-7.45	1.23	1.33
1	Р	250	ARG	CZ-NH2	-7.44	1.23	1.33
3	R	164	ARG	CZ-NH2	-7.44	1.23	1.33
1	В	243	ARG	CZ-NH2	-7.42	1.23	1.33
3	F	85	ARG	CZ-NH2	-7.42	1.23	1.33
1	В	1328	ARG	CZ-NH2	-7.40	1.23	1.33
1	В	1393	ARG	CZ-NH2	-7.40	1.23	1.33
1	Р	243	ARG	CZ-NH2	-7.38	1.23	1.33
1	В	229	ARG	CZ-NH2	-7.38	1.23	1.33
3	F	34	ARG	CZ-NH2	-7.38	1.23	1.33
3	F	161	ARG	CZ-NH2	-7.36	1.23	1.33
3	Q	60	ARG	CZ-NH2	-7.35	1.23	1.33
1	В	105	ARG	CZ-NH2	-7.33	1.24	1.33
3	Е	60	ARG	CZ-NH2	-7.33	1.24	1.33
1	В	1250	ARG	CZ-NH2	-7.32	1.24	1.33
1	В	96	ARG	CZ-NH2	-7.30	1.24	1.33
3	F	156	ARG	CZ-NH2	-7.29	1.24	1.33
1	Р	301	GLN	C-N	7.25	1.44	1.34
1	В	1390	ARG	CZ-NH2	-7.22	1.24	1.33
1	B	301	GLN	C-N	7.10	1.43	1.34



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Р	1394	GLY	N-CA	-6.80	1.37	1.45
1	В	1394	GLY	N-CA	-6.71	1.37	1.45
1	Р	1189	ALA	CA-CB	-6.66	1.43	1.53
1	Р	231	ALA	CA-CB	-6.62	1.43	1.53
1	В	1189	ALA	CA-CB	-6.61	1.43	1.53
1	Р	248	ALA	CA-CB	-6.58	1.43	1.53
1	А	847	GLU	C-N	6.55	1.42	1.33
1	В	248	ALA	CA-CB	-6.54	1.43	1.53
1	Р	237	ALA	CA-CB	-6.50	1.43	1.53
1	0	847	GLU	C-N	6.47	1.42	1.33
1	Р	103	GLY	N-CA	-6.40	1.38	1.45
1	Р	50	ALA	CA-CB	-6.34	1.43	1.53
3	Е	45	ALA	CA-CB	-6.30	1.43	1.53
1	В	103	GLY	N-CA	-6.30	1.38	1.45
3	Q	45	ALA	CA-CB	-6.29	1.43	1.53
3	R	34	ARG	CZ-NH1	-6.29	1.24	1.32
1	Р	1250	ARG	CZ-NH1	-6.29	1.24	1.32
1	В	231	ALA	CA-CB	-6.28	1.43	1.53
3	R	161	ARG	CZ-NH1	-6.28	1.24	1.32
1	Р	1241	ALA	CA-CB	-6.28	1.43	1.53
1	Р	1341	ARG	CZ-NH1	-6.25	1.24	1.32
1	Р	1393	ARG	CZ-NH1	-6.25	1.24	1.32
2	С	320	ALA	CA-CB	-6.24	1.43	1.53
1	Р	96	ARG	CZ-NH1	-6.23	1.24	1.32
1	В	250	ARG	CZ-NH1	-6.22	1.24	1.32
3	R	156	ARG	CZ-NH1	-6.21	1.24	1.32
1	Р	1254	ARG	CZ-NH1	-6.21	1.24	1.32
1	Р	1328	ARG	CZ-NH1	-6.21	1.24	1.32
2	D	320	ALA	CA-CB	-6.20	1.43	1.53
1	Р	250	ARG	CZ-NH1	-6.16	1.24	1.32
1	В	191	ALA	CA-CB	-6.16	1.43	1.53
1	Р	1245	ARG	CZ-NH1	-6.16	1.24	1.32
3	Q	67	ARG	CZ-NH1	-6.13	1.24	1.32
3	Q	31	ARG	CZ-NH1	-6.12	1.24	1.32
1	Р	199	ARG	CZ-NH1	-6.11	1.24	1.32
1	B	1199	ARG	CZ-NH1	-6.11	1.24	1.32
3	E	67	ARG	CZ-NH1	-6.10	1.24	1.32
3	R	131	GLY	N-CA	-6.09	1.38	1.45
3	E	31	ARG	CZ-NH1	-6.09	1.24	1.32
3	Е	203	ARG	CZ-NH1	-6.09	1.24	1.32
1	В	240	ARG	CZ-NH1	-6.08	1.24	1.32
3	R	31	ARG	CZ-NH1	-6.08	1.24	1.32



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	Q	203	ARG	CZ-NH1	-6.08	1.24	1.32
3	Е	206	ARG	CZ-NH1	-6.07	1.24	1.32
1	Р	240	ARG	CZ-NH1	-6.07	1.24	1.32
3	R	164	ARG	CZ-NH1	-6.06	1.24	1.32
3	F	31	ARG	CZ-NH1	-6.06	1.24	1.32
3	F	164	ARG	CZ-NH1	-6.06	1.24	1.32
1	Р	1199	ARG	CZ-NH1	-6.06	1.24	1.32
1	В	105	ARG	CZ-NH1	-6.05	1.24	1.32
1	Р	243	ARG	CZ-NH1	-6.04	1.24	1.32
3	Q	206	ARG	CZ-NH1	-6.03	1.24	1.32
1	В	50	ALA	CA-CB	-6.03	1.43	1.53
1	В	243	ARG	CZ-NH1	-6.01	1.24	1.32
3	R	96	GLY	N-CA	-6.00	1.38	1.45
3	F	128	ALA	CA-CB	-6.00	1.43	1.53
1	В	1211	ALA	CA-CB	-5.99	1.43	1.53
1	В	1221	ARG	CZ-NH1	-5.99	1.24	1.32
1	Р	1211	ALA	CA-CB	-5.98	1.43	1.53
3	R	85	ARG	CZ-NH1	-5.98	1.24	1.32
3	Е	60	ARG	CZ-NH1	-5.97	1.24	1.32
3	F	34	ARG	CZ-NH1	-5.96	1.24	1.32
1	В	1132	ARG	CZ-NH1	-5.96	1.24	1.32
1	Р	1132	ARG	CZ-NH1	-5.93	1.24	1.32
3	Q	60	ARG	CZ-NH1	-5.93	1.24	1.32
1	Р	1131	ARG	CZ-NH1	-5.92	1.24	1.32
1	В	1131	ARG	CZ-NH1	-5.92	1.24	1.32
1	Р	1197	ARG	CZ-NH1	-5.91	1.24	1.32
1	Р	1221	ARG	CZ-NH1	-5.91	1.24	1.32
3	F	96	GLY	N-CA	-5.91	1.38	1.45
1	В	96	ARG	CZ-NH1	-5.91	1.24	1.32
3	Q	59	ALA	CA-CB	-5.88	1.43	1.53
1	В	1328	ARG	CZ-NH1	-5.86	1.24	1.32
1	В	229	ARG	CZ-NH1	-5.86	1.24	1.32
3	F	156	ARG	CZ-NH1	-5.84	1.24	1.32
1	Р	227	GLY	N-CA	-5.83	1.38	1.45
3	F	85	ARG	CZ-NH1	-5.83	1.24	1.32
1	В	1250	ARG	CZ-NH1	-5.81	1.24	1.32
1	В	199	ARG	CZ-NH1	-5.80	1.24	1.32
1	В	1197	ARG	CZ-NH1	-5.79	1.24	1.32
3	F	161	ARG	CZ-NH1	-5.77	1.24	1.32
1	В	1393	ARG	CZ-NH1	-5.77	1.24	1.32
3	F	131	GLY	N-CA	-5.77	1.38	1.45
1	В	227	GLY	N-CA	-5.76	1.38	1.45



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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	R	83	ILE	N-CA	-5.76	1.42	1.46
3	Ε	59	ALA	CA-CB	-5.75	1.43	1.53
3	F	83	ILE	N-CA	-5.74	1.42	1.46
3	R	32	ALA	CA-CB	-5.73	1.43	1.53
1	В	1390	ARG	CZ-NH1	-5.72	1.24	1.32
3	F	32	ALA	CA-CB	-5.66	1.43	1.53
3	R	85	ARG	CD-NE	-5.56	1.38	1.46
1	Р	199	ARG	CD-NE	-5.55	1.38	1.46
1	Р	1245	ARG	CD-NE	-5.51	1.38	1.46
1	В	199	ARG	CD-NE	-5.51	1.38	1.46
1	Р	223	PRO	CA-CB	-5.47	1.46	1.53
1	Р	240	ARG	CD-NE	-5.44	1.38	1.46
1	В	240	ARG	CD-NE	-5.42	1.38	1.46
1	Р	1254	ARG	CD-NE	-5.42	1.38	1.46
3	F	85	ARG	CD-NE	-5.40	1.38	1.46
3	R	34	ARG	CD-NE	-5.36	1.38	1.46
1	Р	1250	ARG	CD-NE	-5.35	1.38	1.46
3	R	161	ARG	CD-NE	-5.34	1.38	1.46
3	Q	203	ARG	CD-NE	-5.32	1.38	1.46
1	В	223	PRO	CA-CB	-5.32	1.46	1.53
1	В	1132	ARG	CD-NE	-5.31	1.38	1.46
1	Р	250	ARG	CD-NE	-5.31	1.38	1.46
1	Р	1132	ARG	CD-NE	-5.31	1.38	1.46
3	R	142	SER	CA-CB	-5.30	1.45	1.52
3	Е	203	ARG	CD-NE	-5.29	1.38	1.46
3	F	34	ARG	CD-NE	-5.29	1.38	1.46
1	В	1199	ARG	CD-NE	-5.27	1.38	1.46
3	R	77	PRO	CA-CB	-5.25	1.47	1.53
3	Q	60	ARG	CD-NE	-5.25	1.39	1.46
3	R	164	ARG	CD-NE	-5.24	1.39	1.46
1	Р	1341	ARG	CD-NE	-5.23	1.39	1.46
1	Р	1199	ARG	CD-NE	-5.22	1.39	1.46
1	В	250	ARG	CD-NE	-5.20	1.39	1.46
1	Р	243	ARG	CD-NE	-5.18	1.39	1.46
1	Р	1393	ARG	CD-NE	-5.18	1.39	1.46
3	F	164	ARG	CD-NE	-5.17	1.39	1.46
1	В	1221	ARG	CD-NE	-5.16	1.39	1.46
3	F	161	ARG	CD-NE	-5.16	1.39	1.46
1	Р	96	ARG	CD-NE	-5.15	1.39	1.46
1	В	1390	ARG	CD-NE	-5.14	1.39	1.46
3	Е	60	ARG	CD-NE	-5.13	1.39	1.46
3	E	67	ARG	CD-NE	-5.13	1.39	1.46



Mol	Chain	Res	Type	Atoms	Ζ	Observed(Å)	Ideal(Å)
1	В	105	ARG	CD-NE	-5.13	1.39	1.46
1	В	1393	ARG	CD-NE	-5.13	1.39	1.46
1	В	96	ARG	CD-NE	-5.13	1.39	1.46
3	F	31	ARG	CD-NE	-5.11	1.39	1.46
1	Р	1221	ARG	CD-NE	-5.09	1.39	1.46
3	Q	31	ARG	CD-NE	-5.09	1.39	1.46
3	Q	67	ARG	CD-NE	-5.09	1.39	1.46
1	В	243	ARG	CD-NE	-5.08	1.39	1.46
3	R	31	ARG	CD-NE	-5.08	1.39	1.46
1	В	1250	ARG	CD-NE	-5.08	1.39	1.46
3	F	142	SER	CA-CB	-5.07	1.46	1.52
1	В	229	ARG	CD-NE	-5.07	1.39	1.46
3	Q	206	ARG	CD-NE	-5.06	1.39	1.46
3	Е	31	ARG	CD-NE	-5.06	1.39	1.46
1	В	1131	ARG	CD-NE	-5.05	1.39	1.46
1	Р	1131	ARG	CD-NE	-5.05	1.39	1.46
3	F	77	PRO	CA-CB	-5.04	1.47	1.53
3	E	206	ARG	CD-NE	-5.03	1.39	1.46

All (589) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	С	295	ARG	CA-C-N	22.15	147.90	120.88
2	С	295	ARG	C-N-CA	22.15	147.90	120.88
2	D	295	ARG	CA-C-N	22.04	147.77	120.88
2	D	295	ARG	C-N-CA	22.04	147.77	120.88
1	0	589	GLN	O-C-N	10.01	132.38	122.07
1	А	589	GLN	O-C-N	9.99	132.35	122.07
3	R	82	LEU	CA-C-N	9.46	129.40	122.59
3	R	82	LEU	C-N-CA	9.46	129.40	122.59
3	F	82	LEU	CA-C-N	9.42	129.37	122.59
3	F	82	LEU	C-N-CA	9.42	129.37	122.59
1	Р	469	ASP	CA-CB-CG	8.88	121.48	112.60
1	В	469	ASP	CA-CB-CG	8.79	121.39	112.60
1	В	1127	ASN	CA-CB-CG	8.41	121.01	112.60
1	Р	1127	ASN	CA-CB-CG	8.38	120.98	112.60
1	А	589	GLN	CA-C-N	-7.85	109.63	120.38
1	А	589	GLN	C-N-CA	-7.85	109.63	120.38
1	В	259	PHE	CA-CB-CG	7.84	121.64	113.80
1	0	589	GLN	CA-C-N	-7.83	109.66	120.38
1	0	589	GLN	C-N-CA	-7.83	109.66	120.38
1	Р	259	PHE	CA-CB-CG	7.81	121.61	113.80



