

Full wwPDB X-ray Structure Validation Report (i)

Sep 11, 2023 - 02:11 PM JST

PDB ID	:	8198
Title	:	Crystal structure of TePixD Y8F
Authors	:	Hu, R.; Lin, L.; Lu, Q.
Deposited on	:	2023-02-06
Resolution	:	2.54 Å(reported)

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

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

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

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.54 Å.

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



Metric	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar resolution} \ (\# Entries, resolution range(Å))$	
R_{free}	130704	$1284 \ (2.56-2.52)$	
Clashscore	141614	$1332 \ (2.56-2.52)$	
Ramachandran outliers	138981	1315 (2.56-2.52)	
Sidechain outliers	138945	1315 (2.56-2.52)	
RSRZ outliers	127900	$1272 \ (2.56-2.52)$	

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

Mol	Chain	Length	Quality of chain			
1	Δ	163	.%	20%		1 / 0/
	11	100	% *	2070		1470
1	В	163	67%	18%	•	13%
1	С	163	61%	23%	•	14%
1	D	163	% 72%	14%	•	13%
1	Е	163	% 66%	21%		13%
1	F	163	% 66%	21%	•	12%



Mol	Chain	Length	Quality of chain						
1	G	163	68%	17%	•	14%			
1	Н	163	64%	21%	·	13%			
1	Ι	163	71%	15%	•	13%			
1	J	163	72%	13%	•	13%			
1	Κ	163	% 63%	21%	•	14%			
1	L	163	4% 61%	24%	•	13%			
1	М	163	2% 54%	31%	•	14%			
1	Ν	163	.% 59%	26%	•	14%			
1	Ο	163	48%	31%	7%	14%			
1	Р	163	<u>4%</u> 60%	25%	•	13%			
1	Q	163	.% 6 5%	20%	•	14%			
1	R	163	65%	19%	•	14%			
1	S	163	.%56%	28%	•	13%			
1	Т	163	% • 62%	23%	•	14%			

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
2	FMN	Т	9201	-	-	Х	-



2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 23005 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$		Chan	recorded		A	Joins			ZeroOcc	AltConf	Trace
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	А	140	Total	C	N	0	S	0	0	0
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$				1113	703	189	210	<u></u>			
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	В	141	Total	C	N	0	S	0	0	0
$\begin{array}{c c c c c c c c c c c c c c c c c c c $				1136	715	199	211	11	_	_	_
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	1	C	140	Total	С	Ν	0	S	0	0	0
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$		Ũ		1119	706	192	210	11	Ŭ		
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	1	D	141	Total	С	Ν	Ο	\mathbf{S}	0	0	0
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$				1128	710	196	211	11	Ŭ	Ŭ	
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	E	142	Total	С	Ν	Ο	\mathbf{S}	0	0	0
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$			112	1154	724	206	213	11	0	0	0
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	1	F	1/13	Total	С	Ν	Ο	\mathbf{S}	0	0	0
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	Ľ	140	1148	721	202	214	11	0	0	0
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	1	С	140	Total	С	Ν	0	\mathbf{S}	0	0	0
$ \begin{array}{ c c c c c c c c c c c c c c c c c c c$		G	140	1119	703	196	209	11	0	0	0
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	1	п	1.41	Total	С	Ν	0	\mathbf{S}	0	0	0
$\begin{array}{ c c c c c c c c c c c c c c c c c c c$		11	141	1128	710	197	210	11			U
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	т	1.41	Total	С	Ν	0	\mathbf{S}	0	0	0
1 I I I I I I I I I I I I I I I I I I I		1	141	1116	704	193	208	11	0	0	0
	1	T	1.41	Total	С	Ν	0	\mathbf{S}	0	0	0
$\begin{array}{ c c c c c c c c c c c c c c c c c c c$		J	141	1130	711	199	209	11	0	0	0
1 K 140 Total C N O S 0	1	K	140	Total	С	Ν	0	S	0	0	0
$\begin{array}{ c c c c c c c c c c c c c c c c c c c$		IX	140	1097	690	188	209	10	0	0	0
1 I Total C N O S 0	1	т	1.41	Total	С	Ν	0	S	0	0	0
$\begin{array}{ c c c c c c c c c c c c c c c c c c c$			141	1119	705	194	209	11	0	0	0
1 M Ital C N O S 0 0	1	М	140	Total	С	Ν	0	S	0	0	0
$\begin{array}{ c c c c c c c c c c c c c c c c c c c$		11/1	140	1113	702	192	208	11	0	0	0
1 N 140 Total C N O S 0	1	N	140	Total	С	Ν	0	S	0	0	0
$\begin{array}{ c c c c c c c c c c c c c c c c c c c$		IN	140	1104	697	189	208	10	0	0	0
1 O Ital C N O S O O	1	0	140	Total	С	Ν	0	S	0	0	0
$ \begin{vmatrix} 1 \\ -1 \\ -1 \\ -1 \\ -1 \\ -1 \\ -1 \\ -1 $			140	1108	701	189	208	10		U	U
1 D 141 Total C N O S O	1	р	1./1	Total	С	Ν	Ο	S	0	0	0
$\begin{array}{ c c c c c c c c c c c c c c c c c c c$		Г	141	1078	680	184	205	9		U	U

• Molecule 1 is a protein called Tll0078 protein.



Atoms			ZeroOcc
N	0	C	

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	0	140	Total	С	Ν	0	S	0	0	0
1	Q	140	1125	708	198	208	11	0	0	U
1	1 D	D 140	Total	С	Ν	0	S	0	0	0
I K	140	1113	703	195	205	10	0	0	U	
1	C	C 141	Total	С	Ν	0	S	0	0	0
1 5	141	1118	704	192	211	11	0	0	0	
1 T	140	Total	С	Ν	0	S	0	0	0	
		1110	704	10/	210	11	0	0	0	

There are 420 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	-19	MET	-	initiating methionine	UNP Q8DMN3
А	-18	GLY	-	expression tag	UNP Q8DMN3
А	-17	SER	-	expression tag	UNP Q8DMN3
А	-16	SER	-	expression tag	UNP Q8DMN3
А	-15	HIS	-	expression tag	UNP Q8DMN3
А	-14	HIS	-	expression tag	UNP Q8DMN3
А	-13	HIS	-	expression tag	UNP Q8DMN3
А	-12	HIS	-	expression tag	UNP Q8DMN3
А	-11	HIS	-	expression tag	UNP Q8DMN3
А	-10	HIS	-	expression tag	UNP Q8DMN3
А	-9	SER	-	expression tag	UNP Q8DMN3
А	-8	SER	-	expression tag	UNP Q8DMN3
А	-7	GLY	-	expression tag	UNP Q8DMN3
А	-6	LEU	-	expression tag	UNP Q8DMN3
А	-5	VAL	-	expression tag	UNP Q8DMN3
А	-4	PRO	-	expression tag	UNP Q8DMN3
А	-3	ARG	-	expression tag	UNP Q8DMN3
А	-2	GLY	-	expression tag	UNP Q8DMN3
А	-1	SER	-	expression tag	UNP Q8DMN3
А	0	HIS	-	expression tag	UNP Q8DMN3
А	8	PHE	TYR	conflict	UNP Q8DMN3
В	981	MET	-	initiating methionine	UNP Q8DMN3
В	982	GLY	-	expression tag	UNP Q8DMN3
В	983	SER	-	expression tag	UNP Q8DMN3
В	984	SER	-	expression tag	UNP Q8DMN3
В	985	HIS	-	expression tag	UNP Q8DMN3
В	986	HIS	-	expression tag	UNP Q8DMN3
В	987	HIS	-	expression tag	UNP Q8DMN3
В	988	HIS	-	expression tag	UNP Q8DMN3
В	989	HIS	-	expression tag	UNP Q8DMN3
В	990	HIS	-	expression tag	UNP Q8DMN3



Chain	Residue	Modelled	Actual Comment		Reference
В	991	SER	-	expression tag	UNP Q8DMN3
В	992	SER	-	expression tag	UNP Q8DMN3
В	993	GLY	-	expression tag	UNP Q8DMN3
В	994	LEU	-	expression tag	UNP Q8DMN3
В	995	VAL	-	expression tag	UNP Q8DMN3
В	996	PRO	-	expression tag	UNP Q8DMN3
В	997	ARG	-	expression tag	UNP Q8DMN3
В	998	GLY	-	expression tag	UNP Q8DMN3
В	999	SER	-	expression tag	UNP Q8DMN3
В	1000	HIS	-	expression tag	UNP Q8DMN3
В	1008	PHE	TYR	conflict	UNP Q8DMN3
С	1981	MET	-	initiating methionine	UNP Q8DMN3
С	1982	GLY	-	expression tag	UNP Q8DMN3
С	1983	SER	-	expression tag	UNP Q8DMN3
С	1984	SER	-	expression tag	UNP Q8DMN3
С	1985	HIS	-	expression tag	UNP Q8DMN3
С	1986	HIS	_	expression tag	UNP Q8DMN3
С	1987	HIS	-	expression tag	UNP Q8DMN3
С	1988	HIS	_	expression tag	UNP Q8DMN3
С	1989	HIS	-	expression tag	UNP Q8DMN3
С	1990	HIS	-	expression tag	UNP Q8DMN3
С	1991	SER	-	expression tag	UNP Q8DMN3
С	1992	SER	-	expression tag	UNP Q8DMN3
С	1993	GLY	-	expression tag	UNP Q8DMN3
С	1994	LEU	-	expression tag	UNP Q8DMN3
С	1995	VAL	-	expression tag	UNP Q8DMN3
С	1996	PRO	-	expression tag	UNP Q8DMN3
С	1997	ARG	-	expression tag	UNP Q8DMN3
С	1998	GLY	-	expression tag	UNP Q8DMN3
С	1999	SER	-	expression tag	UNP Q8DMN3
С	2000	HIS	-	expression tag	UNP Q8DMN3
С	2008	PHE	TYR	conflict	UNP Q8DMN3
D	2981	MET	-	initiating methionine	UNP Q8DMN3
D	2982	GLY	-	expression tag	UNP Q8DMN3
D	2983	SER	-	expression tag	UNP Q8DMN3
D	2984	SER	-	expression tag	UNP Q8DMN3
D	2985	HIS	-	expression tag	UNP Q8DMN3
D	2986	HIS	-	expression tag	UNP Q8DMN3
D	2987	HIS	_	expression tag	UNP Q8DMN3
D	2988	HIS	-	expression tag	UNP Q8DMN3
D	2989	HIS	-	expression tag	UNP Q8DMN3
D	2990	HIS	-	expression tag	UNP Q8DMN3