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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
5	К	63	DG	C4'-C3'-O3'	7.72	121.58	110.00
2	С	120	PHE	CA-CB-CG	-7.54	106.26	113.80
1	Р	187	ARG	NE-CZ-NH2	7.50	125.95	119.20
1	Р	232	PHE	CA-CB-CG	7.44	121.24	113.80
1	В	232	PHE	CA-CB-CG	7.20	121.00	113.80
5	К	47	DC	O3'-P-O5'	-7.19	93.22	104.00
5	K	64	DG	O5'-C5'-C4'	7.05	121.37	110.80
2	D	294	ASN	N-CA-C	-7.04	103.65	111.82
2	С	294	ASN	N-CA-C	-7.00	103.70	111.82
3	R	160	ASN	CA-CB-CG	6.92	119.52	112.60
3	R	89	SER	CA-C-N	6.91	129.87	120.54
3	R	89	SER	C-N-CA	6.91	129.87	120.54
5	К	62	DT	C4'-C3'-O3'	-6.85	99.72	110.00
1	Р	197	PHE	CA-CB-CG	6.81	120.61	113.80
1	Р	219	ASP	CA-CB-CG	6.75	119.35	112.60
1	Р	225	ASN	CA-CB-CG	6.74	119.34	112.60
1	Р	301	GLN	O-C-N	-6.72	115.00	122.12
2	D	176	ARG	CB-CG-CD	6.71	126.74	111.30
3	F	160	ASN	CA-CB-CG	6.71	119.31	112.60
1	Р	94	ASN	CA-CB-CG	6.70	119.30	112.60
1	Р	1253	ASN	CA-CB-CG	6.68	119.28	112.60
3	R	187	PHE	CA-CB-CG	6.68	120.48	113.80
1	В	197	PHE	CA-CB-CG	6.67	120.47	113.80
1	В	301	GLN	O-C-N	-6.65	115.07	122.12
3	Q	44	HIS	CA-CB-CG	6.65	120.45	113.80
3	Е	44	HIS	CA-CB-CG	6.64	120.44	113.80
1	Р	158	ASP	CA-CB-CG	6.63	119.23	112.60
3	Ε	195	ASP	CA-CB-CG	6.60	119.20	112.60
1	В	225	ASN	CA-CB-CG	6.59	119.19	112.60
3	Q	195	ASP	CA-CB-CG	6.55	119.15	112.60
3	Ε	73	PHE	CA-CB-CG	6.54	120.34	113.80
1	Р	1187	PHE	CA-CB-CG	6.51	120.31	113.80
1	Р	54	ASP	CA-CB-CG	6.49	119.09	112.60
3	Q	73	PHE	CA-CB-CG	6.49	120.29	113.80
1	В	94	ASN	CA-CB-CG	6.48	119.08	112.60
1	В	1187	PHE	CA-CB-CG	6.48	120.28	113.80
5	K	64	DG	C5'-C4'-O4'	6.47	119.10	109.40
3	Q	43	ASN	CA-CB-CG	6.47	119.07	112.60
3	Е	196	ASP	CA-CB-CG	6.47	119.07	112.60
1	Р	1207	ASP	CA-CB-CG	6.47	119.07	112.60
3	Q	196	ASP	CA-CB-CG	6.47	119.07	112.60
3	F	187	PHE	CA-CB-CG	6.45	120.25	113.80



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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	Р	1164	ASN	CA-CB-CG	6.45	119.05	112.60
3	Е	43	ASN	CA-CB-CG	6.43	119.03	112.60
1	В	1164	ASN	CA-CB-CG	6.43	119.03	112.60
1	В	966	ARG	NE-CZ-NH2	6.42	124.98	119.20
1	В	1207	ASP	CA-CB-CG	6.41	119.01	112.60
2	D	325	ASP	CA-CB-CG	6.39	118.99	112.60
6	L	43	DG	C2'-C3'-O3'	-6.38	101.93	111.50
1	В	175	HIS	CA-CB-CG	6.36	120.16	113.80
1	В	1210	ASP	CA-CB-CG	6.33	118.93	112.60
1	Р	1201	ASP	N-CA-C	6.33	118.70	111.11
1	В	54	ASP	CA-CB-CG	6.32	118.92	112.60
1	Р	1210	ASP	CA-CB-CG	6.32	118.92	112.60
1	Р	966	ARG	NE-CZ-NH2	6.30	124.87	119.20
1	В	187	ARG	NE-CZ-NH2	6.30	124.87	119.20
1	В	1201	ASP	N-CA-C	6.30	118.67	111.11
1	В	1193	HIS	CA-CB-CG	6.29	120.09	113.80
1	В	255	ASP	CA-CB-CG	6.28	118.88	112.60
1	В	1131	ARG	CD-NE-CZ	6.28	133.19	124.40
1	Р	1131	ARG	CD-NE-CZ	6.28	133.19	124.40
3	R	145	ASP	CA-CB-CG	6.26	118.86	112.60
1	Р	1193	HIS	CA-CB-CG	6.25	120.05	113.80
1	Р	234	ASP	CA-CB-CG	6.24	118.84	112.60
2	С	325	ASP	CA-CB-CG	6.23	118.83	112.60
1	В	97	HIS	CA-C-N	6.23	131.59	123.00
1	В	97	HIS	C-N-CA	6.23	131.59	123.00
1	Р	168	PHE	CA-CB-CG	6.21	120.01	113.80
3	Q	57	PHE	CA-CB-CG	6.21	120.01	113.80
3	Ε	57	PHE	CA-CB-CG	6.21	120.01	113.80
1	Р	255	ASP	CA-CB-CG	6.19	118.79	112.60
5	Κ	47	DC	C2'-C3'-O3'	-6.19	102.21	111.50
3	R	136	PHE	CA-CB-CG	6.18	119.98	113.80
5	Κ	46	DA	O3'-P-O5'	6.18	113.27	104.00
1	Р	243	ARG	CA-CB-CG	6.17	126.44	114.10
1	Р	1242	ASN	CA-CB-CG	6.17	118.77	112.60
1	B	243	ARG	CA-CB-CG	6.17	126.44	114.10
1	В	1132	ARG	CD-NE-CZ	6.15	133.01	124.40
1	В	1221	ARG	CD-NE-CZ	6.14	133.00	124.40
1	Р	1221	ARG	CD-NE-CZ	6.14	132.99	124.40
1	В	164	GLN	CA-C-N	6.13	131.46	123.00
1	B	164	GLN	C-N-CA	6.13	131.46	123.00
1	В	$\overline{234}$	ASP	CA-CB-CG	6.12	118.72	112.60
1	Р	198	TYR	N-CA-CB	6.11	118.87	110.01



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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	Р	1132	ARG	CD-NE-CZ	6.10	132.94	124.40
1	Р	97	HIS	CA-C-N	6.09	131.41	123.00
1	Р	97	HIS	C-N-CA	6.09	131.41	123.00
1	Р	1339	ASP	CA-CB-CG	6.08	118.68	112.60
3	Е	62	ASN	CA-CB-CG	6.08	118.67	112.60
1	Р	164	GLN	CA-C-N	6.08	131.38	123.00
1	Р	164	GLN	C-N-CA	6.08	131.38	123.00
1	Р	1328	ARG	CD-NE-CZ	6.07	132.90	124.40
1	Р	1331	GLN	N-CA-C	6.07	123.73	110.80
1	Р	201	ILE	N-CA-CB	6.07	117.65	110.55
1	Р	243	ARG	CG-CD-NE	6.07	125.35	112.00
1	В	229	ARG	CD-NE-CZ	6.06	132.89	124.40
1	В	201	ILE	N-CA-CB	6.06	117.64	110.55
3	R	27	ASP	CA-CB-CG	6.05	118.66	112.60
1	В	1056	ARG	NE-CZ-NH2	6.05	124.65	119.20
1	В	1328	ARG	CD-NE-CZ	6.05	132.87	124.40
3	Q	62	ASN	CA-CB-CG	6.05	118.65	112.60
1	В	243	ARG	CG-CD-NE	6.04	125.30	112.00
3	R	147	ASP	CA-CB-CG	6.04	118.64	112.60
1	В	105	ARG	CD-NE-CZ	6.04	132.86	124.40
1	В	224	GLU	CA-C-N	6.03	131.50	123.00
1	В	224	GLU	C-N-CA	6.03	131.50	123.00
3	R	156	ARG	CD-NE-CZ	6.03	132.84	124.40
1	Р	224	GLU	CA-C-N	6.02	131.48	123.00
1	Р	224	GLU	C-N-CA	6.02	131.48	123.00
3	Е	138	ASN	CA-CB-CG	6.00	118.61	112.60
1	В	198	TYR	N-CA-CB	6.00	118.71	110.01
3	F	145	ASP	CA-CB-CG	6.00	118.60	112.60
3	Ε	138	ASN	CB-CA-C	5.99	120.64	109.86
1	В	263	ILE	N-CA-CB	5.98	117.14	110.62
1	Р	1056	ARG	NE-CZ-NH2	5.98	124.58	119.20
3	Е	42	ASP	CA-C-N	5.97	128.21	120.44
3	Ε	42	ASP	C-N-CA	5.97	128.21	120.44
1	Р	1341	ARG	CD-NE-CZ	5.97	132.76	124.40
1	Р	118	ILE	CA-C-N	5.96	130.85	122.74
1	Р	118	ILE	C-N-CA	5.96	130.85	122.74
3	F	156	ARG	CD-NE-CZ	5.96	132.75	124.40
3	Q	66	ILE	CA-C-N	5.96	131.78	123.07
3	Q	66	ILE	C-N-CA	5.96	131.78	123.07
1	Р	263	ILE	N-CA-CB	5.96	117.12	110.62
3	Q	42	ASP	CA-C-N	5.96	128.19	120.44
3	Q	42	ASP	C-N-CA	5.96	$1\overline{28.19}$	120.44



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	Р	96	ARG	CD-NE-CZ	5.96	132.74	124.40
3	Q	42	ASP	CA-CB-CG	5.95	118.55	112.60
1	Р	103	GLY	N-CA-C	5.95	119.44	110.75
3	Е	66	ILE	CA-C-N	5.95	131.75	123.07
3	Е	66	ILE	C-N-CA	5.95	131.75	123.07
3	Е	42	ASP	CA-CB-CG	5.95	118.55	112.60
1	В	122	MET	CA-C-N	5.94	131.25	122.99
1	В	122	MET	C-N-CA	5.94	131.25	122.99
3	F	27	ASP	CA-CB-CG	5.94	118.54	112.60
1	Р	165	PHE	CA-CB-CG	5.93	119.73	113.80
1	В	96	ARG	CD-NE-CZ	5.93	132.70	124.40
1	В	118	ILE	CA-C-N	5.92	130.79	122.74
1	В	118	ILE	C-N-CA	5.92	130.79	122.74
3	Е	60	ARG	CD-NE-CZ	5.92	132.68	124.40
3	Q	63	VAL	CA-C-N	5.92	130.29	122.30
3	Q	63	VAL	C-N-CA	5.92	130.29	122.30
1	Р	122	MET	CA-C-N	5.91	131.21	122.99
1	Р	122	MET	C-N-CA	5.91	131.21	122.99
1	Р	1339	ASP	CA-C-N	5.91	128.20	120.28
1	Р	1339	ASP	C-N-CA	5.91	128.20	120.28
3	Q	60	ARG	CD-NE-CZ	5.91	132.67	124.40
2	С	124	ARG	CA-CB-CG	5.91	125.92	114.10
3	R	31	ARG	CD-NE-CZ	5.91	132.67	124.40
1	Р	1390	ARG	NE-CZ-NH2	5.91	124.52	119.20
1	Р	1244	ILE	N-CA-CB	5.90	117.45	110.55
1	Р	1250	ARG	CD-NE-CZ	5.89	132.64	124.40
1	В	1339	ASP	CA-C-N	5.88	128.16	120.28
1	В	1339	ASP	C-N-CA	5.88	128.16	120.28
1	В	103	GLY	N-CA-C	5.87	119.16	110.42
3	E	63	VAL	CA-C-N	5.87	130.22	122.30
3	E	63	VAL	C-N-CA	5.87	130.22	122.30
5	K	32	DA	C5'-C4'-C3'	-5.87	106.10	114.90
3	F	31	ARG	CD-NE-CZ	5.86	132.61	124.40
1	В	1244	ILE	N-CA-CB	5.85	117.40	110.55
3	Q	31	ARG	CD-NE-CZ	5.85	132.59	124.40
6	L	30	DG	C4'-C3'-O3'	-5.84	101.24	110.00
1	В	548	ARG	CA-C-N	5.82	130.54	121.76
1	В	548	ARG	C-N-CA	5.82	130.54	121.76
6	L	47	DT	C5'-C4'-O4'	5.81	118.12	109.40
3	E	31	ARG	CD-NE-CZ	5.81	132.53	124.40
3	F	147	ASP	CA-CB-CG	5.81	118.41	112.60
1	В	166	LYS	CA-C-N	5.80	131.18	122.99



Mol	Chain	$\mathbf{Res}$	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	В	166	LYS	C-N-CA	5.80	131.18	122.99
1	В	1395	LYS	CA-CB-CG	5.80	125.71	114.10
1	В	1192	GLN	CA-C-N	5.80	128.37	120.54
1	В	1192	GLN	C-N-CA	5.80	128.37	120.54
1	Р	548	ARG	CA-C-N	5.80	130.52	121.76
1	Р	548	ARG	C-N-CA	5.80	130.52	121.76
3	Q	74	TYR	CA-C-N	5.79	130.71	122.72
3	Q	74	TYR	C-N-CA	5.79	130.71	122.72
2	С	294	ASN	CA-C-N	5.79	130.79	122.40
2	С	294	ASN	C-N-CA	5.79	130.79	122.40
6	L	56	DT	O3'-P-O5'	-5.78	95.33	104.00
1	В	1250	ARG	CD-NE-CZ	5.78	132.49	124.40
1	В	235	MET	CA-C-N	5.77	127.94	120.44
1	В	235	MET	C-N-CA	5.77	127.94	120.44
3	Q	25	GLU	CA-C-N	5.77	127.94	120.44
3	Q	25	GLU	C-N-CA	5.77	127.94	120.44
3	Е	25	GLU	CA-C-N	5.77	127.94	120.44
3	Ε	25	GLU	C-N-CA	5.77	127.94	120.44
3	R	92	ASP	CA-CB-CG	5.76	118.36	112.60
1	В	1197	ARG	CA-C-N	5.76	128.22	120.50
1	В	1197	ARG	C-N-CA	5.76	128.22	120.50
3	F	129	ASP	CA-C-N	5.76	127.99	120.28
3	F	129	ASP	C-N-CA	5.76	127.99	120.28
1	Р	153	LEU	CA-C-N	5.75	127.92	120.44
1	Р	153	LEU	C-N-CA	5.75	127.92	120.44
1	Р	1197	ARG	CA-C-N	5.75	128.20	120.50
1	Р	1197	ARG	C-N-CA	5.75	128.20	120.50
1	Р	235	MET	CA-C-N	5.75	127.91	120.44
1	Р	235	MET	C-N-CA	5.75	127.91	120.44
2	D	294	ASN	CA-C-N	5.74	130.73	122.40
2	D	294	ASN	C-N-CA	5.74	130.73	122.40
1	В	165	PHE	CA-CB-CG	5.73	119.53	113.80
1	Р	1192	GLN	CA-C-N	5.72	128.26	120.54
1	Р	1192	GLN	C-N-CA	5.72	128.26	120.54
3	Ε	27	ASP	CA-CB-CG	5.70	118.30	112.60
3	R	161	ARG	N-CA-CB	5.70	118.43	109.94
3	Е	74	TYR	CA-C-N	5.70	130.58	122.72
3	Е	74	TYR	C-N-CA	5.70	130.58	122.72
3	R	129	ASP	CA-C-N	5.69	127.90	120.28
3	R	129	ASP	C-N-CA	5.69	127.90	120.28
2	C	137	HIS	$CB-C\overline{G-CD2}$	-5.68	123.82	131.20
1	В	100	VAL	CA-C-N	5.68	131.05	123.10

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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	В	100	VAL	C-N-CA	5.68	131.05	123.10
3	Q	27	ASP	CA-CB-CG	5.68	118.28	112.60
1	В	103	GLY	CA-C-N	5.67	130.97	122.58
1	В	103	GLY	C-N-CA	5.67	130.97	122.58
3	F	161	ARG	N-CA-CB	5.67	118.39	109.94
3	Q	56	GLU	CA-C-N	5.67	128.13	120.65
3	Q	56	GLU	C-N-CA	5.67	128.13	120.65
1	Р	100	VAL	CA-C-N	5.66	131.02	123.10
1	Р	100	VAL	C-N-CA	5.66	131.02	123.10
2	С	330	GLU	N-CA-CB	5.66	118.25	109.48
1	Р	163	VAL	CA-C-N	5.65	130.97	123.05
1	Р	163	VAL	C-N-CA	5.65	130.97	123.05
2	D	330	GLU	N-CA-CB	5.65	118.24	109.48
3	F	26	LEU	CA-C-N	5.65	127.78	120.44
3	F	26	LEU	C-N-CA	5.65	127.78	120.44
1	В	249	ILE	N-CA-CB	5.65	117.16	110.55
1	В	244	ILE	N-CA-CB	5.64	116.55	110.62
1	Р	1387	GLU	N-CA-CB	5.64	118.42	110.12
1	Р	101	VAL	CA-C-N	5.64	130.18	122.34
1	Р	101	VAL	C-N-CA	5.64	130.18	122.34
1	Р	1287	LEU	N-CA-CB	5.64	118.19	110.01
1	Р	528	ARG	NE-CZ-NH2	5.64	124.27	119.20
1	В	1188	ILE	N-CA-CB	5.63	116.77	110.51
3	Е	67	ARG	CG-CD-NE	5.63	124.40	112.00
1	Р	244	ILE	N-CA-CB	5.63	116.53	110.62
6	L	33	DG	C4'-C3'-O3'	-5.63	101.56	110.00
3	Q	67	ARG	CG-CD-NE	5.62	124.38	112.00
3	Q	46	PHE	N-CA-CB	5.62	118.32	109.94
3	R	26	LEU	CA-C-N	5.62	127.75	120.44
3	R	26	LEU	C-N-CA	5.62	127.75	120.44
3	Ε	56	GLU	CA-C-N	5.62	128.07	120.65
3	Ε	56	GLU	C-N-CA	5.62	128.07	120.65
2	D	137	HIS	CB-CG-CD2	-5.62	123.89	131.20
1	Р	256	ARG	CD-NE-CZ	5.62	132.26	124.40
1	В	256	ARG	CD-NE-CZ	5.61	132.26	124.40
3	F	92	ASP	CA-CB-CG	5.61	118.20	112.60
1	В	163	VAL	CA-C-N	5.60	130.90	123.05
1	В	163	VAL	C-N-CA	5.60	130.90	123.05
1	P	$112\overline{6}$	ASP	CA-CB-CG	5.60	$118.2\overline{0}$	112.60
1	В	101	VAL	CA-C-N	5.60	130.13	122.34
1	В	101	VAL	C-N-CA	5.60	130.13	122.34
1	Р	249	ILE	N-CA-CB	5.60	117.10	110.55



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	В	1387	GLU	N-CA-CB	5.60	118.35	110.12
1	Р	1188	ILE	N-CA-CB	5.59	116.72	110.51
3	Е	46	PHE	N-CA-CB	5.59	118.27	109.94
3	F	88	LEU	CA-C-N	5.59	130.67	121.39
3	F	88	LEU	C-N-CA	5.59	130.67	121.39
6	L	39	DG	C4'-C3'-O3'	-5.59	101.62	110.00
1	Р	103	GLY	CA-C-N	5.58	130.84	122.58
1	Р	103	GLY	C-N-CA	5.58	130.84	122.58
5	K	57	DC	C4'-C3'-O3'	-5.57	101.64	110.00
1	В	1126	ASP	CA-CB-CG	5.56	118.16	112.60
1	Р	149	PRO	CA-C-N	5.56	127.67	120.44
1	Р	149	PRO	C-N-CA	5.56	127.67	120.44
3	F	24	PRO	CA-C-N	5.56	127.67	120.44
3	F	24	PRO	C-N-CA	5.56	127.67	120.44
1	В	104	VAL	CA-C-N	5.56	130.16	122.77
1	В	104	VAL	C-N-CA	5.56	130.16	122.77
1	В	528	ARG	NE-CZ-NH2	5.56	124.20	119.20
1	В	193	ASP	CA-CB-CG	5.56	118.16	112.60
2	D	287	THR	CA-CB-OG1	5.56	117.94	109.60
3	R	148	LYS	CG-CD-CE	5.55	124.08	111.30
2	С	287	THR	CA-CB-OG1	5.55	117.93	109.60
2	С	295	ARG	CB-CA-C	5.55	120.28	111.51
1	Р	99	ARG	CA-C-N	5.55	130.71	122.99
1	Р	99	ARG	C-N-CA	5.55	130.71	122.99
1	Р	186	LYS	CA-CB-CG	5.54	125.19	114.10
3	R	129	ASP	CA-CB-CG	5.54	118.14	112.60
6	L	43	DG	O3'-P-O5'	-5.54	95.69	104.00
1	В	1216	GLU	CA-C-N	5.53	127.53	120.56
1	В	1216	GLU	C-N-CA	5.53	127.53	120.56
1	Р	1216	GLU	CA-C-N	5.51	127.51	120.56
1	Р	1216	GLU	C-N-CA	5.51	127.51	120.56
1	Р	1328	ARG	CB-CG-CD	5.51	123.97	111.30
1	В	99	ARG	CA-C-N	5.50	130.64	122.99
1	В	99	ARG	C-N-CA	5.50	130.64	122.99
1	В	228	VAL	CA-C-N	5.50	127.59	120.44
1	В	228	VAL	C-N-CA	5.50	127.59	120.44
1	В	149	PRO	CA-C-N	5.50	127.59	120.44
1	В	149	PRO	C-N-CA	5.50	127.59	120.44
1	Р	167	GLN	CA-C-N	5.50	130.31	122.72
1	Р	167	GLN	C-N-CA	5.50	130.31	122.72
1	P	1396	ASP	CA-C-N	5.50	130.26	123.12
1	Р	1396	ASP	C-N-CA	5.50	130.26	123.12



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	D	295	ARG	CB-CA-C	5.49	120.19	111.51
1	В	1399	PRO	CA-C-N	5.49	129.04	120.75
1	В	1399	PRO	C-N-CA	5.49	129.04	120.75
1	В	403	GLN	OE1-CD-NE2	-5.49	117.11	122.60
3	R	128	ALA	CA-C-N	5.48	129.26	121.42
3	R	128	ALA	C-N-CA	5.48	129.26	121.42
1	Р	117	ASP	CA-C-N	5.48	130.61	122.99
1	Р	117	ASP	C-N-CA	5.48	130.61	122.99
1	В	1197	ARG	CD-NE-CZ	5.48	132.07	124.40
1	В	1396	ASP	CA-C-N	5.47	130.23	123.12
1	В	1396	ASP	C-N-CA	5.47	130.23	123.12
3	F	128	ALA	CA-C-N	5.47	129.24	121.42
3	F	128	ALA	C-N-CA	5.47	129.24	121.42
3	Q	44	HIS	CA-C-N	5.46	127.54	120.44
3	Q	44	HIS	C-N-CA	5.46	127.54	120.44
1	В	1212	ILE	N-CA-CB	5.46	116.35	110.62
3	Е	44	HIS	CA-C-N	5.46	127.54	120.44
3	Е	44	HIS	C-N-CA	5.46	127.54	120.44
1	Р	1212	ILE	N-CA-CB	5.46	116.35	110.62
3	Е	43	ASN	CA-C-N	5.45	127.53	120.44
3	Е	43	ASN	C-N-CA	5.45	127.53	120.44
3	Q	43	ASN	CA-C-N	5.45	127.53	120.44
3	Q	43	ASN	C-N-CA	5.45	127.53	120.44
2	D	323	LEU	CA-C-N	5.45	128.50	120.82
2	D	323	LEU	C-N-CA	5.45	128.50	120.82
1	Р	227	GLY	CA-C-N	5.45	127.42	120.56
1	Р	227	GLY	C-N-CA	5.45	127.42	120.56
3	R	155	VAL	N-CA-CB	5.45	116.92	110.55
5	Κ	56	DT	C2'-C3'-O3'	5.44	119.66	111.50
3	Q	46	PHE	CA-CB-CG	5.44	119.24	113.80
1	Р	403	GLN	OE1-CD-NE2	-5.43	117.17	122.60
3	Ε	46	PHE	CA-CB-CG	5.43	119.23	113.80
3	R	24	PRO	CA-C-N	5.43	127.50	120.44
3	R	24	PRO	C-N-CA	5.43	127.50	120.44
3	F	155	VAL	N-CA-CB	5.42	116.90	110.55
1	Р	1399	PRO	CA-C-N	5.42	128.94	120.75
1	Р	1399	PRO	C-N-CA	5.42	128.94	120.75
2	С	116	ARG	NE-CZ-NH2	5.41	124.07	119.20
1	В	117	ASP	CA-C-N	5.41	130.51	122.99
1	В	117	ASP	C-N-CA	5.41	130.51	122.99
1	Р	218	ARG	CA-C-N	5.40	127.52	120.28
1	Р	218	ARG	C-N-CA	5.40	127.52	120.28



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	Р	1197	ARG	CD-NE-CZ	5.40	131.95	124.40
1	Р	1384	SER	N-CA-CB	5.39	117.83	110.01
1	В	1221	ARG	CA-CB-CG	5.38	124.87	114.10
2	С	323	LEU	CA-C-N	5.38	128.41	120.82
2	С	323	LEU	C-N-CA	5.38	128.41	120.82
1	Р	1221	ARG	CA-CB-CG	5.38	124.86	114.10
1	Р	1322	GLN	CA-CB-CG	5.38	124.86	114.10
3	Q	139	GLN	CB-CG-CD	5.38	121.74	112.60
1	В	227	GLY	CA-C-N	5.38	127.33	120.56
1	В	227	GLY	C-N-CA	5.38	127.33	120.56
3	F	91	LEU	CA-C-N	5.37	127.42	120.44
3	F	91	LEU	C-N-CA	5.37	127.42	120.44
1	В	48	VAL	N-CA-CB	5.37	117.84	110.54
1	В	363	ARG	NE-CZ-NH2	5.36	124.03	119.20
1	В	1322	GLN	CA-CB-CG	5.36	124.83	114.10
3	F	129	ASP	CA-CB-CG	5.36	117.96	112.60
1	Р	243	ARG	CD-NE-CZ	5.36	131.91	124.40
1	В	250	ARG	CA-C-N	5.36	127.26	120.72
1	В	250	ARG	C-N-CA	5.36	127.26	120.72
3	Q	62	ASN	CA-C-N	5.35	130.41	122.71
3	Q	62	ASN	C-N-CA	5.35	130.41	122.71
1	В	233	GLN	CA-C-N	5.35	127.71	120.65
1	В	233	GLN	C-N-CA	5.35	127.71	120.65
3	R	91	LEU	CA-C-N	5.35	127.39	120.44
3	R	91	LEU	C-N-CA	5.35	127.39	120.44
1	В	194	ARG	NE-CZ-NH2	5.34	124.01	119.20
1	В	186	LYS	CA-CB-CG	5.34	124.78	114.10
1	Р	363	ARG	NE-CZ-NH2	5.34	124.00	119.20
1	Р	1241	ALA	CA-C-N	5.34	127.70	120.65
1	Р	1241	ALA	C-N-CA	5.34	127.70	120.65
1	В	194	ARG	N-CA-CB	-5.34	102.28	110.12
2	С	299	GLN	CA-C-N	5.33	127.74	120.54
2	С	299	GLN	C-N-CA	5.33	127.74	120.54
1	В	243	ARG	CD-NE-CZ	5.33	131.87	124.40
3	F	98	ILE	N-CA-CB	5.33	116.79	110.55
2	D	299	GLN	CA-C-N	5.32	127.72	120.54
2	D	299	GLN	C-N-CA	5.32	127.72	120.54
1	Р	233	GLN	CA-C-N	5.32	127.67	120.65
1	Р	233	GLN	C-N-CA	5.32	127.67	120.65
3	R	123	GLU	CA-C-N	5.32	127.72	120.54
3	R	123	GLU	C-N-CA	5.32	127.72	120.54
1	Р	156	ARG	CA-C-N	5.31	$1\overline{27.67}$	120.44



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Mol	Chain	Res	Type	Atoms Z		$Observed(^{o})$	$Ideal(^{o})$
1	Р	156	ARG	C-N-CA	5.31	127.67	120.44
3	R	34	ARG	N-CA-CB	5.31	117.85	109.83
3	F	148	LYS	CG-CD-CE	5.31	123.52	111.30
3	Q	67	ARG	CD-NE-CZ	5.31	131.84	124.40
1	Р	48	VAL	N-CA-CB	5.31	117.76	110.54
3	R	138	ASN	OD1-CG-ND2	-5.31	117.29	122.60
1	В	1328	ARG	CB-CG-CD	5.31	123.50	111.30
3	Е	67	ARG	CA-CB-CG	5.30	124.71	114.10
3	F	123	GLU	CA-C-N	5.30	127.70	120.54
3	F	123	GLU	C-N-CA	5.30	127.70	120.54
5	K	56	DT	C4'-C3'-O3'	-5.30	102.05	110.00
3	R	144	SER	CA-C-N	5.30	127.69	120.54
3	R	144	SER	C-N-CA	5.30	127.69	120.54
3	F	161	ARG	CA-C-N	5.29	127.37	120.28
3	F	161	ARG	C-N-CA	5.29	127.37	120.28
1	Р	162	GLY	CA-C-N	5.29	128.96	121.66
1	Р	162	GLY	C-N-CA	5.29	128.96	121.66
1	В	1220	ALA	CA-C-N	5.29	127.68	120.54
1	В	1220	ALA	C-N-CA	5.29	127.68	120.54
1	Р	250	ARG	CA-C-N	5.29	127.17	120.72
1	Р	250	ARG	C-N-CA	5.29	127.17	120.72
3	Е	67	ARG	CD-NE-CZ	5.29	131.80	124.40
1	В	1188	ILE	CA-C-N	5.29	127.31	120.44
1	В	1188	ILE	C-N-CA	5.29	127.31	120.44
2	D	123	LEU	CB-CG-CD2	-5.29	94.84	110.70
2	С	290	ASP	N-CA-C	5.28	118.88	112.23
1	Р	1188	ILE	CA-C-N	5.28	127.30	120.44
1	Р	1188	ILE	C-N-CA	5.28	127.30	120.44
2	D	290	ASP	N-CA-C	5.28	118.88	112.23
3	R	85	ARG	CA-CB-CG	5.28	124.65	114.10
3	F	144	SER	CA-C-N	5.27	127.66	120.54
3	F	144	SER	C-N-CA	5.27	127.66	120.54
3	Е	62	ASN	CA-C-N	5.27	130.30	122.71
3	Е	62	ASN	C-N-CA	5.27	130.30	122.71
3	F	34	ARG	N-CA-CB	5.27	117.79	109.83
3	R	161	ARG	CA-C-N	5.27	127.34	120.28
3	R	161	ARG	C-N-CA	5.27	127.34	120.28
1	Р	1248	ILE	N-CA-CB	5.26	117.70	110.54
2	D	116	ARG	NE-CZ-NH2	5.26	123.93	119.20
3	F	94	MET	CA-C-N	5.26	127.19	120.56
3	F	94	MET	C-N-CA	5.26	127.19	120.56
1	Р	1164	ASN	N-CA-CB	5.25	117.73	110.17


Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
3	F	147	ASP	CA-C-N	5.25	127.31	120.28
3	F	147	ASP	C-N-CA	5.25	127.31	120.28
3	R	156	ARG	CA-C-N	5.25	127.58	120.65
3	R	156	ARG	C-N-CA	5.25	127.58	120.65
3	Q	67	ARG	CA-CB-CG	5.25	124.59	114.10
3	F	29	GLN	CA-C-N	5.24	127.26	120.44
3	F	29	GLN	C-N-CA	5.24	127.26	120.44
5	Κ	26	DC	C5'-C4'-O4'	5.24	117.26	109.40
5	Κ	63	DG	C4-N9-C1'	-5.24	119.14	127.00
3	R	147	ASP	CA-C-N	5.24	127.31	120.28
3	R	147	ASP	C-N-CA	5.24	127.31	120.28
1	Р	1254	ARG	N-CA-CB	5.24	117.61	110.01
3	R	29	GLN	CA-C-N	5.24	127.25	120.44
3	R	29	GLN	C-N-CA	5.24	127.25	120.44
1	А	966	ARG	NE-CZ-NH2	5.24	123.91	119.20
1	В	191	ALA	CA-C-N	5.24	127.30	120.28
1	В	191	ALA	C-N-CA	5.24	127.30	120.28
1	Р	1220	ALA	CA-C-N	5.24	127.61	120.54
1	Р	1220	ALA	C-N-CA	5.24	127.61	120.54
6	L	48	DC	C5'-C4'-O4'	5.23	117.24	109.40
2	С	151	HIS	CB-CG-CD2	-5.23	124.41	131.20
1	Р	1397	ILE	CA-C-N	5.22	131.36	122.06
1	Р	1397	ILE	C-N-CA	5.22	131.36	122.06
1	В	234	ASP	CA-C-N	5.22	127.27	120.28
1	В	234	ASP	C-N-CA	5.22	127.27	120.28
3	R	94	MET	CA-C-N	5.22	127.13	120.56
3	R	94	MET	C-N-CA	5.22	127.13	120.56
3	Е	29	GLN	CA-C-N	5.21	127.21	120.44
3	Е	29	GLN	C-N-CA	5.21	127.21	120.44
2	D	320	ALA	CA-C-N	5.20	128.26	120.87
2	D	320	ALA	C-N-CA	5.20	128.26	120.87
1	В	194	ARG	CA-C-N	5.20	127.20	120.44
1	В	194	ARG	C-N-CA	5.20	127.20	120.44
5	Κ	62	DT	C2'-C3'-O3'	5.20	119.30	111.50
3	F	156	ARG	CA-C-N	5.20	127.51	120.65
3	F	156	ARG	C-N-CA	5.20	127.51	120.65
1	Р	173	ASP	CA-C-N	5.20	127.19	120.44
1	Р	173	ASP	C-N-CA	5.20	127.19	120.44
1	В	1187	PHE	CA-C-N	5.19	127.30	120.60
1	В	1187	PHE	C-N-CA	5.19	127.30	120.60
3	Q	29	GLN	CA-C-N	5.19	127.18	120.44
3	Q	29	GLN	C-N-CA	5.19	127.18	120.44



Mol	Chain	$\mathbf{Res}$	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	Р	234	ASP	CA-C-N	5.18	127.23	120.28
1	Р	234	ASP	C-N-CA	5.18	127.23	120.28
3	F	80	THR	CA-C-N	5.18	128.46	121.05
3	F	80	THR	C-N-CA	5.18	128.46	121.05
1	Р	240	ARG	N-CA-CB	5.18	117.52	110.01
1	В	1164	ASN	N-CA-CB	5.18	117.62	110.17
1	Р	1250	ARG	N-CA-CB	5.17	117.65	109.94
3	Е	206	ARG	N-CA-CB	5.17	117.72	110.12
3	Q	26	LEU	CA-C-N	5.17	127.16	120.44
3	Q	26	LEU	C-N-CA	5.17	127.16	120.44
3	Е	26	LEU	CA-C-N	5.17	127.16	120.44
3	Е	26	LEU	C-N-CA	5.17	127.16	120.44
2	D	151	HIS	CB-CG-CD2	-5.17	124.48	131.20
1	Р	559	GLN	OE1-CD-NE2	-5.17	117.44	122.60
3	Q	206	ARG	N-CA-CB	5.17	117.71	110.12
1	В	1246	LYS	CA-C-N	5.16	127.15	120.44
1	В	1246	LYS	C-N-CA	5.16	127.15	120.44
2	С	6	GLN	OE1-CD-NE2	-5.16	117.44	122.60
1	Р	1388	GLU	N-CA-CB	5.16	117.50	110.01
1	Р	1286	LEU	CA-C-N	5.16	127.15	120.44
1	Р	1286	LEU	C-N-CA	5.16	127.15	120.44
3	R	80	THR	CA-C-N	5.16	128.43	121.05
3	R	80	THR	C-N-CA	5.16	128.43	121.05
1	Р	1391	ARG	CD-NE-CZ	5.15	131.61	124.40
3	R	154	LYS	CA-C-N	5.15	127.05	120.56
3	R	154	LYS	C-N-CA	5.15	127.05	120.56
1	0	932	ASP	CB-CA-C	5.14	115.64	109.31
1	0	966	ARG	NE-CZ-NH2	5.14	123.83	119.20
6	L	66	DT	C5'-C4'-O4'	5.13	117.10	109.40
6	L	59	DT	C5'-C4'-O4'	5.13	117.09	109.40
1	Р	255	ASP	CA-C-N	5.13	127.11	120.44
1	Р	255	ASP	C-N-CA	5.13	127.11	120.44
1	Р	1187	PHE	CA-C-N	5.12	127.21	120.60
1	Р	1187	PHE	C-N-CA	5.12	127.21	120.60
1	Р	1190	VAL	N-CA-CB	5.12	116.54	110.55
1	В	192	SER	CA-C-N	5.12	127.09	120.44
1	В	192	SER	C-N-CA	5.12	127.09	120.44
1	Р	521	ARG	NE-CZ-NH2	5.11	123.80	119.20
1	В	240	ARG	N-CA-CB	5.11	117.42	110.01
1	В	521	ARG	NE-CZ-NH2	5.11	123.80	119.20
1	В	559	GLN	OE1-CD-NE2	-5.11	117.49	122.60
1	В	1190	VAL	N-CA-CB	5.11	116.53	110.55



Mol	Chain	$\mathbf{Res}$	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	Р	185	PRO	CA-C-N	5.10	131.07	122.87
1	Р	185	PRO	C-N-CA	5.10	131.07	122.87
1	В	185	PRO	CA-C-N	5.09	131.06	122.87
1	В	185	PRO	C-N-CA	5.09	131.06	122.87
1	В	174	TYR	CA-C-N	5.09	127.10	120.28
1	В	174	TYR	C-N-CA	5.09	127.10	120.28
1	Р	157	LEU	CA-C-N	5.08	127.09	120.28
1	Р	157	LEU	C-N-CA	5.08	127.09	120.28
3	R	148	LYS	CA-C-N	5.08	127.05	120.44
3	R	148	LYS	C-N-CA	5.08	127.05	120.44
3	F	148	LYS	CA-C-N	5.08	127.04	120.44
3	F	148	LYS	C-N-CA	5.08	127.04	120.44
3	Е	40	ASP	CA-C-N	5.08	127.39	120.54
3	Е	40	ASP	C-N-CA	5.08	127.39	120.54
1	Р	123	ILE	CA-C-N	5.08	130.55	122.94
1	Р	123	ILE	C-N-CA	5.08	130.55	122.94
3	F	85	ARG	CA-CB-CG	5.07	124.25	114.10
1	Р	1239	SER	CA-C-N	5.07	128.67	120.55
1	Р	1239	SER	C-N-CA	5.07	128.67	120.55
3	Q	27	ASP	N-CA-CB	5.07	117.36	110.01
1	В	1388	GLU	N-CA-CB	5.07	117.36	110.01
3	Е	27	ASP	N-CA-CB	5.07	117.36	110.01
5	Κ	18	DT	C5'-C4'-O4'	5.07	117.00	109.40
1	Р	154	LYS	N-CA-CB	5.07	117.36	110.01
1	А	932	ASP	CB-CA-C	5.07	115.54	109.31
1	В	1250	ARG	N-CA-CB	5.07	117.49	109.94
1	Р	174	TYR	CA-CB-CG	5.06	123.01	113.90
1	Р	549	GLN	N-CA-C	-5.06	98.81	107.61
3	Q	139	GLN	OE1-CD-NE2	-5.06	117.54	122.60
1	В	1198	ILE	CA-C-N	5.05	128.47	120.89
1	В	1198	ILE	C-N-CA	5.05	128.47	120.89
6	L	68	DT	C5'-C4'-O4'	5.05	116.98	109.40
1	В	123	ILE	CA-C-N	5.04	130.51	122.94
1	В	123	ILE	C-N-CA	5.04	130.51	122.94
2	D	176	ARG	CA-CB-CG	-5.04	104.02	114.10
1	Р	1198	ILE	CA-C-N	5.04	128.45	120.89
1	Р	1198	ILE	C-N-CA	5.04	128.45	120.89
1	В	1239	SER	CA-C-N	5.04	128.61	120.55
1	B	1239	SER	C-N-CA	5.04	$128.6\overline{1}$	$120.\overline{55}$
3	R	157	THR	CA-C-N	5.03	127.02	120.28
3	R	157	THR	C-N-CA	5.03	127.02	120.28
3	Ε	186	ARG	NE-CZ-NH2	5.03	123.72	119.20



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
3	R	31	ARG	CB-CG-CD	5.03	122.86	111.30
1	Р	1336	GLU	CA-C-N	5.02	129.11	120.72
1	Р	1336	GLU	C-N-CA	5.02	129.11	120.72
3	R	146	LEU	N-CA-CB	5.02	117.50	110.12
3	R	87	VAL	CA-C-N	5.02	128.82	120.94
3	R	87	VAL	C-N-CA	5.02	128.82	120.94
1	В	255	ASP	CA-C-N	5.02	126.97	120.44
1	В	255	ASP	C-N-CA	5.02	126.97	120.44
1	В	549	GLN	N-CA-C	-5.02	98.88	107.61
3	F	157	THR	CA-C-N	5.02	127.00	120.28
3	F	157	THR	C-N-CA	5.02	127.00	120.28
1	Р	102	VAL	CA-C-N	5.02	128.55	120.97
1	Р	102	VAL	C-N-CA	5.02	128.55	120.97
1	Р	1207	ASP	N-CA-CB	5.02	117.45	110.07
3	Q	163	ARG	NE-CZ-NH2	5.01	123.71	119.20
1	Р	548	ARG	NE-CZ-NH2	5.00	123.70	119.20
1	В	247	GLU	N-CA-CB	5.00	117.48	110.12
2	С	324	LEU	CA-C-N	5.00	130.44	122.59
2	С	324	LEU	C-N-CA	5.00	130.44	122.59
3	F	85	ARG	CD-NE-CZ	5.00	131.41	124.40
3	R	85	ARG	CD-NE-CZ	5.00	131.40	124.40
2	С	153	HIS	CB-CG-CD2	-5.00	124.70	131.20
5	K	15	DA	C2'-C3'-O3'	-5.00	104.00	111.50

There are no chirality outliers.

Mol	Chain	$\mathbf{Res}$	Type	Group
1	А	1058	ARG	Sidechain
1	А	966	ARG	Sidechain
1	А	967	ARG	Sidechain
1	В	528	ARG	Sidechain
1	В	966	ARG	Sidechain
2	С	120	PHE	Sidechain
2	С	138	ARG	Sidechain
2	С	300	ARG	Sidechain
2	С	327	ARG	Sidechain
2	С	4	TYR	Sidechain
2	С	89	ARG	Sidechain
2	D	116	ARG	Sidechain
2	D	138	ARG	Sidechain
2	D	300	ARG	Sidechain



Mol	Chain	Res	Type	Group
2	D	327	ARG	Sidechain
2	D	4	TYR	Sidechain
2	D	89	ARG	Sidechain
3	Е	101	TYR	Sidechain
3	Е	140	ARG	Sidechain
3	Е	161	ARG	Sidechain
3	Е	164	ARG	Sidechain
5	Κ	11	DT	Sidechain
5	Κ	12	DC	Sidechain
5	Κ	14	DG	Sidechain
5	Κ	18	DT	Sidechain
5	Κ	28	DC	Sidechain
5	Κ	29	DG	Sidechain
5	Κ	36	DC	Sidechain
5	K	4	DG	Sidechain
5	Κ	44	DA	Sidechain
5	Κ	45	DT	Sidechain
5	Κ	46	DA	Sidechain
5	Κ	49	DA	Sidechain
5	Κ	52	DC	Sidechain
5	Κ	54	DT	Sidechain
5	Κ	58	DC	Sidechain
5	Κ	63	DG	Sidechain
5	Κ	66	DA	Sidechain
5	Κ	71	DC	Sidechain
5	Κ	8	DA	Sidechain
6	L	29	DA	Sidechain
6	L	30	DG	Sidechain
6	L	31	DG	Sidechain
6	L	37	DA	Sidechain
6	L	38	DC	Sidechain
6	L	39	DG	Sidechain
6	L	46	DA	Sidechain
6	L	47	DT	Sidechain
6	L	49	DT	Sidechain
6	L	50	DT	Sidechain
6	L	51	DT	Sidechain
6	L	56	DT	Sidechain
6	L	59	DT	Sidechain
6	L	68	DT	Sidechain
6	L	76	DT	Sidechain
6	L	83	DT	Sidechain

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		1	1 0	
Mol	Chain	Res	Type	Group
6	L	86	DG	Sidechain
1	0	1058	ARG	Sidechain
1	0	966	ARG	Sidechain
1	0	967	ARG	Sidechain
1	Р	189	ARG	Sidechain
1	Р	528	ARG	Sidechain
1	Р	966	ARG	Sidechain
3	Q	101	TYR	Sidechain
3	Q	140	ARG	Sidechain

## 5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	11840	11707	11705	76	0
1	В	11840	11706	11705	95	0
1	0	11840	11707	11705	79	0
1	Р	11840	11706	11705	99	0
2	С	3531	3451	3450	71	0
2	D	3531	3451	3450	71	0
3	Е	1722	1719	1718	15	0
3	F	1619	1627	1626	15	0
3	Q	1722	1719	1718	16	0
3	R	1619	1627	1626	15	0
4	G	583	564	563	25	0
4	Ι	583	564	563	9	0
4	М	583	564	563	9	0
4	S	583	564	563	27	0
5	Κ	1496	815	816	13	0
6	L	1497	823	822	6	0
7	А	1	0	0	0	0
7	В	1	0	0	0	0
7	0	1	0	0	0	0
7	Р	1	0	0	0	0
8	A	31	12	12	0	0
8	В	31	12	12	0	0
8	0	31	12	12	0	0
8	Р	31	12	12	0	0



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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	66557	64362	64346	526	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 4.