Chain	Residue	Modelled	Actual	Comment	Reference	
D	2991	SER	-	expression tag	UNP Q8DMN3	
D	2992	SER	-	expression tag	UNP Q8DMN3	
D	2993	GLY	-	expression tag	UNP Q8DMN3	
D	2994	LEU	-	expression tag	UNP Q8DMN3	
D	2995	VAL	-	expression tag	UNP Q8DMN3	
D	2996	PRO	-	expression tag	UNP Q8DMN3	
D	2997	ARG	-	expression tag	UNP Q8DMN3	
D	2998	GLY	-	expression tag	UNP Q8DMN3	
D	2999	SER	-	expression tag	UNP Q8DMN3	
D	3000	HIS	-	expression tag	UNP Q8DMN3	
D	3008	PHE	TYR	conflict	UNP Q8DMN3	
E	3981	MET	-	initiating methionine	UNP Q8DMN3	
E	3982	GLY	-	expression tag	UNP Q8DMN3	
E	3983	SER	-	expression tag	UNP Q8DMN3	
E	3984	SER	-	expression tag	UNP Q8DMN3	
E	3985	HIS	-	expression tag	UNP Q8DMN3	
E	3986	HIS	-	expression tag	UNP Q8DMN3	
E	3987	HIS	-	expression tag	UNP Q8DMN3	
E	3988	HIS	-	expression tag	UNP Q8DMN3	
Ε	3989	HIS	-	expression tag	UNP Q8DMN3	
E	3990	HIS	-	expression tag	UNP Q8DMN3	
Ε	3991	SER	-	expression tag	UNP Q8DMN3	
Ε	3992	SER	-	expression tag	UNP Q8DMN3	
E	3993	GLY	-	expression tag	UNP Q8DMN3	
E	3994	LEU	-	expression tag	UNP Q8DMN3	
E	3995	VAL	-	expression tag	UNP Q8DMN3	
E	3996	PRO	-	expression tag	UNP Q8DMN3	
E	3997	ARG	-	expression tag	UNP Q8DMN3	
E	3998	GLY	-	expression tag	UNP Q8DMN3	
E	3999	SER	-	expression tag	UNP Q8DMN3	
E	4000	HIS	-	expression tag	UNP Q8DMN3	
E	4008	PHE	TYR	conflict	UNP Q8DMN3	
F	4981	MET	-	initiating methionine	UNP Q8DMN3	
F	4982	GLY	-	expression tag	UNP Q8DMN3	
F	4983	SER	-	expression tag	UNP Q8DMN3	
F	4984	SER	-	expression tag	UNP Q8DMN3	
F	4985	HIS	-	expression tag	UNP Q8DMN3	
F	4986	HIS	-	expression tag	UNP Q8DMN3	
F	4987	HIS	-	expression tag	UNP Q8DMN3	
F	4988	HIS	-	expression tag	UNP Q8DMN3	
F	4989	HIS	-	expression tag	UNP Q8DMN3	
F	4990	HIS	-	expression tag	UNP Q8DMN3	



Chain	Residue	Modelled	Actual	Comment	Reference
F	4991	SER	-	expression tag	UNP Q8DMN3
F	4992	SER	_	expression tag	UNP Q8DMN3
F	4993	GLY	-	expression tag	UNP Q8DMN3
F	4994	LEU	-	expression tag	UNP Q8DMN3
F	4995	VAL	-	expression tag	UNP Q8DMN3
F	4996	PRO	-	expression tag	UNP Q8DMN3
F	4997	ARG	-	expression tag	UNP Q8DMN3
F	4998	GLY	-	expression tag	UNP Q8DMN3
F	4999	SER	-	expression tag	UNP Q8DMN3
F	5000	HIS	-	expression tag	UNP Q8DMN3
F	5008	PHE	TYR	conflict	UNP Q8DMN3
G	5981	MET	-	initiating methionine	UNP Q8DMN3
G	5982	GLY	-	expression tag	UNP Q8DMN3
G	5983	SER	-	expression tag	UNP Q8DMN3
G	5984	SER	-	expression tag	UNP Q8DMN3
G	5985	HIS	-	expression tag	UNP Q8DMN3
G	5986	HIS	-	expression tag	UNP Q8DMN3
G	5987	HIS	-	expression tag	UNP Q8DMN3
G	5988	HIS	-	expression tag	UNP Q8DMN3
G	5989	HIS	-	expression tag	UNP Q8DMN3
G	5990	HIS	-	expression tag	UNP Q8DMN3
G	5991	SER	-	expression tag	UNP Q8DMN3
G	5992	SER	-	expression tag	UNP Q8DMN3
G	5993	GLY	-	expression tag	UNP Q8DMN3
G	5994	LEU	-	expression tag	UNP Q8DMN3
G	5995	VAL	-	expression tag	UNP Q8DMN3
G	5996	PRO	-	expression tag	UNP Q8DMN3
G	5997	ARG	-	expression tag	UNP Q8DMN3
G	5998	GLY	-	expression tag	UNP Q8DMN3
G	5999	SER	-	expression tag	UNP Q8DMN3
G	6000	HIS	-	expression tag	UNP Q8DMN3
G	6008	PHE	TYR	conflict	UNP Q8DMN3
H	6981	MET	-	initiating methionine	UNP Q8DMN3
H	6982	GLY	-	expression tag	UNP Q8DMN3
H	6983	SER	-	expression tag	UNP Q8DMN3
H	6984	SER	-	expression tag	UNP Q8DMN3
H	6985	HIS	-	expression tag	UNP Q8DMN3
H	6986	HIS	-	expression tag	UNP Q8DMN3
H	6987	HIS	-	expression tag	UNP Q8DMN3
H	6988	HIS	-	expression tag	UNP Q8DMN3
H	6989	HIS	-	expression tag	UNP Q8DMN3
H	6990	HIS	-	expression tag	UNP Q8DMN3



Chain	Residue	Modelled	Actual	Comment	Reference
Н	6991	SER	_	expression tag	UNP Q8DMN3
Н	6992	SER	-	expression tag	UNP Q8DMN3
Н	6993	GLY	_	expression tag	UNP Q8DMN3
Н	6994	LEU	-	expression tag	UNP Q8DMN3
Н	6995	VAL	_	expression tag	UNP Q8DMN3
Н	6996	PRO	-	expression tag	UNP Q8DMN3
Н	6997	ARG	-	expression tag	UNP Q8DMN3
Н	6998	GLY	-	expression tag	UNP Q8DMN3
Н	6999	SER	-	expression tag	UNP Q8DMN3
Н	7000	HIS	-	expression tag	UNP Q8DMN3
Н	7008	PHE	TYR	conflict	UNP Q8DMN3
Ι	7981	MET	-	initiating methionine	UNP Q8DMN3
Ι	7982	GLY	-	expression tag	UNP Q8DMN3
Ι	7983	SER	-	expression tag	UNP Q8DMN3
Ι	7984	SER	-	expression tag	UNP Q8DMN3
Ι	7985	HIS	-	expression tag	UNP Q8DMN3
Ι	7986	HIS	-	expression tag	UNP Q8DMN3
Ι	7987	HIS	-	expression tag	UNP Q8DMN3
Ι	7988	HIS	-	expression tag	UNP Q8DMN3
Ι	7989	HIS	-	expression tag	UNP Q8DMN3
Ι	7990	HIS	-	expression tag	UNP Q8DMN3
Ι	7991	SER	-	expression tag	UNP Q8DMN3
Ι	7992	SER	-	expression tag	UNP Q8DMN3
I	7993	GLY	-	expression tag	UNP Q8DMN3
Ι	7994	LEU	-	expression tag	UNP Q8DMN3
I	7995	VAL	-	expression tag	UNP Q8DMN3
I	7996	PRO	-	expression tag	UNP Q8DMN3
I	7997	ARG	-	expression tag	UNP Q8DMN3
I	7998	GLY	-	expression tag	UNP Q8DMN3
I	7999	SER	-	expression tag	UNP Q8DMN3
I	8000	HIS	-	expression tag	UNP Q8DMN3
I	8008	PHE	TYR	conflict	UNP Q8DMN3
J	8981	MET	-	initiating methionine	UNP Q8DMN3
J	8982	GLY	-	expression tag	UNP Q8DMN3
J	8983	SER	-	expression tag	UNP Q8DMN3
J	8984	SER	-	expression tag	UNP Q8DMN3
J	8985	HIS	-	expression tag	UNP Q8DMN3
J	8986	HIS	-	expression tag	UNP Q8DMN3
J	8987	HIS	-	expression tag	UNP Q8DMN3
J	8988	HIS	-	expression tag	UNP Q8DMN3
J	8989	HIS	-	expression tag	UNP Q8DMN3
J	8990	HIS	_	expression tag	UNP Q8DMN3



Chain	Residue	Modelled	Actual	Comment	Reference
J	8991	SER	-	expression tag	UNP Q8DMN3
J	8992	SER	-	expression tag	UNP Q8DMN3
J	8993	GLY	_	expression tag	UNP Q8DMN3
J	8994	LEU	_	expression tag	UNP Q8DMN3
J	8995	VAL	-	expression tag	UNP Q8DMN3
J	8996	PRO	-	expression tag	UNP Q8DMN3
J	8997	ARG	-	expression tag	UNP Q8DMN3
J	8998	GLY	-	expression tag	UNP Q8DMN3
J	8999	SER	-	expression tag	UNP Q8DMN3
J	9000	HIS	-	expression tag	UNP Q8DMN3
J	9008	PHE	TYR	conflict	UNP Q8DMN3
K	81	MET	-	initiating methionine	UNP Q8DMN3
K	82	GLY	-	expression tag	UNP Q8DMN3
K	83	SER	-	expression tag	UNP Q8DMN3
K	84	SER	-	expression tag	UNP Q8DMN3
K	85	HIS	-	expression tag	UNP Q8DMN3
K	86	HIS	-	expression tag	UNP Q8DMN3
K	87	HIS	-	expression tag	UNP Q8DMN3
K	88	HIS	-	expression tag	UNP Q8DMN3
K	89	HIS	-	expression tag	UNP Q8DMN3
K	90	HIS	-	expression tag	UNP Q8DMN3
K	91	SER	-	expression tag	UNP Q8DMN3
K	92	SER	-	expression tag	UNP Q8DMN3
K	93	GLY	-	expression tag	UNP Q8DMN3
K	94	LEU	-	expression tag	UNP Q8DMN3
K	95	VAL	-	expression tag	UNP Q8DMN3
K	96	PRO	-	expression tag	UNP Q8DMN3
K	97	ARG	-	expression tag	UNP Q8DMN3
K	98	GLY	-	expression tag	UNP Q8DMN3
K	99	SER	-	expression tag	UNP Q8DMN3
K	100	HIS	-	expression tag	UNP Q8DMN3
K	108	PHE	TYR	conflict	UNP Q8DMN3
L	981	MET	-	initiating methionine	UNP Q8DMN3
L	982	GLY	-	expression tag	UNP Q8DMN3
L	983	SER	-	expression tag	UNP Q8DMN3
L	984	SER	-	expression tag	UNP Q8DMN3
L	985	HIS	-	expression tag	UNP Q8DMN3
L	986	HIS	-	expression tag	UNP Q8DMN3
L	987	HIS	-	expression tag	UNP Q8DMN3
L	988	HIS	-	expression tag	UNP Q8DMN3
L	989	HIS	-	expression tag	UNP Q8DMN3
L	990	HIS	-	expression tag	UNP Q8DMN3