All (526) 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)
2:C:158:ALA:HB1	2:D:123:LEU:HG	1.19	1.18
2:C:162:TYR:HB3	2:D:124:ARG:HG3	1.23	1.15
2:C:158:ALA:CB	2:D:123:LEU:HG	1.82	1.10
2:C:131:ILE:HD11	2:D:163:SER:OG	1.56	1.06
4:S:36:4HH:CL3	4:S:40:VAL:HG21	1.87	1.05
4:G:36:4HH:CL3	4:G:40:VAL:HG21	1.87	1.04
1:B:1127:ASN:O	1:B:1127:ASN:ND2	1.91	1.03
1:P:1127:ASN:O	1:P:1127:ASN:ND2	1.91	1.03
2:C:138:ARG:NH1	2:D:134:ASN:ND2	2.10	0.99
2:C:162:TYR:HB3	2:D:124:ARG:CG	1.93	0.98
2:C:134:ASN:HD21	2:D:138:ARG:HH12	1.12	0.93
2:C:131:ILE:CD1	2:D:163:SER:OG	2.18	0.91
1:B:1107:ARG:NE	4:I:48:GLU:OE1	2.04	0.90
1:P:1107:ARG:NE	4:M:48:GLU:OE1	2.04	0.89
1:A:292:ARG:HD3	4:G:36:4HH:SU	2.14	0.88
1:O:292:ARG:HD3	4:S:36:4HH:SU	2.13	0.88
2:C:138:ARG:NH1	2:D:134:ASN:HD21	1.70	0.87
2:C:138:ARG:HH12	2:D:134:ASN:ND2	1.70	0.86
2:C:158:ALA:CB	2:D:123:LEU:CG	2.51	0.86
2:C:162:TYR:CB	2:D:124:ARG:HG3	2.04	0.86
2:C:162:TYR:CG	2:D:124:ARG:HB2	2.12	0.85
1:P:665:GLN:NE2	1:P:671:ASP:OD2	2.11	0.84
1:B:665:GLN:NE2	1:B:671:ASP:OD2	2.11	0.82
2:C:131:ILE:HD11	2:D:163:SER:HG	1.42	0.82
2:C:123:LEU:HG	2:D:158:ALA:HB1	1.61	0.82
1:P:1127:ASN:HD22	1:P:1127:ASN:C	1.88	0.81
2:C:158:ALA:HB2	2:D:123:LEU:CD2	2.13	0.79
2:C:134:ASN:HD21	2:D:138:ARG:NH1	1.80	0.78
2:C:123:LEU:HD21	2:D:158:ALA:HB2	1.67	0.77
4:G:36:4HH:HT3	4:G:56:ASP:OD1	1.85	0.76
1:B:1127:ASN:HD22	1:B:1127:ASN:C	1.88	0.76
4:S:36:4HH:HT3	4:S:56:ASP:OD1	1.85	0.76
1:A:1412:ASP:OD1	1:A:1413:ALA:N	2.20	0.75



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:0:1412:ASP:OD1	1:O:1413:ALA:N	2.20	0.74
4:G:23:THR:OG1	4:G:25:ASN:OD1	2.04	0.73
2:C:131:ILE:HD11	2:D:163:SER:CB	2.18	0.73
1:B:172:THR:HG21	5:K:21:DC:H5"	1.71	0.72
2:C:124:ARG:HA	2:D:162:TYR:CB	2.20	0.72
4:S:36:4HH:CL3	4:S:40:VAL:CG2	2.68	0.71
1:A:288:ALA:HB1	4:G:44:MET:HE1	1.73	0.71
2:C:124:ARG:HA	2:D:162:TYR:HB3	1.73	0.71
1:O:288:ALA:HB1	4:S:44:MET:HE1	1.73	0.70
4:G:36:4HH:HB2	4:G:36:4HH:HJ2	1.74	0.70
4:S:23:THR:OG1	4:S:25:ASN:OD1	2.04	0.69
4:G:36:4HH:CL3	4:G:40:VAL:CG2	2.68	0.69
4:S:36:4HH:HJ2	4:S:36:4HH:HB2	1.74	0.69
1:P:273:ASP:OD1	1:P:274:TYR:N	2.26	0.69
1:B:273:ASP:OD1	1:B:274:TYR:N	2.26	0.68
1:O:826:LEU:HD21	1:P:827:SER:HA	1.75	0.68
1:A:1298:GLN:N	1:A:1298:GLN:OE1	2.26	0.68
1:A:826:LEU:HD21	1:B:827:SER:HA	1.75	0.67
1:A:784:GLU:OE1	1:A:784:GLU:N	2.28	0.67
1:A:1436:GLU:O	1:A:1436:GLU:OE1	2.13	0.67
4:S:36:4HH:HJ2	4:S:36:4HH:CB	2.25	0.67
5:K:63:DG:C3'	1:P:187:ARG:HD3	2.24	0.67
1:0:1436:GLU:0	1:O:1436:GLU:OE1	2.12	0.67
1:O:1298:GLN:N	1:0:1298:GLN:OE1	2.27	0.67
5:K:63:DG:H3'	1:P:187:ARG:HD3	1.77	0.66
1:O:784:GLU:N	1:O:784:GLU:OE1	2.28	0.66
4:S:46:LEU:HD21	4:S:72:ILE:HD11	1.78	0.65
2:C:158:ALA:HB2	2:D:123:LEU:HD21	1.77	0.65
1:B:1332:THR:O	1:B:1336:GLU:N	2.30	0.65
2:C:123:LEU:HG	2:D:158:ALA:CB	2.26	0.65
1:P:1332:THR:O	1:P:1336:GLU:N	2.30	0.65
4:G:46:LEU:HD21	4:G:72:ILE:HD11	1.78	0.64
1:0:1457:GLU:OE1	1:O:1457:GLU:N	2.28	0.63
3:F:167:MET:HE2	3:F:167:MET:HA	1.79	0.63
3:R:167:MET:HE2	3:R:167:MET:HA	1.79	0.63
4:G:36:4HH:HJ2	4:G:36:4HH:CB	2.25	0.63
1:P:1141:MET:HA	1:P:1141:MET:HE3	1.81	0.63
2:D:314:THR:HA	3:Q:93:MET:HE2	1.81	0.62
4:G:36:4HH:ON	4:G:40:VAL:CG2	2.47	0.62
2:C:162:TYR:HB3	2:D:124:ARG:CB	2.29	0.62
4:S:36:4HH:ON	4:S:40:VAL:CG2	2.47	0.62



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:O:231:ALA:HB2	1:P:665:GLN:CB	2.30	0.62
1:P:1322:GLN:O	1:P:1322:GLN:CD	2.43	0.62
1:A:1457:GLU:OE1	1:A:1457:GLU:N	2.28	0.61
1:P:254:SER:O	1:P:258:LEU:HD22	2.00	0.61
1:B:1322:GLN:O	1:B:1322:GLN:CD	2.43	0.61
1:A:231:ALA:HB2	1:B:665:GLN:CB	2.30	0.61
1:B:1141:MET:HE3	1:B:1141:MET:HA	1.81	0.61
2:C:124:ARG:HB2	2:D:162:TYR:CD1	2.35	0.61
1:B:254:SER:O	1:B:258:LEU:HD22	2.01	0.61
2:C:314:THR:HA	3:E:93:MET:HE2	1.81	0.61
1:O:289:LEU:HD22	4:S:36:4HH:HS3	1.83	0.60
2:C:138:ARG:NH1	2:D:134:ASN:HD22	2.00	0.60
2:C:123:LEU:CG	2:D:158:ALA:CB	2.79	0.60
1:P:788:GLU:OE1	1:P:789:ALA:N	2.35	0.60
1:A:289:LEU:HD22	4:G:36:4HH:HS3	1.83	0.59
4:M:24:ASN:O	4:M:66:GLN:N	2.35	0.59
1:B:788:GLU:OE1	1:B:789:ALA:N	2.35	0.59
2:C:123:LEU:CG	2:D:158:ALA:HB1	2.30	0.59
2:C:162:TYR:CG	2:D:124:ARG:CB	2.85	0.59
5:K:63:DG:C2'	1:P:187:ARG:HD3	2.33	0.59
2:C:158:ALA:HB3	2:C:159:PRO:HD3	1.85	0.59
3:E:10:MET:SD	3:F:18:LEU:HD11	2.43	0.58
4:I:24:ASN:O	4:I:66:GLN:N	2.35	0.58
3:Q:10:MET:SD	3:R:18:LEU:HD11	2.43	0.58
1:B:1142:GLU:OE1	1:B:1142:GLU:N	2.36	0.58
1:P:674:MET:HE3	1:P:674:MET:HA	1.86	0.58
1:P:1107:ARG:HE	4:M:48:GLU:CD	2.12	0.57
1:B:674:MET:HE3	1:B:674:MET:HA	1.85	0.57
1:P:1142:GLU:N	1:P:1142:GLU:OE1	2.36	0.57
1:B:1107:ARG:HE	4:I:48:GLU:CD	2.12	0.56
2:C:124:ARG:HA	2:D:162:TYR:CG	2.41	0.56
1:P:273:ASP:OD1	1:P:273:ASP:C	2.49	0.55
2:C:131:ILE:CD1	2:D:163:SER:CB	2.83	0.55
4:G:36:4HH:HJ3	4:G:37:LEU:N	2.22	0.55
1:O:231:ALA:HB2	1:P:665:GLN:HB2	1.89	0.55
1:A:231:ALA:HB2	1:B:665:GLN:HB2	1.89	0.55
1:B:273:ASP:OD1	1:B:273:ASP:C	2.49	0.55
2:C:123:LEU:CD2	2:D:158:ALA:HB2	2.36	0.55
2:D:328:ASP:OD1	2:D:328:ASP:O	2.25	0.55
1:P:822:VAL:HA	1:P:826:LEU:HD23	1.88	0.55
1:0:764:ASP:N	1:0:764:ASP:OD1	2.40	0.55



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
4:S:36:4HH:HJ3	4:S:37:LEU:N	2.22	0.54
3:F:148:LYS:HD3	3:F:148:LYS:N	2.23	0.54
1:O:236:GLU:OE2	1:O:1307:THR:HG21	2.08	0.54
1:A:764:ASP:N	1:A:764:ASP:OD1	2.40	0.54
1:B:822:VAL:HA	1:B:826:LEU:HD23	1.88	0.54
1:B:1423:CYS:SG	1:B:1430:LEU:HD11	2.48	0.54
1:P:1423:CYS:SG	1:P:1430:LEU:HD11	2.48	0.54
3:E:7:GLU:OE1	3:E:7:GLU:N	2.38	0.54
1:0:1281:GLU:0	1:O:1285:ILE:HD12	2.08	0.54
2:C:79:ASN:CG	3:Q:142:SER:HB3	2.34	0.53
1:A:828:VAL:HG12	1:A:828:VAL:O	2.08	0.53
1:A:1420:PHE:HA	1:A:1423:CYS:SG	2.48	0.53
1:B:1299:ASP:OD1	1:B:1300:LEU:N	2.42	0.53
2:C:328:ASP:OD1	2:C:328:ASP:O	2.25	0.53
1:A:236:GLU:OE2	1:A:1307:THR:HG21	2.08	0.53
1:B:1395:LYS:O	1:B:1395:LYS:HD3	2.09	0.53
3:R:148:LYS:HD3	3:R:148:LYS:N	2.23	0.53
1:A:289:LEU:HD22	4:G:36:4HH:CS	2.39	0.53
1:A:1281:GLU:O	1:A:1285:ILE:HD12	2.08	0.53
1:P:1299:ASP:OD1	1:P:1300:LEU:N	2.42	0.53
1:0:65:GLU:0	1:O:65:GLU:HG3	2.08	0.53
1:O:1420:PHE:HA	1:0:1423:CYS:SG	2.48	0.53
1:P:799:GLU:OE1	1:P:799:GLU:C	2.52	0.53
2:C:123:LEU:HD11	2:D:158:ALA:CB	2.39	0.53
1:O:289:LEU:HD22	4:S:36:4HH:CS	2.39	0.53
1:0:1126:ASP:0	1:0:1127:ASN:OD1	2.27	0.53
1:0:828:VAL:O	1:O:828:VAL:HG12	2.08	0.53
3:Q:124:LEU:C	3:Q:124:LEU:HD23	2.34	0.53
1:A:65:GLU:O	1:A:65:GLU:HG3	2.08	0.53
1:B:799:GLU:C	1:B:799:GLU:OE1	2.52	0.52
1:B:1441:GLU:OE1	1:B:1441:GLU:N	2.37	0.52
1:P:1258:LEU:HD21	1:P:1380:MET:HG2	1.90	0.52
3:E:124:LEU:C	3:E:124:LEU:HD23	2.34	0.52
1:P:1441:GLU:OE1	1:P:1441:GLU:N	2.37	0.52
1:A:1126:ASP:O	1:A:1127:ASN:OD1	2.27	0.52
1:B:1258:LEU:HD21	1:B:1380:MET:HG2	1.90	0.52
2:C:158:ALA:HB2	2:D:123:LEU:CG	2.31	0.52
2:D:79:ASN:CG	3:E:142:SER:HB3	2.34	0.52
1:A:122:MET:HE1	1:A:177:GLN:HB3	1.90	0.52
3:Q:7:GLU:OE1	3:Q:7:GLU:N	2.38	0.52
1:P:217:LEU:HG	1:P:221:LEU:HD12	1.91	0.52