Chain	Residue	Modelled	Actual	Comment	Reference
L	991	SER	-	expression tag	UNP Q8DMN3
L	992	SER	-	expression tag	UNP Q8DMN3
L	993	GLY	-	expression tag	UNP Q8DMN3
L	994	LEU	-	expression tag	UNP Q8DMN3
L	995	VAL	-	expression tag	UNP Q8DMN3
L	996	PRO	-	expression tag	UNP Q8DMN3
L	997	ARG	-	expression tag	UNP Q8DMN3
L	998	GLY	-	expression tag	UNP Q8DMN3
L	999	SER	-	expression tag	UNP Q8DMN3
L	1000	HIS	-	expression tag	UNP Q8DMN3
L	1008	PHE	TYR	conflict	UNP Q8DMN3
М	1981	MET	-	initiating methionine	UNP Q8DMN3
М	1982	GLY	-	expression tag	UNP Q8DMN3
М	1983	SER	-	expression tag	UNP Q8DMN3
М	1984	SER	-	expression tag	UNP Q8DMN3
М	1985	HIS	-	expression tag	UNP Q8DMN3
М	1986	HIS	-	expression tag	UNP Q8DMN3
М	1987	HIS	-	expression tag	UNP Q8DMN3
М	1988	HIS	-	expression tag	UNP Q8DMN3
М	1989	HIS	-	expression tag	UNP Q8DMN3
М	1990	HIS	-	expression tag	UNP Q8DMN3
М	1991	SER	-	expression tag	UNP Q8DMN3
М	1992	SER	-	expression tag	UNP Q8DMN3
М	1993	GLY	-	expression tag	UNP Q8DMN3
М	1994	LEU	-	expression tag	UNP Q8DMN3
М	1995	VAL	-	expression tag	UNP Q8DMN3
М	1996	PRO	-	expression tag	UNP Q8DMN3
М	1997	ARG	-	expression tag	UNP Q8DMN3
М	1998	GLY	-	expression tag	UNP Q8DMN3
М	1999	SER	-	expression tag	UNP Q8DMN3
М	2000	HIS	-	expression tag	UNP Q8DMN3
М	2008	PHE	TYR	conflict	UNP Q8DMN3
N	2981	MET	-	initiating methionine	UNP Q8DMN3
N	2982	GLY	-	expression tag	UNP Q8DMN3
N	2983	SER	-	expression tag	UNP Q8DMN3
N	2984	SER	-	expression tag	UNP Q8DMN3
N	2985	HIS	-	expression tag	UNP Q8DMN3
N	2986	HIS	-	expression tag	UNP Q8DMN3
N	2987	HIS	-	expression tag	UNP Q8DMN3
N	2988	HIS	-	expression tag	UNP Q8DMN3
N	2989	HIS	-	expression tag	UNP Q8DMN3
N	2990	HIS	-	expression tag	UNP Q8DMN3

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Chain	Residue	Modelled	Actual	Comment	Reference
N	2991	SER	-	expression tag	UNP Q8DMN3
N	2992	SER	_	expression tag	UNP Q8DMN3
N	2993	GLY	-	expression tag	UNP Q8DMN3
N	2994	LEU	-	expression tag	UNP Q8DMN3
N	2995	VAL	-	expression tag	UNP Q8DMN3
N	2996	PRO	-	expression tag	UNP Q8DMN3
N	2997	ARG	-	expression tag	UNP Q8DMN3
N	2998	GLY	-	expression tag	UNP Q8DMN3
N	2999	SER	-	expression tag	UNP Q8DMN3
N	3000	HIS	-	expression tag	UNP Q8DMN3
N	3008	PHE	TYR	conflict	UNP Q8DMN3
0	3981	MET	-	initiating methionine	UNP Q8DMN3
0	3982	GLY	-	expression tag	UNP Q8DMN3
0	3983	SER	-	expression tag	UNP Q8DMN3
0	3984	SER	-	expression tag	UNP Q8DMN3
0	3985	HIS	-	expression tag	UNP Q8DMN3
0	3986	HIS	-	expression tag	UNP Q8DMN3
0	3987	HIS	-	expression tag	UNP Q8DMN3
0	3988	HIS	-	expression tag	UNP Q8DMN3
0	3989	HIS	-	expression tag	UNP Q8DMN3
0	3990	HIS	-	expression tag	UNP Q8DMN3
0	3991	SER	-	expression tag	UNP Q8DMN3
0	3992	SER	-	expression tag	UNP Q8DMN3
0	3993	GLY	-	expression tag	UNP Q8DMN3
0	3994	LEU	-	expression tag	UNP Q8DMN3
0	3995	VAL	-	expression tag	UNP Q8DMN3
0	3996	PRO	-	expression tag	UNP Q8DMN3
0	3997	ARG	-	expression tag	UNP Q8DMN3
0	3998	GLY	-	expression tag	UNP Q8DMN3
0	3999	SER	-	expression tag	UNP Q8DMN3
0	4000	HIS	-	expression tag	UNP Q8DMN3
0	4008	PHE	TYR	conflict	UNP Q8DMN3
P	4981	MET	-	initiating methionine	UNP Q8DMN3
Р	4982	GLY	-	expression tag	UNP Q8DMN3
P	4983	SER	-	expression tag	UNP Q8DMN3
Р	4984	SER	-	expression tag	UNP Q8DMN3
Р	4985	HIS	-	expression tag	UNP Q8DMN3
Р	4986	HIS	-	expression tag	UNP Q8DMN3
Р	4987	HIS	-	expression tag	UNP Q8DMN3
Р	4988	HIS	-	expression tag	UNP Q8DMN3
Р	4989	HIS	-	expression tag	UNP Q8DMN3
P	4990	HIS	-	expression tag	UNP Q8DMN3



Chain	Residue	Modelled	Actual	Comment	Reference
Р	4991	SER	-	expression tag	UNP Q8DMN3
Р	4992	SER	-	expression tag	UNP Q8DMN3
Р	4993	GLY	_	expression tag	UNP Q8DMN3
Р	4994	LEU	-	expression tag	UNP Q8DMN3
Р	4995	VAL	-	expression tag	UNP Q8DMN3
Р	4996	PRO	-	expression tag	UNP Q8DMN3
Р	4997	ARG	-	expression tag	UNP Q8DMN3
Р	4998	GLY	-	expression tag	UNP Q8DMN3
Р	4999	SER	-	expression tag	UNP Q8DMN3
Р	5000	HIS	-	expression tag	UNP Q8DMN3
Р	5008	PHE	TYR	conflict	UNP Q8DMN3
Q	5981	MET	-	initiating methionine	UNP Q8DMN3
Q	5982	GLY	-	expression tag	UNP Q8DMN3
Q	5983	SER	-	expression tag	UNP Q8DMN3
Q	5984	SER	-	expression tag	UNP Q8DMN3
Q	5985	HIS	-	expression tag	UNP Q8DMN3
Q	5986	HIS	-	expression tag	UNP Q8DMN3
Q	5987	HIS	-	expression tag	UNP Q8DMN3
Q	5988	HIS	-	expression tag	UNP Q8DMN3
Q	5989	HIS	-	expression tag	UNP Q8DMN3
Q	5990	HIS	-	expression tag	UNP Q8DMN3
Q	5991	SER	-	expression tag	UNP Q8DMN3
Q	5992	SER	-	expression tag	UNP Q8DMN3
Q	5993	GLY	-	expression tag	UNP Q8DMN3
Q	5994	LEU	-	expression tag	UNP Q8DMN3
Q	5995	VAL	-	expression tag	UNP Q8DMN3
Q	5996	PRO	-	expression tag	UNP Q8DMN3
Q	5997	ARG	-	expression tag	UNP Q8DMN3
Q	5998	GLY	-	expression tag	UNP Q8DMN3
Q	5999	SER	-	expression tag	UNP Q8DMN3
Q	6000	HIS	-	expression tag	UNP Q8DMN3
Q	6008	PHE	TYR	conflict	UNP Q8DMN3
R	6981	MET	-	initiating methionine	UNP Q8DMN3
R	6982	GLY	-	expression tag	UNP Q8DMN3
R	6983	SER	-	expression tag	UNP Q8DMN3
R	6984	SER	-	expression tag	UNP Q8DMN3
R	6985	HIS	-	expression tag	UNP Q8DMN3
R	6986	HIS	-	expression tag	UNP Q8DMN3
R	6987	HIS	-	expression tag	UNP Q8DMN3
R	6988	HIS	-	expression tag	UNP Q8DMN3
R	6989	HIS	-	expression tag	UNP Q8DMN3
R	6990	HIS	-	expression tag	UNP Q8DMN3