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:828:VAL:HG12	1:B:828:VAL:O	2.10	0.52
1:B:665:GLN:C	1:B:665:GLN:OE1	2.53	0.52
1:O:122:MET:HE1	1:0:177:GLN:HB3	1.90	0.52
2:D:158:ALA:HB3	2:D:159:PRO:HD3	1.91	0.52
1:A:44:MET:HE3	1:A:1433:ALA:HB2	1.92	0.52
1:P:63:THR:HG21	1:P:1407:GLU:HG3	1.92	0.52
1:P:665:GLN:OE1	1:P:665:GLN:C	2.53	0.52
1:P:732:GLU:H	1:P:732:GLU:CD	2.18	0.52
3:E:10:MET:HE3	3:E:14:LEU:HD22	1.92	0.51
1:P:1161:VAL:HG12	1:P:1161:VAL:O	2.10	0.51
1:O:44:MET:HE3	1:O:1433:ALA:HB2	1.92	0.51
1:B:1246:LYS:HD2	1:B:1246:LYS:O	2.11	0.51
1:P:91:ASP:C	1:P:91:ASP:OD1	2.54	0.51
1:B:63:THR:HG21	1:B:1407:GLU:HG3	1.92	0.51
4:G:62:ILE:HG22	4:G:62:ILE:O	2.10	0.51
1:P:828:VAL:HG12	1:P:828:VAL:O	2.10	0.51
2:C:124:ARG:HB2	2:D:162:TYR:CG	2.46	0.51
2:C:134:ASN:ND2	2:D:138:ARG:NH1	2.57	0.51
1:P:1319:LEU:HD12	1:P:1320:ASN:N	2.26	0.51
3:Q:10:MET:HE3	3:Q:14:LEU:HD22	1.92	0.51
1:B:217:LEU:HG	1:B:221:LEU:HD12	1.91	0.51
5:K:63:DG:H4'	1:P:189:ARG:HG3	1.93	0.51
6:L:39:DG:H3'	3:Q:157:THR:HG23	1.93	0.51
1:B:1161:VAL:HG12	1:B:1161:VAL:O	2.09	0.50
1:B:1319:LEU:HD12	1:B:1320:ASN:N	2.26	0.50
2:D:370:GLN:OE1	2:D:370:GLN:O	2.29	0.50
4:S:62:ILE:HG22	4:S:62:ILE:O	2.10	0.50
1:B:1257:MET:SD	1:B:1257:MET:C	2.95	0.50
2:D:358:LEU:HG	2:D:362:ILE:HD11	1.94	0.50
1:B:732:GLU:CD	1:B:732:GLU:H	2.18	0.50
1:O:200:LEU:HD12	1:O:1378:LEU:HD22	1.94	0.50
2:C:370:GLN:OE1	2:C:370:GLN:O	2.29	0.50
1:P:1196:GLU:N	1:P:1196:GLU:OE1	2.45	0.50
1:P:1257:MET:C	1:P:1257:MET:SD	2.95	0.50
1:B:1107:ARG:CZ	4:I:48:GLU:OE1	2.59	0.50
2:C:356:ASP:C	2:C:356:ASP:OD1	2.55	0.50
1:A:1361:GLU:OE1	1:A:1361:GLU:HA	2.12	0.50
2:D:356:ASP:OD1	2:D:356:ASP:C	2.55	0.50
1:A:200:LEU:HD12	1:A:1378:LEU:HD22	1.94	0.50
1:B:91:ASP:C	1:B:91:ASP:OD1	2.54	0.50
2:C:162:TYR:CD1	2:D:124:ARG:HD2	2.47	0.50



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:O:1361:GLU:OE1	1:O:1361:GLU:HA	2.12	0.50
1:P:1107:ARG:CZ	4:M:48:GLU:OE1	2.60	0.50
2:C:134:ASN:ND2	2:D:138:ARG:HH12	1.95	0.49
1:A:1163:ASP:OD1	1:A:1164:ASN:N	2.45	0.49
2:C:358:LEU:HG	2:C:362:ILE:HD11	1.94	0.49
3:F:16:GLN:C	3:F:16:GLN:OE1	2.55	0.49
5:K:63:DG:H3'	1:P:187:ARG:CD	2.41	0.49
1:0:1163:ASP:OD1	1:O:1164:ASN:N	2.45	0.49
1:A:1376:SER:O	1:A:1379:VAL:HG22	2.12	0.49
1:B:1196:GLU:N	1:B:1196:GLU:OE1	2.45	0.49
4:G:36:4HH:CB	4:G:36:4HH:CJ	2.90	0.49
1:P:244:ILE:HD13	3:Q:41:LEU:HD21	1.94	0.49
1:A:235:MET:HA	1:A:235:MET:HE2	1.95	0.49
2:D:75:ASN:HD21	3:E:146:LEU:HB2	1.78	0.49
1:O:732:GLU:N	1:O:732:GLU:OE1	2.46	0.49
3:R:16:GLN:C	3:R:16:GLN:OE1	2.55	0.49
4:S:2:THR:OG1	4:S:3:ILE:N	2.45	0.49
5:K:63:DG:H1'	5:K:64:DG:C8	2.48	0.49
1:A:732:GLU:OE1	1:A:732:GLU:N	2.46	0.49
2:C:124:ARG:CB	2:D:162:TYR:CG	2.96	0.49
4:I:36:4HH:O	4:I:40:VAL:HG23	2.12	0.49
4:M:36:4HH:O	4:M:40:VAL:HG23	2.11	0.49
1:0:1376:SER:O	1:O:1379:VAL:HG22	2.12	0.49
4:S:36:4HH:ON	4:S:40:VAL:HG21	2.06	0.48
1:A:1211:ALA:O	1:A:1215:MET:HG2	2.13	0.48
4:G:36:4HH:ON	4:G:40:VAL:HG23	2.14	0.48
1:O:235:MET:HE2	1:O:235:MET:HA	1.95	0.48
3:R:56:GLU:OE1	3:R:56:GLU:HA	2.13	0.48
1:B:1376:SER:O	1:B:1379:VAL:HG22	2.13	0.48
2:C:123:LEU:CG	2:D:158:ALA:HB2	2.44	0.48
1:0:1237:SER:OG	1:0:1238:LYS:N	2.45	0.48
1:P:782:ALA:O	1:P:785:ASN:N	2.47	0.48
1:B:244:ILE:HD13	3:E:41:LEU:HD21	1.94	0.48
2:C:391:LEU:HD13	2:C:428:TYR:CE2	2.49	0.48
4:G:2:THR:OG1	4:G:3:ILE:N	2.45	0.48
2:C:75:ASN:HD21	3:Q:146:LEU:HB2	1.78	0.48
2:C:106:LEU:HB2	2:D:113:TYR:CD1	2.49	0.48
1:0:1211:ALA:O	1:O:1215:MET:HG2	2.13	0.48
1:P:1376:SER:O	1:P:1379:VAL:HG22	2.13	0.48
3:F:56:GLU:OE1	3:F:56:GLU:HA	2.13	0.48
4:S:11:ILE:HG23	4:S:12:GLY:N	2.29	0.48



Interatomic Clash				
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:A:1237:SER:OG	1:A:1238:LYS:N	2.45	0.47	
1:B:1161:VAL:O	1:B:1161:VAL:CG1	2.62	0.47	
2:D:292:ASP:CG	2:D:295:ARG:HA	2.39	0.47	
2:C:292:ASP:CG	2:C:295:ARG:HA	2.39	0.47	
4:S:36:4HH:ON	4:S:40:VAL:HG23	2.13	0.47	
1:P:1161:VAL:O	1:P:1161:VAL:CG1	2.62	0.47	
1:B:1275:LEU:HD12	1:B:1347:ASP:O	2.14	0.47	
4:G:11:ILE:HG23	4:G:12:GLY:N	2.29	0.47	
1:B:94:ASN:OD1	1:B:95:SER:N	2.47	0.47	
1:B:1322:GLN:O	1:B:1322:GLN:OE1	2.32	0.47	
2:D:375:PRO:HA	2:D:440:TYR:OH	2.15	0.47	
2:D:391:LEU:HD13	2:D:428:TYR:CE2	2.49	0.47	
1:A:62:ASN:OD1	1:A:63:THR:N	2.48	0.47	
1:B:184:ILE:HG23	1:B:185:PRO:HD2	1.97	0.47	
1:B:285:LEU:HD13	4:I:41:GLU:OE2	2.15	0.47	
1:B:774:GLU:N	1:B:774:GLU:OE1	2.48	0.47	
1:P:774:GLU:N	1:P:774:GLU:OE1	2.48	0.47	
1:P:1322:GLN:O	1:P:1322:GLN:OE1	2.31	0.47	
1:B:782:ALA:O	1:B:785:ASN:N	2.47	0.47	
2:C:162:TYR:CB	2:D:124:ARG:CB	2.93	0.47	
2:C:375:PRO:HA	2:C:440:TYR:OH	2.15	0.47	
1:P:184:ILE:HG23	1:P:185:PRO:HD2	1.97	0.47	
3:R:180:ILE:HG23	3:R:184:VAL:HG21	1.96	0.47	
2:D:391:LEU:HD13	2:D:428:TYR:CD2	2.50	0.47	
3:F:25:GLU:CD	3:F:25:GLU:H	2.23	0.47	
1:0:588:GLU:0	1:O:592:GLN:HG3	2.15	0.47	
1:A:588:GLU:O	1:A:592:GLN:HG3	2.15	0.46	
1:B:824:LYS:HG2	1:B:824:LYS:O	2.15	0.46	
1:P:1117:TRP:O	1:P:1121:MET:HG2	2.14	0.46	
1:P:1320:ASN:ND2	3:Q:49:ASP:OD2	2.49	0.46	
1:0:62:ASN:OD1	1:O:63:THR:N	2.48	0.46	
1:P:1275:LEU:HD12	1:P:1347:ASP:O	2.15	0.46	
3:R:25:GLU:CD	3:R:25:GLU:H	2.23	0.46	
4:S:28:PHE:CE1	4:S:65:VAL:HG22	2.51	0.46	
3:E:5:HIS:CD2	3:E:7:GLU:OE1	2.69	0.46	
1:A:12:LEU:HD21	1:A:46:ALA:HB2	1.97	0.46	
3:F:39:ASP:OD1	3:F:39:ASP:N	2.49	0.46	
3:F:180:ILE:HG23	3:F:184:VAL:HG21	1.96	0.46	
4:G:28:PHE:CE1	4:G:65:VAL:HG22	2.51	0.46	
1:P:824:LYS:O	1:P:824:LYS:HG2	2.15	0.46	
3:Q:140:ARG:HD2	3:Q:140:ARG:O	2.15	0.46	



	jue page	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:C:138:ARG:HH11	2:D:134:ASN:HD21	1.56	0.46
1:P:285:LEU:HD13	4:M:41:GLU:OE2	2.15	0.46
1:B:1117:TRP:O	1:B:1121:MET:HG2	2.14	0.46
1:P:1391:ARG:HA	1:P:1391:ARG:NE	2.30	0.46
4:S:57:GLU:OE1	4:S:57:GLU:N	2.45	0.46
1:O:1285:ILE:HD12	1:O:1285:ILE:H	1.81	0.46
1:B:542:PHE:CD2	1:B:876:LEU:HD21	2.51	0.46
1:B:782:ALA:O	1:B:785:ASN:CB	2.64	0.46
2:C:426:ASN:OD1	2:C:430:ALA:HB3	2.16	0.46
2:D:426:ASN:OD1	2:D:430:ALA:HB3	2.16	0.46
4:G:57:GLU:OE1	4:G:57:GLU:N	2.46	0.46
1:O:349:LYS:HE3	1:O:353:TYR:CZ	2.51	0.46
1:A:8:ARG:HH21	1:A:8:ARG:HG3	1.80	0.46
1:B:664:SER:OG	1:B:665:GLN:HG3	2.15	0.46
2:C:391:LEU:HD13	2:C:428:TYR:CD2	2.50	0.46
3:Q:5:HIS:CD2	3:Q:7:GLU:OE1	2.69	0.46
1:B:1320:ASN:ND2	3:E:49:ASP:OD2	2.49	0.45
1:P:664:SER:OG	1:P:665:GLN:HG3	2.15	0.45
1:P:679:GLU:OE1	1:P:679:GLU:HA	2.16	0.45
1:A:1285:ILE:HD12	1:A:1285:ILE:H	1.81	0.45
2:C:355:ASN:OD1	2:C:355:ASN:N	2.49	0.45
4:G:36:4HH:OM	4:G:37:LEU:HA	2.17	0.45
1:B:679:GLU:OE1	1:B:679:GLU:HA	2.16	0.45
3:R:39:ASP:OD1	3:R:39:ASP:N	2.49	0.45
2:C:106:LEU:HD13	2:D:113:TYR:CG	2.51	0.45
1:O:1275:LEU:HD23	1:O:1380:MET:HE2	1.98	0.45
3:R:121:TYR:CZ	3:R:125:ILE:HD11	2.52	0.45
3:R:190:ASP:C	3:R:190:ASP:OD1	2.59	0.45
1:B:1375:MET:HG2	1:B:1419:LEU:HD11	1.98	0.45
1:O:247:GLU:OE1	1:O:247:GLU:HA	2.17	0.45
1:O:765:ARG:HH11	1:P:748:VAL:HG23	1.81	0.45
1:P:782:ALA:O	1:P:785:ASN:CB	2.65	0.45
1:A:349:LYS:HE3	1:A:353:TYR:CZ	2.51	0.45
1:B:611:LEU:C	1:B:611:LEU:HD23	2.42	0.45
5:K:38:DA:C2	6:L:54:DA:C2	3.05	0.45
1:A:247:GLU:HA	1:A:247:GLU:OE1	2.17	0.45
1:O:1213:GLU:OE1	1:P:813:ARG:NE	2.49	0.45
1:P:542:PHE:CD2	1:P:876:LEU:HD21	2.51	0.45
1:O:8:ARG:HH21	1:O:8:ARG:HG3	1.80	0.45
1:A:640:ARG:O	1:A:643:THR:HG22	2.17	0.45
1:A:1213:GLU:OE1	1:B:813:ARG:NE	2.49	0.45