Chain	Residue	Modelled	Actual	Comment	Reference
R	6991	SER	-	expression tag	UNP Q8DMN3
R	6992	SER	-	expression tag	UNP Q8DMN3
R	6993	GLY	-	expression tag	UNP Q8DMN3
R	6994	LEU	-	expression tag	UNP Q8DMN3
R	6995	VAL	-	expression tag	UNP Q8DMN3
R	6996	PRO	-	expression tag	UNP Q8DMN3
R	6997	ARG	-	expression tag	UNP Q8DMN3
R	6998	GLY	-	expression tag	UNP Q8DMN3
R	6999	SER	-	expression tag	UNP Q8DMN3
R	7000	HIS	-	expression tag	UNP Q8DMN3
R	7008	PHE	TYR	conflict	UNP Q8DMN3
S	7981	MET	-	initiating methionine	UNP Q8DMN3
S	7982	GLY	-	expression tag	UNP Q8DMN3
S	7983	SER	-	expression tag	UNP Q8DMN3
S	7984	SER	-	expression tag	UNP Q8DMN3
S	7985	HIS	-	expression tag	UNP Q8DMN3
S	7986	HIS	-	expression tag	UNP Q8DMN3
S	7987	HIS	-	expression tag	UNP Q8DMN3
S	7988	HIS	-	expression tag	UNP Q8DMN3
S	7989	HIS	-	expression tag	UNP Q8DMN3
S	7990	HIS	-	expression tag	UNP Q8DMN3
S	7991	SER	-	expression tag	UNP Q8DMN3
S	7992	SER	-	expression tag	UNP Q8DMN3
S	7993	GLY	-	expression tag	UNP Q8DMN3
S	7994	LEU	-	expression tag	UNP Q8DMN3
S	7995	VAL	-	expression tag	UNP Q8DMN3
S	7996	PRO	-	expression tag	UNP Q8DMN3
S	7997	ARG	-	expression tag	UNP Q8DMN3
S	7998	GLY	-	expression tag	UNP Q8DMN3
S	7999	SER	-	expression tag	UNP Q8DMN3
S	8000	HIS	-	expression tag	UNP Q8DMN3
S	8008	PHE	TYR	conflict	UNP Q8DMN3
Т	8981	MET	-	initiating methionine	UNP Q8DMN3
Т	8982	GLY	-	expression tag	UNP Q8DMN3
Т	8983	SER	-	expression tag	UNP Q8DMN3
Т	8984	SER	-	expression tag	UNP Q8DMN3
Т	8985	HIS	-	expression tag	UNP Q8DMN3
Т	8986	HIS	-	expression tag	UNP Q8DMN3
Т	8987	HIS	-	expression tag	UNP Q8DMN3
Т	8988	HIS	-	expression tag	UNP Q8DMN3
Т	8989	HIS	-	expression tag	UNP Q8DMN3
Т	8990	HIS	-	expression tag	UNP Q8DMN3

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Chain	Residue	Modelled	Actual	$\operatorname{Comment}$	Reference
Т	8991	SER	-	expression tag	UNP Q8DMN3
Т	8992	SER	-	expression tag	UNP Q8DMN3
Т	8993	GLY	-	expression tag	UNP Q8DMN3
Т	8994	LEU	-	expression tag	UNP Q8DMN3
Т	8995	VAL	-	expression tag	UNP Q8DMN3
Т	8996	PRO	-	expression tag	UNP Q8DMN3
Т	8997	ARG	-	expression tag	UNP Q8DMN3
Т	8998	GLY	-	expression tag	UNP Q8DMN3
Т	8999	SER	-	expression tag	UNP Q8DMN3
Т	9000	HIS	-	expression tag	UNP Q8DMN3
Т	9008	PHE	TYR	conflict	UNP Q8DMN3

• Molecule 2 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf							
2	2 1	1	Total C N O P	0	0							
2	Π	T	31 17 4 9 1	0	0							
2	В	1	Total C N O P	0	0							
2	D	1	31 17 4 9 1	0	0							
0	<u>р</u> С	C 1	Total C N O P	0	0							
	U		31 17 4 9 1	0	0							
0	2 D	Л	Л	Л	Л	Л	Л	Л	1	Total C N O P	0	0
		1	31 17 4 9 1	0	0							
0	9 E	1	Total C N O P	0	0							
	Ľ		31 17 4 9 1	0								



 \mathbf{S}

Т

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Mol	Chain	Residues		Ato	oms			ZeroOcc	AltConf		
2	F	1	Total	С	Ν	0	Р	0	0		
			31	17	4	9	1		-		
2	G	1	Total	С	Ν	Ο	Р	0	0		
		1	31	17	4	9	1	0	0		
2	н	1	Total	\mathbf{C}	Ν	Ο	Р	0	0		
2	11	1	31	17	4	9	1	0	0		
9	т	1	Total	С	Ν	Ο	Р	0	0		
2	1	1	31	17	4	9	1	0	0		
9	т	1	Total	С	Ν	Ο	Р	0	0		
Z	J	1	31	17	4	9	1	0			
0	V	K 1	Total	С	Ν	Ο	Р	0	0		
Ζ	n		31	17	4	9	1	U	0		
0	т	т	1	Total	С	Ν	Ο	Р	0	0	
Ζ	L	1	31	17	4	9	1	0	0		
0	м	1	Total	С	Ν	Ο	Р	0	0		
Ζ	IVI	1	31	17	4	9	1	0			
0	N	1	Total	С	Ν	Ο	Р	0	0		
2	IN	1	31	17	4	9	1	0	0		
0	0	1	Total	С	Ν	Ο	Р	0	0		
2	0	O	0	1	31	17	4	9	1	0	0
0	Б	1	Total	С	Ν	0	Р	0	0		
2	Р	1	31	17	4	9	1	0	0		
0	0	1	Total	С	Ν	0	Р	0	0		
2	Q		31	17	4	9	1	0	0		
	D	1	Total	С	Ν	0	Р	0	0		
2	R		91	17	1	0	1	0	0		

Total

Total

С

С



Р

0

Ν

Ν

Р

3 Residue-property plots (i)

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



• Molecule 1: Tll0078 protein





• Molecule 1: Tll0078 protein





• Molecule 1: Tll0078 protein





• Molecule 1: Tll0078 protein





• Molecule 1: Tll0078 protein







• Molecule 1: Tll0078 protein













4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	82.27Å 162.04Å 135.87Å	Deperitor
a, b, c, α , β , γ	90.00° 92.60° 90.00°	Depositor
$\mathbf{P}_{\text{assolution}}(\hat{\mathbf{A}})$	35.88 - 2.54	Depositor
Resolution (A)	135.73 - 2.54	EDS
% Data completeness	98.4 (35.88-2.54)	Depositor
(in resolution range)	$98.4\ (135.73\text{-}2.54)$	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.46 (at 2.55 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
P. P.	0.203 , 0.262	Depositor
n, n_{free}	0.205 , 0.257	DCC
R_{free} test set	5750 reflections (5.00%)	wwPDB-VP
Wilson B-factor $(Å^2)$	48.8	Xtriage
Anisotropy	0.349	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.32 , 43.6	EDS
L-test for $twinning^2$	$< L >=0.51, < L^2>=0.34$	Xtriage
Estimated twinning fraction	0.017 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	23005	wwPDB-VP
Average B, all atoms $(Å^2)$	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.37% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



¹Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: FMN

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	Bond lengths		Bond	angles
	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.66	0/1133	0.75	0/1524
1	В	0.59	0/1156	0.74	0/1552
1	С	0.58	0/1139	0.73	0/1531
1	D	0.62	0/1148	0.73	0/1543
1	Е	0.61	0/1175	0.75	0/1577
1	F	0.58	0/1168	0.75	0/1568
1	G	0.56	0/1138	0.74	0/1528
1	Н	0.55	0/1148	0.75	0/1543
1	Ι	0.56	0/1136	0.72	0/1529
1	J	0.61	0/1150	0.75	0/1545
1	Κ	0.56	0/1116	0.71	0/1504
1	L	0.50	0/1140	0.69	0/1535
1	М	0.52	0/1133	0.69	0/1524
1	Ν	0.51	0/1124	0.73	0/1514
1	0	0.51	0/1128	0.73	0/1518
1	Р	0.52	0/1097	0.69	0/1482
1	Q	0.55	0/1145	0.74	0/1538
1	R	0.53	0/1133	0.68	0/1524
1	S	0.59	0/1138	0.70	0/1532
1	Т	0.58	0/1139	0.75	0/1532
All	All	0.56	0/22784	0.73	0/30643

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.



5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	1113	0	1093	30	0
1	В	1136	0	1125	21	0
1	С	1119	0	1101	33	0
1	D	1128	0	1110	18	0
1	Е	1154	0	1145	22	0
1	F	1148	0	1134	27	0
1	G	1119	0	1107	21	0
1	Н	1128	0	1112	29	0
1	Ι	1116	0	1090	23	0
1	J	1130	0	1117	30	0
1	K	1097	0	1061	27	0
1	L	1119	0	1089	45	0
1	М	1113	0	1093	51	0
1	N	1104	0	1075	44	0
1	0	1108	0	1083	67	0
1	Р	1078	0	1029	40	0
1	Q	1125	0	1115	29	0
1	R	1113	0	1094	31	0
1	S	1118	0	1088	44	0
1	Т	1119	0	1097	40	0
2	А	31	0	19	2	0
2	В	31	0	19	0	0
2	С	31	0	19	4	0
2	D	31	0	19	1	0
2	Е	31	0	19	1	0
2	F	31	0	19	2	0
2	G	31	0	19	2	0
2	Н	31	0	19	4	0
2	Ι	31	0	19	2	0
2	J	31	0	19	3	0
2	K	31	0	19	0	0
2	L	31	0	19	2	0
2	М	31	0	19	1	0
2	N	31	0	19	2	0
2	0	31	0	19	4	0
2	Р	31	0	19	4	0
2	Q	31	0	19	1	0



	f = f = f = f = f = f = f = f = f = f =					
Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	R	31	0	19	1	0
2	S	31	0	19	0	0
2	Т	31	0	19	9	0
All	All	23005	0	22338	633	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 14.

All (633) 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)
1:Q:6101:MET:HE3	1:Q:6106:ILE:HD11	1.25	1.10
1:I:8093:MET:HA	1:I:8093:MET:HE2	1.35	1.09
1:P:5017:SER:HB2	1:P:5019:PRO:HD2	1.44	0.99
1:S:8111:LEU:HD22	1:T:9086:ARG:HH12	1.26	0.99
1:S:8111:LEU:HD22	1:T:9086:ARG:NH1	1.80	0.97
1:T:9093:MET:HE2	1:T:9093:MET:HA	1.44	0.96
1:J:9017:SER:OG	1:J:9019:PRO:HD2	1.66	0.95
1:H:7090:ASN:ND2	1:H:7141:GLN:HE22	1.62	0.95
1:T:9007:ILE:HG22	1:T:9078:VAL:HB	1.47	0.93
1:R:7025:MET:SD	1:R:7095:LEU:HB2	2.10	0.91
1:H:7090:ASN:HD22	1:H:7141:GLN:HE22	0.96	0.90
1:S:8001:MET:HE2	1:S:8001:MET:HA	1.50	0.89
1:F:5041:LEU:HB2	1:F:5093:MET:HE1	1.54	0.89
1:J:9101:MET:HE3	1:J:9106:ILE:CD1	2.04	0.87
1:T:9072:HIS:CD2	2:T:9201:FMN:HM82	2.09	0.87
1:T:9072:HIS:HD2	2:T:9201:FMN:HM82	1.37	0.87
1:M:2017:SER:OG	1:M:2019:PRO:HD2	1.75	0.87
1:Q:6101:MET:CE	1:Q:6106:ILE:HD11	2.04	0.87
1:I:8025:MET:CE	1:I:8093:MET:HG3	2.05	0.87
1:O:4025:MET:HE1	1:O:4094:ARG:HA	1.55	0.86
1:M:2091:TRP:HH2	1:M:2140:SER:CB	1.89	0.86
1:O:4091:TRP:HH2	1:O:4140:SER:HB2	1.40	0.86
1:C:2027:LYS:HE3	2:C:2201:FMN:H5'2	1.57	0.85
1:M:2041:LEU:HD12	1:M:2050:GLN:HB2	1.57	0.85
1:R:7095:LEU:HD21	1:R:7097:GLN:HG3	1.59	0.83
1:S:8041:LEU:HD21	1:S:8048:PHE:CD1	2.14	0.83
1:H:7090:ASN:HD22	1:H:7141:GLN:NE2	1.77	0.82
1:R:7045:ASN:O	1:R:7045:ASN:ND2	2.13	0.82
1:L:1001:MET:HG3	1:Q:6125:THR:HG22	1.63	0.81
1:N:3017:SER:HB2	1:N:3019:PRO:HD2	1.63	0.80



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:I:8093:MET:HA	1:I:8093:MET:CE	2.10	0.79
1:O:4035:ASP:HB3	1:O:4058:LYS:HG3	1.65	0.78
1:L:1040:MET:HE3	1:L:1094:ARG:HG2	1.67	0.77
1:J:9101:MET:HE3	1:J:9106:ILE:HG13	1.67	0.77
1:Q:6041:LEU:HD11	1:Q:6048:PHE:CD1	2.19	0.77
1:I:8017:SER:OG	1:I:8019:PRO:HD2	1.85	0.77
1:N:3084:GLU:OE2	1:O:4127:GLU:HG3	1.84	0.77
1:S:8041:LEU:HD21	1:S:8048:PHE:HD1	1.50	0.77
1:J:9101:MET:HE3	1:J:9106:ILE:HD11	1.66	0.77
1:J:9101:MET:HE3	1:J:9106:ILE:CG1	2.14	0.76
1:I:8025:MET:HE1	1:I:8093:MET:HG3	1.68	0.76
1:R:7009:LEU:HD22	1:R:7121:PRO:HB2	1.67	0.76
1:Q:6013:THR:O	1:Q:6016:LEU:HD23	1.86	0.76
1:T:9093:MET:HA	1:T:9093:MET:CE	2.16	0.75
1:D:3027:LYS:HD2	2:D:3201:FMN:H5'2	1.69	0.75
1:O:4040:MET:CE	1:O:4137:TYR:HB2	2.17	0.75
1:K:197:GLN:HB2	1:K:200:GLU:HG3	1.68	0.75
1:J:9091:TRP:CE2	1:J:9094:ARG:HD2	2.22	0.74
1:P:5007:ILE:HG22	1:P:5078:VAL:HB	1.69	0.74
1:N:3121:PRO:HA	1:N:3124:MET:HG3	1.67	0.74
1:P:5016:LEU:HD21	1:P:5021:LEU:HG	1.68	0.74
1:R:7119:PHE:CZ	1:R:7121:PRO:HG3	2.22	0.74
1:N:3093:MET:HA	1:N:3093:MET:HE2	1.70	0.73
1:A:16:LEU:HD21	1:A:21:LEU:HD21	1.71	0.73
1:Q:6101:MET:HE3	1:Q:6106:ILE:CD1	2.12	0.73
1:T:9066:ILE:HD11	2:T:9201:FMN:C4A	2.17	0.73
1:M:2091:TRP:CH2	1:M:2140:SER:HB2	2.23	0.73
1:Q:6010:SER:O	1:Q:6047:MET:HE3	1.87	0.73
1:I:8025:MET:O	1:I:8029:GLU:HG3	1.88	0.73
1:A:125:THR:HG22	1:F:5001:MET:HE1	1.71	0.72
1:H:7090:ASN:ND2	1:H:7141:GLN:NE2	2.34	0.72
1:G:6095:LEU:HD21	1:G:6097:GLN:HG3	1.70	0.72
1:M:2091:TRP:HH2	1:M:2140:SER:HB2	1.53	0.72
1:N:3006:LEU:HD12	1:N:3007:ILE:N	2.05	0.71
1:C:2091:TRP:CH2	1:C:2140:SER:HB2	2.25	0.71
1:Q:6001:MET:HE3	1:Q:6001:MET:N	2.05	0.71
1:B:1076:GLU:OE1	1:B:1122:ARG:NH1	2.24	0.71
1:G:6017:SER:OG	1:G:6019:PRO:HG2	1.90	0.71
1:A:28:SER:HB3	1:A:93:MET:HG2	1.72	0.71
1:O:4066:ILE:HG22	1:O:4072:HIS:CE1	2.25	0.71
1:S:8001:MET:HA	1:S:8001:MET:CE	2.21	0.71



Atom_1	Atom_2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:125:THR:HG22	1:F:5001:MET:CE	2.20	0.70
1:D:3000:HIS:O	1:D:3001:MET:HB2	1.91	0.70
1:M:2093:MET:HA	1:M:2093:MET:HE2	1.73	0.70
1:I:8101:MET:HG2	1:I:8106:ILE:HD11	1.72	0.70
1:P:5017:SER:CB	1:P:5019:PRO:HD2	2.19	0.70
1:C:2021:LEU:HD13	1:C:2095:LEU:HD21	1.75	0.69
1:O:4007:ILE:HG22	1:O:4078:VAL:HB	1.75	0.69
1:H:7021:LEU:HD13	1:H:7095:LEU:HD21	1.75	0.69
1:M:2041:LEU:CD1	1:M:2050:GLN:HB2	2.22	0.69
1:Q:6125:THR:H	1:Q:6128:GLN:NE2	1.90	0.69
1:J:9076:GLU:HG3	1:J:9122:ARG:NH1	2.08	0.69
1:N:3084:GLU:OE2	1:0:4127:GLU:CG	2.41	0.69
1:R:7110:ARG:O	1:R:7114:SER:HB3	1.93	0.69
1:M:2091:TRP:CE3	1:M:2094:ARG:CB	2.76	0.69
1:H:7076:GLU:OE1	1:H:7122:ARG:NH1	2.26	0.68
1:M:2017:SER:O	1:M:2021:LEU:HD12	1.92	0.68
1:O:4095:LEU:HD23	1:O:4096:VAL:N	2.08	0.68
1:L:1041:LEU:HD11	1:L:1048:PHE:HD1	1.58	0.68
1:L:1057:GLN:NE2	1:L:1061:GLU:OE2	2.26	0.68
1:M:2069:ASP:OD1	1:M:2071:ARG:HG3	1.92	0.68
1:P:5066:ILE:HG22	1:P:5072:HIS:HE1	1.57	0.68
1:G:6028:SER:HB3	1:G:6093:MET:HG2	1.76	0.67
1:R:7040:MET:HE2	1:R:7094:ARG:HB3	1.75	0.67
1:R:7041:LEU:HD12	1:R:7042:CYS:N	2.08	0.67
1:F:5090:ASN:ND2	1:F:5141:GLN:HE22	1.93	0.67
1:C:2091:TRP:HH2	1:C:2140:SER:HB2	1.58	0.67
1:M:2021:LEU:HD23	1:M:2095:LEU:HD11	1.75	0.67
1:O:4008:PHE:CE1	1:O:4050:GLN:HB3	2.29	0.67
1:G:6024:ILE:HG13	1:G:6071:ARG:NH1	2.10	0.66
1:O:4040:MET:HE3	1:O:4137:TYR:HB2	1.77	0.66
1:O:4066:ILE:HG22	1:O:4072:HIS:HE1	1.60	0.66
1:O:4041:LEU:N	1:O:4093:MET:HE1	2.11	0.65
1:P:5055:ASP:HB3	1:P:5058:LYS:HG2	1.78	0.65
1:P:5033:LEU:HD13	1:P:5033:LEU:O	1.96	0.65
1:T:9003:LEU:HD21	1:T:9086:ARG:HG3	1.76	0.65
1:A:40:MET:HE2	1:A:133:LEU:HD22	1.79	0.65
1:M:2055:ASP:O	1:M:2059:VAL:HG23	1.97	0.65
1:M:2091:TRP:CH2	1:M:2140:SER:CB	2.75	0.65
1:M:2024:ILE:HG13	1:M:2071:ARG:HH21	1.62	0.65
1:Q:6076:GLU:HG3	1:Q:6122:ARG:NH1	2.12	0.65
1:T:9135:GLU:O	1:T:9139:MET:HG3	1.97	0.64



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:I:8025:MET:HE1	1:I:8093:MET:C	2.18	0.64
1:L:1041:LEU:HD11	1:L:1048:PHE:CD1	2.33	0.64
1:T:9037:ILE:CG2	1:T:9052:LEU:HD12	2.28	0.64
1:M:2063:TYR:CE2	1:M:2067:LEU:HD11	2.33	0.64
1:L:1025:MET:SD	1:L:1095:LEU:HB2	2.37	0.64
1:N:3009:LEU:HD22	1:N:3121:PRO:HB2	1.79	0.64
1:B:1025:MET:CE	1:B:1093:MET:HG3	2.28	0.64
1:E:4090:ASN:ND2	1:E:4141:GLN:OE1	2.31	0.64
1:E:4116:ALA:CB	1:E:4120:GLN:HG3	2.28	0.64
1:F:5041:LEU:CB	1:F:5093:MET:HE1	2.28	0.64
1:E:4125:THR:HG22	1:J:9001:MET:HE1	1.80	0.63
1:J:9097:GLN:HB2	1:J:9100:GLU:HG3	1.79	0.63
1:J:9101:MET:CE	1:J:9106:ILE:HD11	2.28	0.63
1:K:116:LEU:HD21	1:K:121:LEU:HD21	1.81	0.63
1:D:3009:LEU:HD22	1:D:3121:PRO:HB2	1.81	0.63
1:S:8045:ASN:O	1:S:8045:ASN:OD1	2.17	0.63
1:B:1025:MET:O	1:B:1029:GLU:HG3	1.97	0.62
1:S:8018:TYR:N	1:S:8019:PRO:HD2	2.14	0.62
1:J:9098:LEU:HA	1:J:9101:MET:HE2	1.81	0.62
1:J:9013:THR:HG22	1:J:9073:HIS:HD2	1.65	0.62
1:T:9069:ASP:OD1	1:T:9070:PRO:HD2	1.99	0.62
1:O:4069:ASP:OD1	1:O:4071:ARG:HG3	1.99	0.62
1:L:1025:MET:HA	1:L:1025:MET:CE	2.29	0.61
1:R:7127:GLU:OE1	1:R:7127:GLU:HA	1.99	0.61
1:P:5066:ILE:HD11	2:P:5201:FMN:C4A	2.30	0.61
1:L:1110:ARG:HD2	1:L:1118:THR:C	2.20	0.61
1:S:8091:TRP:CE3	1:S:8094:ARG:CB	2.84	0.61
1:A:125:THR:CG2	1:F:5001:MET:HE1	2.30	0.61
1:T:9066:ILE:HD11	2:T:9201:FMN:N5	2.15	0.61
1:J:9091:TRP:CD2	1:J:9094:ARG:HD2	2.36	0.61
1:D:3025:MET:HE1	1:D:3093:MET:HG3	1.83	0.60
1:J:9027:LYS:HE2	2:J:9201:FMN:P	2.41	0.60
1:Q:6063:TYR:CE2	1:Q:6067:LEU:HD11	2.35	0.60
1:S:8111:LEU:O	1:T:9086:ARG:HD2	2.02	0.60
1:T:9037:ILE:HG21	1:T:9052:LEU:HD12	1.82	0.60
1:H:7108:ARG:HD3	1:I:8090:ASN:OD1	2.01	0.60
1:T:9003:LEU:HD11	1:T:9086:ARG:HE	1.66	0.60
1:E:4116:ALA:HB1	1:E:4120:GLN:HG3	1.83	0.60
1:M:2091:TRP:HH2	1:M:2140:SER:HB3	1.66	0.60
1:P:5093:MET:HE2	1:P:5093:MET:HA	1.82	0.60
1:R:7041:LEU:N	1:R:7093:MET:HE1	2.16	0.60