	sus puge	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:784:GLU:HA	1:B:787:LEU:HG	1.99	0.45
3:F:134:MET:N	3:F:134:MET:HE2	2.32	0.45
1:O:12:LEU:HD21	1:O:46:ALA:HB2	1.97	0.45
1:A:275:MET:HE1	1:A:1134:HIS:ND1	2.31	0.44
1:A:1127:ASN:OD1	1:A:1127:ASN:C	2.60	0.44
2:D:355:ASN:N	2:D:355:ASN:OD1	2.48	0.44
1:O:640:ARG:O	1:O:643:THR:HG22	2.17	0.44
1:0:1127:ASN:OD1	1:0:1127:ASN:C	2.60	0.44
1:A:765:ARG:HH11	1:B:748:VAL:HG23	1.81	0.44
1:A:1275:LEU:HD23	1:A:1380:MET:HE2	1.98	0.44
1:B:232:PHE:CZ	1:B:1240:VAL:HG11	2.53	0.44
3:F:190:ASP:C	3:F:190:ASP:OD1	2.60	0.44
4:I:58:GLU:OE1	4:I:71:TYR:OH	2.31	0.44
1:O:275:MET:HE1	1:0:1134:HIS:CE1	2.52	0.44
1:P:1375:MET:HG2	1:P:1419:LEU:HD11	1.98	0.44
1:B:750:ASN:HB3	1:B:761:LYS:HB3	2.00	0.44
1:B:839:ARG:HG2	1:B:839:ARG:HH21	1.82	0.44
1:P:691:ASP:OD1	1:P:780:ARG:HB3	2.17	0.44
1:B:1104:TYR:CE1	1:B:1107:ARG:NH1	2.86	0.44
5:K:40:DA:C2	6:L:52:DA:C2	3.05	0.44
1:O:51:LEU:O	1:O:52:ILE:HD13	2.18	0.44
1:P:632:MET:HE1	1:P:818:PHE:HB3	1.99	0.44
1:P:784:GLU:HA	1:P:787:LEU:HG	1.98	0.44
3:R:134:MET:N	3:R:134:MET:HE2	2.32	0.44
4:S:36:4HH:OM	4:S:37:LEU:HA	2.17	0.44
1:O:152:GLU:OE1	1:O:152:GLU:N	2.51	0.44
1:O:275:MET:HE1	1:0:1134:HIS:ND1	2.31	0.44
1:P:611:LEU:HD23	1:P:611:LEU:C	2.42	0.44
1:A:275:MET:HE1	1:A:1134:HIS:CE1	2.52	0.44
1:A:1121:MET:HA	1:A:1124:VAL:HG12	1.99	0.44
1:P:750:ASN:HB3	1:P:761:LYS:HB3	2.00	0.44
1:A:1387:GLU:C	1:A:1387:GLU:OE1	2.61	0.44
2:D:399:ARG:O	2:D:403:ASP:OD2	2.36	0.44
4:I:64:THR:HG22	4:I:65:VAL:N	2.33	0.44
1:P:1213:GLU:H	1:P:1213:GLU:CD	2.26	0.44
3:Q:180:ILE:HG22	3:Q:181:THR:N	2.33	0.44
1:0:1274:ARG:HG3	1:O:1357:TRP:CZ3	2.53	0.43
1:O:1380:MET:HE3	1:O:1380:MET:HB3	1.96	0.43
1:A:51:LEU:O	1:A:52:ILE:HD13	2.18	0.43
1:B:782:ALA:O	1:B:785:ASN:HB3	2.18	0.43
1:O:1401:ARG:HB3	1:O:1428:MET:HE2	1.99	0.43



	h i c	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
4:S:36:4HH:CB	4:S:36:4HH:CJ	2.90	0.43
1:B:215:ARG:HG2	1:B:1325:MET:HE2	2.01	0.43
1:B:89:THR:C	1:B:90:LEU:HD12	2.43	0.43
1:B:632:MET:HE1	1:B:818:PHE:HB3	2.00	0.43
1:B:691:ASP:OD1	1:B:780:ARG:HB3	2.17	0.43
2:D:358:LEU:HA	2:D:361:MET:SD	2.59	0.43
1:P:105:ARG:HD2	1:P:105:ARG:C	2.44	0.43
1:P:1104:TYR:CE1	1:P:1107:ARG:NH1	2.86	0.43
1:P:1338:LEU:N	1:P:1338:LEU:HD23	2.32	0.43
4:M:64:THR:HG22	4:M:65:VAL:N	2.33	0.43
1:A:1401:ARG:HB3	1:A:1428:MET:HE2	1.99	0.43
3:E:180:ILE:HG22	3:E:181:THR:N	2.33	0.43
5:K:63:DG:C5'	1:P:189:ARG:HG3	2.49	0.43
1:O:1121:MET:HA	1:O:1124:VAL:HG12	1.99	0.43
1:P:839:ARG:HG2	1:P:839:ARG:HH21	1.82	0.43
1:A:1285:ILE:HD11	3:F:108:ARG:NH1	2.34	0.43
1:0:1129:VAL:O	1:O:1130:GLU:C	2.61	0.43
1:O:1285:ILE:HD11	3:R:108:ARG:NH1	2.34	0.43
2:C:124:ARG:CA	2:D:162:TYR:CG	3.01	0.43
2:C:358:LEU:HA	2:C:361:MET:SD	2.59	0.43
1:O:782:ALA:C	1:O:783:ARG:HD3	2.43	0.43
1:O:1107:ARG:NH2	4:S:47:GLU:OE2	2.50	0.43
3:Q:127:LEU:HD23	3:Q:127:LEU:C	2.44	0.43
2:C:399:ARG:O	2:C:403:ASP:OD2	2.36	0.43
1:O:105:ARG:HD2	1:O:105:ARG:C	2.44	0.43
1:O:1235:ILE:HG21	1:P:675:ILE:HD13	2.01	0.43
1:P:89:THR:C	1:P:90:LEU:HD12	2.43	0.43
1:P:1436:GLU:O	1:P:1438:ILE:HG23	2.19	0.43
1:P:232:PHE:CZ	1:P:1240:VAL:HG11	2.53	0.43
1:P:775:LEU:HD22	1:P:775:LEU:N	2.34	0.43
2:C:18:ASN:HB3	2:C:20:PHE:CZ	2.53	0.43
2:C:154:ARG:HA	2:D:123:LEU:HD21	2.00	0.43
1:0:782:ALA:O	1:O:783:ARG:HD3	2.19	0.43
1:P:215:ARG:HG2	1:P:1325:MET:HE2	2.00	0.43
1:B:1213:GLU:H	1:B:1213:GLU:CD	2.26	0.42
1:P:782:ALA:O	1:P:785:ASN:HB3	2.18	0.42
3:R:25:GLU:O	3:R:29:GLN:HG3	2.19	0.42
1:A:782:ALA:C	1:A:783:ARG:HD3	2.43	0.42
1:A:1274:ARG:HG3	1:A:1357:TRP:CZ3	2.53	0.42
1:B:1436:GLU:O	1:B:1438:ILE:HG23	2.19	0.42
2:D:175:GLN:HB3	2:D:266:TRP:CE2	2.55	0.42



	sue page	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:P:594:ILE:HD12	1:P:845:HIS:CE1	2.54	0.42
1:P:1247:THR:O	1:P:1251:GLU:OE1	2.37	0.42
4:I:40:VAL:O	4:I:43:VAL:HG12	2.20	0.42
1:0:1118:CYS:SG	1:O:1122:ARG:NH1	2.92	0.42
1:O:1387:GLU:CD	1:O:1387:GLU:C	2.87	0.42
1:P:605:LEU:O	1:P:609:ASP:OD2	2.37	0.42
1:P:745:ASP:OD1	1:P:745:ASP:N	2.51	0.42
1:B:594:ILE:HD12	1:B:845:HIS:CE1	2.55	0.42
1:B:606:ALA:HA	1:B:609:ASP:OD2	2.20	0.42
2:C:158:ALA:CB	2:D:123:LEU:CD2	2.85	0.42
1:O:1202:ILE:HG22	1:O:1202:ILE:O	2.20	0.42
1:P:606:ALA:HA	1:P:609:ASP:OD2	2.20	0.42
1:A:292:ARG:HD3	4:G:36:4HH:CT	2.49	0.42
1:A:1373:THR:O	1:A:1377:ILE:HG12	2.19	0.42
1:A:1387:GLU:C	1:A:1387:GLU:CD	2.87	0.42
1:0:1387:GLU:C	1:O:1387:GLU:OE1	2.61	0.42
1:P:1325:MET:SD	1:P:1325:MET:N	2.90	0.42
1:A:767:TRP:CE3	1:B:717:LEU:HD13	2.55	0.42
1:A:782:ALA:O	1:A:783:ARG:HD3	2.19	0.42
1:A:1129:VAL:O	1:A:1130:GLU:C	2.61	0.42
1:B:605:LEU:O	1:B:609:ASP:OD2	2.37	0.42
1:B:1247:THR:O	1:B:1251:GLU:OE1	2.37	0.42
2:C:131:ILE:HD13	2:D:163:SER:OG	2.15	0.42
2:D:18:ASN:HB3	2:D:20:PHE:CZ	2.55	0.42
3:E:127:LEU:C	3:E:127:LEU:HD23	2.44	0.42
1:O:12:LEU:HD22	1:0:15:TRP:CG	2.55	0.42
1:0:1373:THR:O	1:O:1377:ILE:HG12	2.19	0.42
1:P:695:ILE:N	1:P:695:ILE:HD12	2.35	0.42
4:M:40:VAL:O	4:M:43:VAL:HG12	2.20	0.42
1:A:105:ARG:HD2	1:A:105:ARG:C	2.44	0.42
1:A:152:GLU:OE1	1:A:152:GLU:N	2.51	0.42
1:A:1235:ILE:HG21	1:B:675:ILE:HD13	2.01	0.42
1:B:1395:LYS:HD3	1:B:1395:LYS:C	2.45	0.42
1:O:292:ARG:HD3	4:S:36:4HH:CT	2.49	0.42
1:O:1331:GLN:NE2	1:O:1335:GLU:OE2	2.48	0.42
4:S:64:THR:HG23	4:S:67:ALA:H	1.85	0.42
1:A:45:ALA:HB1	1:A:60:PHE:CE2	2.55	0.42
1:A:780:ARG:O	1:A:783:ARG:N	2.46	0.42
1:B:775:LEU:N	1:B:775:LEU:HD22	2.34	0.42
5:K:63:DG:C3'	1:P:187:ARG:CD	2.94	0.42
1:0:782:ALA:O	1:O:783:ARG:C	2.63	0.42



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:P:94:ASN:OD1	1:P:95:SER:N	2.53	0.42
1:A:12:LEU:HD22	1:A:15:TRP:CG	2.55	0.41
1:A:1068:LEU:C	1:A:1068:LEU:HD23	2.45	0.41
1:B:695:ILE:HD12	1:B:695:ILE:N	2.35	0.41
2:C:131:ILE:HD11	2:D:163:SER:HB2	1.99	0.41
3:R:167:MET:HE1	3:R:183:ALA:HB1	2.01	0.41
3:F:167:MET:HE1	3:F:183:ALA:HB1	2.01	0.41
1:A:1199:ARG:O	1:A:1199:ARG:HG2	2.19	0.41
1:B:288:ALA:HB2	1:B:1106:ILE:HG22	2.03	0.41
1:B:1142:GLU:CD	1:B:1142:GLU:H	2.28	0.41
1:B:1246:LYS:HD2	1:B:1246:LYS:C	2.45	0.41
6:L:55:DG:H2"	6:L:56:DT:C6	2.56	0.41
1:A:12:LEU:HD21	1:A:46:ALA:CB	2.50	0.41
1:B:264:THR:HG23	1:B:265:GLU:N	2.36	0.41
1:B:1331:GLN:OE1	1:B:1331:GLN:N	2.54	0.41
1:O:1068:LEU:C	1:O:1068:LEU:HD23	2.45	0.41
1:O:1407:GLU:OE1	1:O:1407:GLU:HA	2.21	0.41
1:B:141:GLY:O	1:B:143:ARG:NH1	2.54	0.41
2:C:357:GLN:O	2:C:361:MET:SD	2.78	0.41
5:K:13:DA:C2	6:L:79:DG:C2	3.08	0.41
1:O:767:TRP:CE3	1:P:717:LEU:HD13	2.55	0.41
1:A:587:LEU:HD11	1:A:591:LYS:HE2	2.03	0.41
1:B:745:ASP:OD1	1:B:745:ASP:N	2.51	0.41
1:B:1126:ASP:O	1:B:1127:ASN:HB3	2.21	0.41
3:F:25:GLU:O	3:F:29:GLN:HG3	2.19	0.41
1:O:1199:ARG:O	1:O:1199:ARG:HG2	2.19	0.41
1:P:244:ILE:CD1	3:Q:41:LEU:HD21	2.51	0.41
1:P:141:GLY:O	1:P:143:ARG:NH1	2.54	0.41
1:A:246:LEU:O	1:A:249:ILE:CG2	2.69	0.41
1:B:232:PHE:CZ	1:B:1338:LEU:HA	2.56	0.41
1:B:1403:LEU:HD13	1:B:1428:MET:HE3	2.03	0.41
1:B:1411:LEU:HB2	1:B:1416:ILE:HD11	2.03	0.41
6:L:44:DG:H5"	3:R:140:ARG:CZ	2.51	0.41
1:O:12:LEU:HD21	1:O:46:ALA:CB	2.50	0.41
1:O:46:ALA:O	1:O:49:THR:HG22	2.21	0.41
1:P:264:THR:HG23	1:P:265:GLU:N	2.36	0.41
4:S:7:VAL:O	4:S:11:ILE:HG22	2.21	0.41
1:A:1118:CYS:SG	1:A:1122:ARG:NH1	2.92	0.41
1:B:1232:LYS:O	1:B:1235:ILE:HG22	2.21	0.41
4:G:64:THR:HG23	4:G:67:ALA:H	1.85	0.41
5:K:63:DG:C4'	1:P:189:ARG:HG3	2.51	0.41



	sue page	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:O:45:ALA:HB1	1:O:60:PHE:CE2	2.55	0.41
1:O:281:ARG:HD2	1:O:281:ARG:C	2.46	0.41
1:0:1117:TRP:CE3	1:O:1121:MET:HE1	2.56	0.41
1:P:288:ALA:HB2	1:P:1106:ILE:HG22	2.02	0.41
1:P:1142:GLU:H	1:P:1142:GLU:CD	2.28	0.41
1:P:1227:THR:O	1:P:1230:GLU:HG3	2.21	0.41
1:P:1403:LEU:HD13	1:P:1428:MET:HE3	2.03	0.41
3:Q:108:ARG:NH1	3:Q:111:ASN:HD21	2.19	0.41
1:A:1407:GLU:HA	1:A:1407:GLU:OE1	2.21	0.41
1:B:1335:GLU:HA	1:B:1338:LEU:HG	2.03	0.41
1:B:1338:LEU:HD23	1:B:1338:LEU:N	2.36	0.41
3:E:108:ARG:NH1	3:E:111:ASN:HD21	2.19	0.41
1:P:604:TRP:CH2	1:P:608:GLN:HG3	2.56	0.41
4:S:36:4HH:O	4:S:40:VAL:HG23	2.21	0.41
1:A:281:ARG:C	1:A:281:ARG:HD2	2.46	0.40
2:D:357:GLN:O	2:D:361:MET:SD	2.78	0.40
3:E:140:ARG:HD2	3:E:140:ARG:O	2.22	0.40
4:G:36:4HH:O	4:G:40:VAL:HG23	2.21	0.40
4:M:29:VAL:HG13	4:M:30:GLU:N	2.36	0.40
1:A:788:GLU:O	1:A:792:LEU:HD13	2.21	0.40
1:A:1202:ILE:O	1:A:1202:ILE:HG22	2.20	0.40
2:D:201:ILE:HD13	2:D:289:ILE:HD11	2.02	0.40
1:P:1411:LEU:HB2	1:P:1416:ILE:HD11	2.03	0.40
1:A:1107:ARG:NH2	4:G:47:GLU:OE2	2.50	0.40
2:C:162:TYR:CD2	2:D:124:ARG:HB2	2.54	0.40
2:C:440:TYR:CD1	2:C:440:TYR:N	2.90	0.40
1:O:246:LEU:O	1:O:249:ILE:CG2	2.69	0.40
1:O:1387:GLU:OE1	1:O:1388:GLU:N	2.54	0.40
1:P:275:MET:HA	1:P:275:MET:HE3	2.04	0.40
1:A:1117:TRP:CE3	1:A:1121:MET:HE1	2.56	0.40
1:B:1325:MET:SD	1:B:1325:MET:N	2.90	0.40
2:C:124:ARG:CB	2:D:162:TYR:CD1	3.04	0.40
2:C:201:ILE:HD13	2:C:289:ILE:HD11	2.02	0.40
3:E:9:PHE:CE1	3:F:16:GLN:HG2	2.57	0.40
3:F:42:ASP:OD1	3:F:43:ASN:N	2.54	0.40
1:0:87:TYR:CG	1:O:136:LEU:HD23	2.56	0.40
1:O:587:LEU:HD11	1:O:591:LYS:HE2	2.03	0.40
1:0:788:GLU:O	1:O:792:LEU:HD13	2.21	0.40
1:A:594:ILE:HD12	1:A:845:HIS:CE1	2.56	0.40
1:A:782:ALA:O	1:A:783:ARG:C	2.63	0.40
1:B:275:MET:HE3	1:B:275:MET:HA	2.04	0.40