Atom-1	Atom-2	Interatomic	Clash
	1100111-2	distance (Å)	overlap (Å)
1:O:4051:THR:HG21	1:O:4088:PHE:CE2	2.37	0.60
1:C:2073:HIS:ND1	1:C:2074:SER:OG	2.28	0.60
1:M:2051:THR:O	1:M:2052:LEU:HD23	2.03	0.59
1:B:1125:THR:H	1:B:1128:GLN:NE2	2.00	0.59
1:J:9101:MET:CE	1:J:9106:ILE:CD1	2.79	0.59
1:M:2024:ILE:CG1	1:M:2071:ARG:HH21	2.15	0.59
1:L:1041:LEU:HD12	1:L:1042:CYS:N	2.17	0.59
1:N:3097:GLN:HB2	1:N:3100:GLU:HG3	1.83	0.59
1:O:4109:LEU:HG	1:O:4132:PHE:CE1	2.37	0.59
1:J:9027:LYS:HE2	2:J:9201:FMN:O3P	2.03	0.59
1:K:124:ILE:HG13	1:K:171:ARG:NH1	2.17	0.59
1:O:4091:TRP:CE3	1:O:4094:ARG:CB	2.86	0.59
1:P:5066:ILE:HG22	1:P:5072:HIS:CE1	2.38	0.59
1:C:2050:GLN:NE2	1:C:2052:LEU:HD21	2.17	0.58
1:T:9091:TRP:CD2	1:T:9094:ARG:HD2	2.37	0.58
1:C:2017:SER:HB2	1:C:2019:PRO:HD2	1.84	0.58
2:L:1201:FMN:O4'	2:L:1201:FMN:N1	2.36	0.58
1:M:2062:THR:O	1:M:2066:ILE:HG13	2.03	0.58
1:O:4032:ASN:HB3	1:O:4037:ILE:O	2.04	0.58
1:O:4023:ASP:HB3	1:O:4071:ARG:HH12	1.68	0.58
1:G:6011:CYS:SG	1:G:6122:ARG:NH2	2.77	0.58
1:S:8013:THR:HG22	1:S:8073:HIS:HD2	1.68	0.58
1:L:1040:MET:CE	1:L:1094:ARG:HG2	2.33	0.58
1:O:4066:ILE:HD11	2:O:4201:FMN:C4A	2.32	0.58
1:C:2027:LYS:CE	2:C:2201:FMN:H5'2	2.30	0.58
1:B:1098:LEU:HD13	1:B:1106:ILE:HD11	1.85	0.57
1:P:5072:HIS:ND1	2:P:5201:FMN:HM82	2.19	0.57
1:H:7017:SER:OG	1:H:7019:PRO:HD2	2.04	0.57
1:H:7043:TYR:HD1	1:H:7048:PHE:CE1	2.22	0.57
1:C:2084:GLU:OE1	1:D:3131:ARG:NH2	2.37	0.57
1:J:9076:GLU:HG3	1:J:9122:ARG:HH12	1.69	0.57
1:S:8020:ASP:O	1:S:8024:ILE:HG13	2.04	0.57
1:B:1006:LEU:HB2	1:B:1080:PHE:HD1	1.69	0.57
1:O:4011:CYS:SG	1:O:4047:MET:CE	2.92	0.57
1:R:7066:ILE:HG22	1:R:7072:HIS:CE1	2.40	0.57
1:S:8057:GLN:NE2	1:S:8061:GLU:OE2	2.38	0.57
1:S:8045:ASN:HD22	1:S:8118:THR:HB	1.69	0.57
1:C:2104:ASP:HB3	1:C:2108:ARG:HH11	1.69	0.57
1:K:227:GLU:O	1:K:231:ARG:HG2	2.04	0.57
1:N:3091:TRP:HH2	1:N:3140:SER:HB3	1.69	0.57
1:S:8093:MET:HE2	1:S:8093:MET:HA	1.87	0.57



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:N:3050:GLN:HE21	1:N:3052:LEU:HD21	1.69	0.57
1:N:3057:GLN:HG3	1:S:8076:GLU:OE2	2.05	0.57
1:O:4095:LEU:HD22	1:O:4097:GLN:HG3	1.87	0.56
1:F:5041:LEU:HD23	1:F:5095:LEU:HD13	1.86	0.56
1:D:3025:MET:CE	1:D:3093:MET:HG3	2.35	0.56
1:Q:6026:ALA:O	1:Q:6030:VAL:HG23	2.06	0.56
1:F:5097:GLN:HB2	1:F:5100:GLU:HG3	1.86	0.56
1:S:8001:MET:CE	1:S:8001:MET:CA	2.83	0.56
1:E:4009:LEU:HD12	1:E:4009:LEU:C	2.25	0.56
1:A:28:SER:CB	1:A:93:MET:HG2	2.36	0.56
1:E:4127:GLU:HA	1:E:4127:GLU:OE1	2.05	0.56
1:O:4110:ARG:HD2	1:O:4118:THR:C	2.26	0.56
1:B:1018:TYR:N	1:B:1019:PRO:HD2	2.21	0.56
1:E:4084:GLU:OE1	1:F:5127:GLU:HG2	2.05	0.56
1:J:9041:LEU:CD1	1:J:9050:GLN:HB2	2.36	0.55
1:O:4040:MET:HA	1:O:4093:MET:HE3	1.89	0.55
1:B:1101:MET:HE2	1:B:1106:ILE:HB	1.89	0.55
1:L:1069:ASP:OD1	1:L:1071:ARG:HG3	2.06	0.55
1:S:8001:MET:HE2	1:S:8001:MET:CA	2.28	0.55
1:T:9017:SER:O	1:T:9020:ASP:HB2	2.06	0.55
1:C:2025:MET:CE	1:C:2095:LEU:HB2	2.36	0.55
1:G:6016:LEU:HD21	1:G:6021:LEU:CD1	2.36	0.55
1:O:4086:ARG:NH2	1:P:5115:PRO:HA	2.22	0.55
1:R:7093:MET:HE3	1:R:7094:ARG:H	1.70	0.55
1:J:9013:THR:HG23	1:J:9072:HIS:HA	1.89	0.55
1:K:193:MET:HE2	1:K:193:MET:HA	1.88	0.55
1:N:3112:LYS:HE2	1:N:3113:TYR:OH	2.06	0.55
1:P:5066:ILE:CG2	1:P:5072:HIS:HE1	2.20	0.54
1:K:110:SER:O	1:K:147:MET:HE3	2.07	0.54
1:L:1110:ARG:HD2	1:L:1118:THR:O	2.06	0.54
1:L:1110:ARG:O	1:L:1110:ARG:HG2	2.06	0.54
1:M:2095:LEU:HD21	1:M:2097:GLN:HG3	1.88	0.54
1:C:2104:ASP:HB3	1:C:2108:ARG:NH1	2.22	0.54
1:O:4040:MET:HE1	1:O:4137:TYR:HB2	1.87	0.54
1:R:7102:ASP:HB3	1:R:7105:THR:HB	1.90	0.54
1:B:1025:MET:HE1	1:B:1093:MET:HG3	1.89	0.54
1:C:2005:ARG:HB2	1:C:2083:ILE:HD13	1.88	0.54
1:D:3090:ASN:ND2	1:E:4108:ARG:HD2	2.23	0.54
1:L:1032:ASN:ND2	1:L:1093:MET:HG2	2.23	0.54
1:F:5062:THR:O	1:F:5066:ILE:HG13	2.07	0.54
1:O:4024:ILE:HG13	1:O:4071:ARG:NH2	2.23	0.54



Atom_1	Atom_2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:Q:6097:GLN:O	1:Q:6100:GLU:HG2	2.08	0.54
1:H:7023:ASP:OD2	1:H:7027:LYS:HE3	2.09	0.53
1:A:76:GLU:HG3	1:A:122:ARG:NH1	2.23	0.53
1:B:1074:SER:O	1:B:1122:ARG:NH2	2.41	0.53
1:E:4017:SER:OG	1:E:4019:PRO:HD2	2.08	0.53
1:H:7041:LEU:HD13	1:H:7050:GLN:HE21	1.72	0.53
1:L:1011:CYS:HB2	1:L:1073:HIS:CE1	2.43	0.53
1:L:1024:ILE:HG13	1:L:1071:ARG:HH21	1.74	0.53
1:P:5098:LEU:HD12	1:P:5119:PHE:CD2	2.43	0.53
1:G:6093:MET:HA	1:G:6093:MET:HE2	1.90	0.53
1:L:1050:GLN:NE2	1:L:1052:LEU:HD21	2.24	0.53
1:M:2021:LEU:CD2	1:M:2095:LEU:HD11	2.37	0.53
1:A:127:GLU:HG2	1:G:6084:GLU:OE1	2.08	0.53
1:H:7016:LEU:HD21	1:H:7021:LEU:HD21	1.90	0.53
1:H:7062:THR:O	1:H:7066:ILE:HG13	2.09	0.53
1:P:5062:THR:O	1:P:5066:ILE:HG12	2.09	0.53
1:N:3105:THR:HG22	1:N:3106:ILE:HD13	1.91	0.53
1:O:4035:ASP:OD1	1:O:4035:ASP:N	2.40	0.53
1:R:7095:LEU:CD2	1:R:7097:GLN:HG3	2.36	0.53
1:E:4069:ASP:OD1	1:E:4070:PRO:HD2	2.09	0.52
1:J:9041:LEU:HD13	1:J:9050:GLN:HB2	1.91	0.52
1:F:5028:SER:HB3	1:F:5093:MET:HG3	1.91	0.52
1:Q:6009:LEU:HD12	1:Q:6009:LEU:C	2.28	0.52
1:R:7041:LEU:HD11	1:R:7048:PHE:CD1	2.44	0.52
1:N:3026:ALA:O	1:N:3030:VAL:HG23	2.10	0.52
1:O:4093:MET:HE3	1:O:4094:ARG:H	1.75	0.52
1:R:7040:MET:C	1:R:7093:MET:HE1	2.30	0.52
1:S:8017:SER:OG	1:S:8019:PRO:HG2	2.08	0.52
1:N:3069:ASP:OD2	1:N:3071:ARG:HB2	2.09	0.52
1:K:101:MET:CB	1:O:4001:MET:HB2	2.40	0.52
1:N:3025:MET:HE1	1:N:3094:ARG:C	2.29	0.52
1:Q:6041:LEU:HD11	1:Q:6048:PHE:HD1	1.69	0.52
1:Q:6076:GLU:HG3	1:Q:6122:ARG:HH12	1.75	0.52
1:D:3021:LEU:HD13	1:D:3095:LEU:HD21	1.92	0.51
1:E:4104:ASP:O	1:E:4108:ARG:HG3	2.10	0.51
1:G:6038:THR:HB	1:G:6088:PHE:O	2.10	0.51
1:H:7009:LEU:HD22	1:H:7121:PRO:HB2	1.92	0.51
1:K:125:MET:SD	1:K:195:LEU:HB2	2.51	0.51
1:O:4027:LYS:NZ	1:O:4027:LYS:HB3	2.24	0.51
1:B:1017:SER:OG	1:B:1019:PRO:HG2	2.11	0.51
1:G:6069:ASP:HB2	2:G:6201:FMN:O2'	2.11	0.51



Atom_1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:G:6038:THR:HA	1:G:6092:SER:HA	1.93	0.51
1:N:3050:GLN:OE1	2:N:3201:FMN:H6	2.11	0.51
1:O:4024:ILE:HG12	2:O:4201:FMN:C9	2.40	0.51
1:R:7041:LEU:N	1:R:7093:MET:CE	2.74	0.51
1:M:2038:THR:HG23	1:M:2086:ARG:NH1	2.26	0.51
1:N:3089:ILE:HD11	1:O:4112:LYS:HG3	1.91	0.51
1:I:8135:GLU:O	1:I:8139:MET:HG2	2.11	0.51
1:M:2098:LEU:HA	1:M:2101:MET:HE2	1.93	0.51
1:I:8127:GLU:OE1	1:I:8131:ARG:HD2	2.10	0.51
1:S:8108:ARG:HD2	1:T:9089:ILE:HG22	1.93	0.51
1:E:4025:MET:CE	1:E:4093:MET:HG3	2.41	0.50
1:L:1028:SER:HB3	1:L:1093:MET:CG	2.41	0.50
1:P:5050:GLN:NE2	1:P:5093:MET:SD	2.84	0.50
1:R:7069:ASP:HB2	2:R:7201:FMN:O2'	2.11	0.50
1:S:8042:CYS:SG	1:S:8098:LEU:HD13	2.52	0.50
1:S:8135:GLU:O	1:S:8139:MET:HG3	2.12	0.50
1:M:2017:SER:CB	1:M:2019:PRO:HD2	2.41	0.50
1:H:7101:MET:HB2	1:H:7106:ILE:HG13	1.93	0.50
1:L:1009:LEU:HD12	1:L:1009:LEU:C	2.32	0.50
1:S:8042:CYS:SG	1:S:8098:LEU:HD22	2.51	0.50
1:L:1094:ARG:HG3	1:L:1095:LEU:N	2.26	0.50
1:R:7127:GLU:HG3	1:S:8084:GLU:OE1	2.12	0.50
1:C:2135:GLU:O	1:C:2139:MET:HG3	2.12	0.50
1:F:5069:ASP:HB2	2:F:5201:FMN:O2'	2.11	0.50
1:K:202:ASP:O	1:K:206:ILE:HG22	2.12	0.50
1:C:2093:MET:HA	1:C:2093:MET:HE2	1.93	0.50
1:J:9027:LYS:HD2	2:J:9201:FMN:H5'2	1.92	0.50
1:N:3091:TRP:CH2	1:N:3140:SER:HB3	2.45	0.50
1:A:50:GLN:OE1	2:A:201:FMN:H6	2.12	0.50
1:D:3020:ASP:O	1:D:3024:ILE:HG13	2.12	0.50
1:M:2113:TYR:O	1:M:2124:MET:HG2	2.11	0.50
1:I:8025:MET:SD	1:I:8093:MET:HG3	2.52	0.50
1:M:2109:LEU:CD1	1:M:2135:GLU:OE1	2.60	0.50
1:O:4080:PHE:CD2	1:T:9077:ILE:HG22	2.47	0.50
1:P:5021:LEU:HD23	1:P:5024:ILE:HD12	1.92	0.50
1:T:9101:MET:HE2	1:T:9106:ILE:HB	1.94	0.50
1:A:43:TYR:HD2	1:A:48:PHE:CE1	2.30	0.49
1:C:2001:MET:HE1	1:H:7125:THR:HG22	1.94	0.49
1:P:5034:ARG:HG3	1:P:5035:ASP:OD1	2.11	0.49
1:M:2001:MET:HB3	1:S:8001:MET:CE	2.42	0.49
1:M:2135:GLU:O	1:M:2139:MET:HG3	2.12	0.49



Atom-1	Atom-2	Interatomic	Clash
		distance (Å)	overlap (Å)
1:O:4040:MET:HE1	1:O:4137:TYR:HA	1.94	0.49
1:O:4072:HIS:C	1:O:4072:HIS:CD2	2.85	0.49
1:C:2079:GLU:OE2	1:C:2081:LYS:HE2	2.12	0.49
1:L:1016:LEU:HD21	1:L:1021:LEU:HD13	1.94	0.49
1:M:2005:ARG:HB2	1:M:2083:ILE:HD13	1.94	0.49
1:D:3057:GLN:HA	1:I:8076:GLU:HG2	1.95	0.49
1:Q:6018:TYR:N	1:Q:6019:PRO:HD2	2.28	0.49
1:M:2091:TRP:CH2	1:M:2140:SER:HB3	2.45	0.49
1:N:3027:LYS:HD2	2:N:3201:FMN:H5'2	1.93	0.49
1:N:3097:GLN:CB	1:N:3100:GLU:HG3	2.42	0.49
1:P:5093:MET:HG3	1:P:5094:ARG:N	2.26	0.49
1:F:5017:SER:HB2	1:F:5019:PRO:HD2	1.95	0.49
1:A:25:MET:HA	1:A:25:MET:HE3	1.94	0.49
1:I:8025:MET:HE1	1:I:8094:ARG:N	2.28	0.49
1:J:9102:ASP:HB3	1:J:9105:THR:HB	1.94	0.49
1:L:1097:GLN:HB2	1:L:1100:GLU:HG3	1.94	0.49
1:S:8013:THR:HG21	1:S:8070:PRO:O	2.12	0.49
1:K:210:ARG:NH1	1:K:217:ALA:O	2.46	0.48
1:S:8029:GLU:O	1:S:8033:LEU:HB2	2.12	0.48
1:O:4095:LEU:CD2	1:O:4097:GLN:HG3	2.43	0.48
1:P:5045:ASN:O	1:P:5045:ASN:ND2	2.46	0.48
1:T:9024:ILE:HD11	2:T:9201:FMN:HM83	1.94	0.48
1:F:5032:ASN:ND2	1:F:5093:MET:HG2	2.28	0.48
1:M:2032:ASN:HB3	1:M:2037:ILE:O	2.13	0.48
1:O:4110:ARG:HD2	1:O:4119:PHE:N	2.28	0.48
1:Q:6125:THR:H	1:Q:6128:GLN:HE21	1.61	0.48
1:K:169:ASP:OD1	1:K:170:PRO:HD2	2.12	0.48
1:M:2069:ASP:HB2	2:M:2201:FMN:O2'	2.13	0.48
1:M:2093:MET:HA	1:M:2093:MET:CE	2.42	0.48
1:O:4066:ILE:HD11	2:O:4201:FMN:C10	2.42	0.48
1:M:2021:LEU:HD23	1:M:2095:LEU:CD1	2.42	0.48
1:O:4040:MET:HE1	1:0:4137:TYR:CB	2.44	0.48
1:R:7119:PHE:CE2	1:R:7121:PRO:HG3	2.47	0.48
1:B:1009:LEU:HD22	1:B:1121:PRO:HB2	1.96	0.48
1:N:3110:ARG:HD3	1:N:3118:THR:O	2.13	0.48
1:P:5050:GLN:OE1	2:P:5201:FMN:H6	2.13	0.48
1:K:174:SER:HB3	1:K:222:ARG:HH22	1.78	0.48
1:A:17:SER:O	1:A:20:ASP:HB2	2.14	0.48
1:H:7043:TYR:CD1	1:H:7048:PHE:CE1	3.01	0.48
1:K:195:LEU:HD21	1:K:197:GLN:HG2	1.96	0.48
1:L:1050:GLN:OE1	2:L:1201:FMN:H6	2.14	0.48