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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:1307:THR:OG1	1:P:1310:GLU:HG3	2.22	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	1465/1482~(99%)	1423 (97%)	42 (3%)	0	100	100
1	В	1465/1482~(99%)	1413 (96%)	52~(4%)	0	100	100
1	Ο	1465/1482~(99%)	1423 (97%)	42 (3%)	0	100	100
1	Р	1465/1482~(99%)	1413 (96%)	52~(4%)	0	100	100
2	С	438/440 (100%)	426 (97%)	12 (3%)	0	100	100
2	D	438/440 (100%)	426 (97%)	12 (3%)	0	100	100
3	Е	210/240~(88%)	206 (98%)	4 (2%)	0	100	100
3	F	196/240~(82%)	191 (97%)	5 (3%)	0	100	100
3	Q	210/240~(88%)	206 (98%)	4 (2%)	0	100	100
3	R	196/240~(82%)	191 (97%)	5 (3%)	0	100	100
4	G	69/78~(88%)	68 (99%)	1 (1%)	0	100	100
4	Ι	69/78~(88%)	67 (97%)	2(3%)	0	100	100
4	М	69/78~(88%)	66 (96%)	3 (4%)	0	100	100
4	S	69/78~(88%)	68 (99%)	1 (1%)	0	100	100
All	All	7824/8080~(97%)	7587 (97%)	237 (3%)	0	100	100

There are no Ramachandran outliers to report.



#### 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	1269/1281~(99%)	1268 (100%)	1 (0%)	92	95
1	В	1269/1281~(99%)	1267 (100%)	2 (0%)	92	94
1	Ο	1269/1281~(99%)	1268 (100%)	1 (0%)	92	95
1	Р	1269/1281~(99%)	1266 (100%)	3~(0%)	92	94
2	С	376/376~(100%)	369~(98%)	7 (2%)	52	69
2	D	376/376~(100%)	369~(98%)	7 (2%)	52	69
3	Ε	189/212~(89%)	184 (97%)	5(3%)	41	59
3	F	177/212~(84%)	175 (99%)	2 (1%)	70	80
3	Q	189/212~(89%)	185 (98%)	4 (2%)	48	66
3	R	177/212~(84%)	175 (99%)	2 (1%)	70	80
4	G	62/66~(94%)	62 (100%)	0	100	100
4	Ι	62/66~(94%)	62 (100%)	0	100	100
4	М	62/66~(94%)	62 (100%)	0	100	100
4	S	62/66~(94%)	62 (100%)	0	100	100
All	All	6808/6988~(97%)	6774 (100%)	34 (0%)	85	89

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	221	LEU
1	В	1127	ASN
1	В	1213	GLU
2	С	2	SER
2	С	92	SER
2	С	94	LEU
2	С	132	VAL
2	С	209	SER
2	С	287	THR
2	С	355	ASN
2	D	2	SER



	3	1	1 5
Mol	Chain	$\mathbf{Res}$	Type
2	D	92	SER
2	D	94	LEU
2	D	132	VAL
2	D	209	SER
2	D	287	THR
2	D	355	ASN
3	Е	123	GLU
3	Е	138	ASN
3	Е	162	LEU
3	Е	169	TYR
3	Е	181	THR
3	F	25	GLU
3	F	152	GLN
1	0	221	LEU
1	Р	189	ARG
1	Р	1127	ASN
1	Р	1213	GLU
3	Q	123	GLU
3	Q	162	LEU
3	Q	169	TYR
3	Q	181	THR
3	R	25	GLU
3	R	152	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (98) such sidechains are listed below:

Mol	Chain	$\mathbf{Res}$	Type
1	А	242	ASN
1	А	306	GLN
1	А	331	GLN
1	А	367	GLN
1	А	404	GLN
1	А	409	GLN
1	А	472	HIS
1	А	510	HIS
1	А	516	GLN
1	А	652	GLN
1	А	865	GLN
1	А	882	GLN
1	А	930	GLN
1	А	951	HIS
1	А	1077	GLN



Mol	Chain	Res	Type
1	А	1105	GLN
1	А	1109	GLN
1	А	1242	ASN
1	А	1293	GLN
1	В	62	ASN
1	В	78	HIS
1	В	98	GLN
1	В	175	HIS
1	В	306	GLN
1	В	330	HIS
1	В	398	GLN
1	В	418	GLN
1	В	473	ASN
1	В	531	ASN
1	В	559	GLN
1	В	566	GLN
1	В	766	GLN
1	В	864	GLN
1	В	986	ASN
1	В	1006	GLN
1	В	1013	GLN
1	В	1032	GLN
1	В	1091	ASN
1	В	1166	HIS
1	В	1193	HIS
1	В	1342	ASN
1	В	1437	ASN
2	С	75	ASN
2	С	134	ASN
2	С	198	GLN
2	С	435	HIS
2	D	18	ASN
2	D	75	ASN
2	D	134	ASN
2	D	198	GLN
2	D	435	HIS
3	E	8	GLN
3	Е	111	ASN
1	0	242	ASN
1	0	306	GLN
1	Ō	331	GLN
1	0	367	GLN



Mol	Chain	Res	Type
1	0	378	GLN
1	0	404	GLN
1	0	409	GLN
1	0	472	HIS
1	0	480	GLN
1	0	510	HIS
1	0	516	GLN
1	0	865	GLN
1	0	882	GLN
1	0	930	GLN
1	0	951	HIS
1	0	1077	GLN
1	Ο	1105	GLN
1	0	1109	GLN
1	0	1242	ASN
1	0	1293	GLN
1	Р	62	ASN
1	Р	78	HIS
1	Р	97	HIS
1	Р	98	GLN
1	Р	306	GLN
1	Р	330	HIS
1	Р	398	GLN
1	Р	418	GLN
1	Р	473	ASN
1	Р	531	ASN
1	Р	546	GLN
1	Р	559	GLN
1	Р	566	GLN
1	Р	766	GLN
1	Р	864	GLN
1	Р	986	ASN
1	Р	1006	GLN
1	P	1013	GLN
1	Р	1091	ASN
1	Р	1342	ASN
1	Р	1437	ASN
3	Q	8	GLN
3	Q	111	ASN
3	Q	201	GLN
3	R	139	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)

4 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mal	Tune	Chain	Dec	Tiple	Bo	ond leng	$_{\rm ths}$	В	ond ang	les
IVIOI	Type	Unain	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z  > 2
4	4HH	Ι	36	4	$21,\!26,\!27$	0.46	0	$27,\!35,\!37$	1.72	3 (11%)
4	4HH	S	36	4	21,26,27	0.45	0	27,35,37	<mark>3.13</mark>	4 (14%)
4	4HH	М	36	4	21,26,27	0.47	0	27,35,37	1.73	3 (11%)
4	4HH	G	36	4	21,26,27	0.45	0	27,35,37	<mark>3.13</mark>	4 (14%)

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
4	4HH	Ι	36	4	-	6/32/35/37	-
4	4HH	S	36	4	-	5/32/35/37	-
4	4HH	М	36	4	-	6/32/35/37	-
4	4HH	G	36	4	-	5/32/35/37	-

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
4	G	36	$4\mathrm{HH}$	O1P-P-OG	11.65	161.86	107.75
4	S	36	4HH	O1P-P-OG	11.64	161.82	107.75
4	S	36	4HH	OG-P-O2P	-8.87	74.39	109.07
4	G	36	4HH	OG-P-O2P	-8.86	74.46	109.07



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
4	G	36	4HH	P-OG-CB	6.13	157.62	121.68
4	S	36	4HH	P-OG-CB	6.11	157.50	121.68
4	Ι	36	4HH	P-OG-CB	-5.41	89.97	121.68
4	М	36	4HH	P-OG-CB	-5.39	90.07	121.68
4	М	36	4HH	O1P-P-OG	4.65	129.33	107.75
4	Ι	36	4HH	O1P-P-OG	4.64	129.28	107.75
4	М	36	4HH	OG-CB-CA	4.42	112.45	108.14
4	Ι	36	4HH	OG-CB-CA	4.35	112.38	108.14
4	G	36	4HH	OG-CB-CA	2.86	110.93	108.14
4	S	$\overline{36}$	4HH	OG-CB-CA	2.80	110.87	108.14

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	Ι	36	4HH	N-CA-CB-OG
4	Ι	36	4HH	CB-OG-P-O1P
4	М	36	4HH	N-CA-CB-OG
4	М	36	4HH	CB-OG-P-O1P
4	G	36	4HH	CJ-O3P-P-OG
4	S	36	4HH	CJ-O3P-P-OG
4	S	36	4HH	CB-OG-P-O3P
4	G	36	4HH	CB-OG-P-O3P
4	Ι	36	4HH	CO-CP-CQ-NR
4	М	36	4HH	CO-CP-CQ-NR
4	Ι	36	4HH	CO-CP-CQ-OR
4	М	36	4HH	CO-CP-CQ-OR
4	Ι	36	4HH	CB-OG-P-O3P
4	М	36	4HH	CB-OG-P-O3P
4	G	36	4HH	ON-CL3-CM-OM
4	Ι	36	4HH	ON-CL3-CM-OM
4	S	36	4HH	ON-CL3-CM-OM
4	М	36	4HH	ON-CL3-CM-OM
4	G	36	4HH	CT-CS-NR-CQ
4	S	36	4HH	CT-CS-NR-CQ
4	G	36	4HH	CB-OG-P-O2P
4	S	36	4HH	CB-OG-P-O2P

There are no ring outliers.

4 monomers are involved in 33 short contacts:



Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	Ι	36	4HH	1	0
4	S	36	4HH	16	0
4	М	36	4HH	1	0
4	G	36	4HH	15	0

### 5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

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

Mal	Turne	Chain	Dag	Link	Bond lengths			Bond angles		
IVIOI	туре	Unam	nes		Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	ATP	А	1502	7	26,33,33	0.61	0	31,52,52	1.13	3 (9%)
8	ATP	0	1502	7	26,33,33	0.61	0	31,52,52	1.13	3 (9%)
8	ATP	Р	1502	7	26,33,33	0.63	0	31,52,52	1.12	3 (9%)
8	ATP	В	1502	7	26,33,33	0.63	0	31,52,52	1.12	3 (9%)

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
8	ATP	А	1502	7	-	1/18/38/38	0/3/3/3
8	ATP	0	1502	7	-	1/18/38/38	0/3/3/3
8	ATP	Р	1502	7	-	2/18/38/38	0/3/3/3
8	ATP	В	1502	7	-	2/18/38/38	0/3/3/3

There are no bond length outliers.

All (12) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
8	Р	1502	ATP	C5-C6-N6	2.39	123.99	120.35
8	В	1502	ATP	C5-C6-N6	2.37	123.96	120.35
8	А	1502	ATP	C5-C6-N6	2.35	123.92	120.35
8	А	1502	ATP	O2'-C2'-C3'	-2.32	104.30	111.82
8	0	1502	ATP	O2'-C2'-C3'	-2.31	104.36	111.82
8	0	1502	ATP	C5-C6-N6	2.30	123.85	120.35
8	Р	1502	ATP	O2'-C2'-C3'	-2.20	104.72	111.82
8	В	1502	ATP	O2'-C2'-C3'	-2.18	104.77	111.82
8	В	1502	ATP	O3'-C3'-C2'	-2.14	104.90	111.82
8	Р	1502	ATP	O3'-C3'-C2'	-2.13	104.93	111.82
8	0	1502	ATP	O3'-C3'-C2'	-2.08	105.10	111.82
8	А	1502	ATP	O3'-C3'-C2'	-2.07	105.12	111.82

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	А	1502	ATP	PA-O3A-PB-O2B
8	0	1502	ATP	PA-O3A-PB-O2B
8	В	1502	ATP	PA-O3A-PB-O1B
8	В	1502	ATP	PA-O3A-PB-O2B
8	Р	1502	ATP	PA-O3A-PB-O1B
8	Р	1502	ATP	PA-O3A-PB-O2B

There are no ring outliers.

No monomer is involved in short contacts.

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)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	D	1
2	С	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	295:ARG	С	296:ILE	Ν	1.04
1	С	295:ARG	С	296:ILE	Ν	1.03



# 6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-51446. 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









Z Index: 83

#### 6.2.2 Raw map



X Index: 83

Y Index: 83

Z Index: 83

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: 90



Y Index: 90



Z Index: 76

#### 6.3.2 Raw map



X Index: 90

Y Index: 91



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 0.07. 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 shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

#### $emd_{51446}msk_{1.map}$ (i) 6.6.1





# 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  $892~\mathrm{nm^3};$  this corresponds to an approximate mass of 806 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 0.110  ${\rm \AA^{-1}}$ 



# 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 0.110  $\text{\AA}^{-1}$ 



#### 8.2 Resolution estimates (i)

$\begin{array}{ c c c c c c c c c c c c c c c c c c c$	Estimation criterion (FSC cut-off)			
resolution estimate (A)	0.143	0.5	Half-bit	
Reported by author	9.10	-	-	
Author-provided FSC curve	-	-	-	
Unmasked-calculated*	22.68	30.86	23.36	

\*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 22.68 differs from the reported value 9.1 by more than 10 %



# 9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-51446 and PDB model 9GMA. Per-residue inclusion information can be found in section 3 on page 7.

## 9.1 Map-model overlay (i)



The images above show the 3D surface view of the map at the recommended contour level 0.07 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 (0.07).



#### 9.4 Atom inclusion (i)



At the recommended contour level, 54% of all backbone atoms, 54% of all non-hydrogen atoms, are inside the map.



### 9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.07) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score	
All	0.5410	0.0750	
А	0.9440	0.1220	
В	0.9390	0.1190	<b>1</b> 0
С	0.9450	0.1200	1.0
D	0.6710	0.0760	
E	0.9470	0.1300	
F	0.9570	0.1330	
G	0.9830	0.1350	
Ι	0.9640	0.1490	
K	0.6510	0.1010	
L	0.6390	0.0990	
М	0.0360	0.0260	0.0
0	0.0050	0.0160	<0.0
Р	0.0350	0.0200	
Q	0.6600	0.0450	
R	0.1760	0.0320	
S	0.0000	0.0030	