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:M:2112:LYS:HD3	1:M:2113:TYR:CZ	2.48	0.48
1:F:5041:LEU:HD23	1:F:5095:LEU:CD1	2.43	0.48
1:N:3091:TRP:CE3	1:N:3094:ARG:CB	2.96	0.48
1:O:4018:TYR:O	1:O:4021:LEU:HB2	2.14	0.48
1:P:5009:LEU:HD22	1:P:5121:PRO:HB2	1.95	0.48
1:P:5025:MET:HE3	1:P:5025:MET:O	2.14	0.48
1:S:8110:ARG:O	1:S:8114:SER:HB3	2.14	0.48
1:C:2038:THR:HB	1:C:2088:PHE:O	2.13	0.47
1:C:2069:ASP:HB2	2:C:2201:FMN:O2'	2.14	0.47
1:O:4035:ASP:HB3	1:O:4058:LYS:CG	2.40	0.47
1:O:4018:TYR:HB3	1:O:4019:PRO:HD3	1.96	0.47
1:A:25:MET:SD	1:A:95:LEU:HB2	2.54	0.47
1:C:2093:MET:HA	1:C:2093:MET:CE	2.44	0.47
1:P:5066:ILE:HD12	2:P:5201:FMN:C5A	2.45	0.47
1:T:9017:SER:OG	1:T:9019:PRO:HD2	2.14	0.47
1:B:1006:LEU:HB2	1:B:1080:PHE:CD1	2.48	0.47
1:R:7018:TYR:HB3	1:R:7019:PRO:HD3	1.96	0.47
1:C:2055:ASP:O	1:C:2059:VAL:HG23	2.14	0.47
1:M:2127:GLU:HA	1:M:2127:GLU:OE1	2.14	0.47
1:N:3017:SER:O	1:N:3020:ASP:HB2	2.14	0.47
1:N:3040:MET:CE	1:N:3091:TRP:HZ3	2.28	0.47
1:S:8045:ASN:ND2	1:S:8118:THR:HB	2.28	0.47
1:T:9093:MET:HE2	1:T:9093:MET:CA	2.31	0.47
1:I:8003:LEU:HG	1:I:8083:ILE:HD11	1.96	0.47
1:H:7050:GLN:HE22	2:H:7201:FMN:H6	1.80	0.47
1:J:9091:TRP:CZ2	1:J:9094:ARG:HD2	2.48	0.47
1:N:3021:LEU:HA	1:N:3024:ILE:HD12	1.95	0.47
1:O:4037:ILE:HA	1:O:4053:GLU:O	2.14	0.47
1:O:4038:THR:HA	1:O:4092:SER:HA	1.97	0.47
1:Q:6112:LYS:HD3	1:Q:6113:TYR:CE2	2.50	0.47
1:S:8005:ARG:HB2	1:S:8083:ILE:HD13	1.96	0.47
1:B:1057:GLN:HG3	1:G:6076:GLU:OE2	2.15	0.47
1:L:1050:GLN:HG2	1:L:1051:THR:N	2.29	0.47
1:M:2086:ARG:NH2	1:N:3115:PRO:HA	2.29	0.47
1:T:9007:ILE:CG2	1:T:9078:VAL:HB	2.33	0.47
1:T:9016:LEU:HD22	1:T:9016:LEU:HA	1.73	0.47
1:T:9091:TRP:CE3	1:T:9094:ARG:HD3	2.50	0.47
1:E:4057:GLN:HG3	1:J:9076:GLU:OE2	2.15	0.47
1:G:6005:ARG:HB2	1:G:6083:ILE:HD13	1.96	0.47
1:P:5069:ASP:OD1	1:P:5071:ARG:HB2	2.15	0.47
1:A:40:MET:CE	1:A:133:LEU:HD22	2.45	0.47



Atom-1	Atom 2	Interatomic	Clash
	Atom-2	distance (Å)	overlap (Å)
1:E:4012:ALA:HB1	1:E:4016:LEU:HD22	1.97	0.47
1:G:6028:SER:CB	1:G:6093:MET:HG2	2.45	0.47
1:C:2017:SER:H	1:C:2020:ASP:HB2	1.80	0.46
1:O:4062:THR:O	1:O:4066:ILE:HG12	2.14	0.46
1:Q:6028:SER:HB3	1:Q:6093:MET:HG2	1.96	0.46
1:K:156:ARG:HG3	1:K:180:PHE:CE2	2.50	0.46
1:M:2101:MET:HE3	1:M:2106:ILE:HG13	1.97	0.46
1:S:8013:THR:HG23	1:S:8072:HIS:CA	2.46	0.46
1:H:7017:SER:CB	1:H:7019:PRO:HD2	2.45	0.46
1:L:1024:ILE:CG1	1:L:1071:ARG:HH21	2.27	0.46
1:L:1024:ILE:HD11	1:L:1071:ARG:HE	1.81	0.46
1:N:3093:MET:HE2	1:N:3093:MET:CA	2.40	0.46
1:P:5093:MET:HE3	1:P:5093:MET:HB2	1.83	0.46
1:R:7079:GLU:CD	1:R:7081:LYS:HE2	2.35	0.46
1:T:9050:GLN:HE22	2:T:9201:FMN:H6	1.81	0.46
1:N:3084:GLU:OE2	1:O:4127:GLU:HG2	2.16	0.46
1:A:40:MET:SD	1:A:137:TYR:HB2	2.56	0.46
1:I:8076:GLU:HG3	1:I:8122:ARG:NH1	2.30	0.46
1:K:106:LEU:HB2	1:K:180:PHE:HD1	1.80	0.46
1:P:5021:LEU:HA	1:P:5024:ILE:HD12	1.97	0.46
1:R:7028:SER:CB	1:R:7093:MET:HG2	2.46	0.46
1:O:4106:ILE:HD12	1:O:4106:ILE:HA	1.75	0.46
1:S:8037:ILE:HG21	1:S:8052:LEU:HD22	1.98	0.46
1:C:2094:ARG:HE	1:C:2094:ARG:HB2	1.35	0.46
1:E:4118:THR:O	1:E:4120:GLN:HG2	2.16	0.46
1:L:1094:ARG:HE	1:L:1094:ARG:HB2	1.53	0.46
1:S:8098:LEU:HD11	1:S:8136:LEU:HD11	1.98	0.46
1:A:18:TYR:N	1:A:19:PRO:HD2	2.31	0.46
1:H:7055:ASP:O	1:H:7059:VAL:HG23	2.16	0.46
1:N:3112:LYS:HE2	1:N:3113:TYR:CZ	2.51	0.46
1:Q:6017:SER:OG	1:Q:6019:PRO:HG2	2.16	0.46
1:D:3021:LEU:HD23	1:D:3021:LEU:HA	1.56	0.45
1:M:2009:LEU:HD12	1:M:2009:LEU:C	2.37	0.45
1:C:2017:SER:O	1:C:2020:ASP:HB2	2.16	0.45
1:O:4043:TYR:O	1:O:4097:GLN:HA	2.16	0.45
1:D:3041:LEU:HD12	1:D:3042:CYS:N	2.32	0.45
1:B:1042:CYS:SG	1:B:1098:LEU:HD21	2.57	0.45
1:M:2089:ILE:HD11	1:N:3112:LYS:HG3	1.97	0.45
1:E:4069:ASP:OD1	1:E:4071:ARG:HB2	2.16	0.45
1:L:1025:MET:HA	1:L:1025:MET:HE3	1.97	0.45
1:M:2098:LEU:HA	1:M:2101:MET:CE	2.47	0.45



Atom-1	Atom 2	Interatomic	Clash
	Atom-2	distance (\AA)	overlap (Å)
1:Q:6025:MET:CE	1:Q:6093:MET:HG3	2.47	0.45
1:E:4010:SER:O	1:E:4047:MET:HE3	2.17	0.45
1:J:9013:THR:HG23	1:J:9072:HIS:CA	2.47	0.45
1:K:103:LEU:HD21	1:K:186:ARG:HG3	1.98	0.45
1:O:4098:LEU:H	1:O:4098:LEU:HG	1.31	0.45
1:G:6017:SER:O	1:G:6020:ASP:HB2	2.17	0.45
1:K:116:LEU:HD21	1:K:121:LEU:CD2	2.46	0.45
1:A:91:TRP:CD2	1:A:94:ARG:HD3	2.52	0.45
1:M:2063:TYR:HE2	1:M:2067:LEU:HD11	1.78	0.45
1:I:8076:GLU:HG3	1:I:8122:ARG:HH12	1.81	0.45
1:L:1006:LEU:HB2	1:L:1080:PHE:HD1	1.82	0.45
1:M:2086:ARG:HG3	1:N:3111:LEU:O	2.17	0.45
1:N:3025:MET:CE	1:N:3095:LEU:N	2.80	0.45
1:0:4011:CYS:SG	1:O:4047:MET:HE1	2.57	0.45
1:R:7041:LEU:HD12	1:R:7041:LEU:C	2.38	0.45
1:B:1107:ARG:HE	1:B:1107:ARG:HB3	1.67	0.44
1:F:5009:LEU:O	1:F:5075:ALA:HA	2.18	0.44
1:I:8047:MET:HG3	1:I:8121:PRO:HD2	1.99	0.44
1:M:2008:PHE:HE1	1:M:2050:GLN:HE21	1.65	0.44
1:C:2025:MET:HE3	1:C:2095:LEU:HB2	1.97	0.44
1:F:5091:TRP:CD2	1:F:5094:ARG:HD3	2.52	0.44
1:I:8050:GLN:OE1	2:I:8201:FMN:H6	2.17	0.44
1:K:111:CYS:HB3	1:K:173:HIS:CE1	2.52	0.44
1:G:6016:LEU:HD21	1:G:6021:LEU:HD11	1.98	0.44
1:G:6110:ARG:HD3	1:G:6118:THR:C	2.38	0.44
1:O:4007:ILE:CG2	1:O:4078:VAL:HB	2.45	0.44
1:S:8110:ARG:NH2	1:S:8117:ALA:O	2.51	0.44
1:A:102:ASP:C	1:A:104:ASP:N	2.70	0.44
1:D:3003:LEU:HD21	1:D:3086:ARG:HG2	1.99	0.44
1:F:5032:ASN:HD22	1:F:5093:MET:HG2	1.83	0.44
1:F:5078:VAL:CG1	1:F:5126:ALA:HA	2.47	0.44
1:G:6041:LEU:HD13	1:G:6050:GLN:HB2	1.99	0.44
1:R:7066:ILE:CG2	1:R:7072:HIS:CE1	3.01	0.44
1:B:1025:MET:SD	1:B:1095:LEU:HB2	2.57	0.44
1:F:5065:ARG:HA	1:F:5068:LYS:HE3	2.00	0.44
2:I:8201:FMN:H1'1	2:I:8201:FMN:H9	1.76	0.44
1:K:222:ARG:NH1	1:P:5057:GLN:HE21	2.16	0.44
1:O:4066:ILE:CD1	2:O:4201:FMN:C10	2.96	0.44
1:C:2024:ILE:HD13	2:C:2201:FMN:HM83	2.00	0.44
1:K:156:ARG:HG3	1:K:180:PHE:CZ	2.53	0.44
1:B:1001:MET:CE	1:G:6125:THR:HG22	2.48	0.43


Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:B:1025:MET:HE3	1:B:1093:MET:HG3	1.99	0.43
1:I:8025:MET:SD	1:I:8095:LEU:HB2	2.58	0.43
1:M:2101:MET:HB3	1:M:2106:ILE:HG12	2.00	0.43
1:S:8013:THR:HG23	1:S:8072:HIS:HA	2.00	0.43
1:H:7122:ARG:HG2	1:H:7122:ARG:HH11	1.82	0.43
1:L:1025:MET:CE	1:L:1025:MET:CA	2.96	0.43
1:L:1080:PHE:CD2	1:Q:6077:ILE:HG22	2.54	0.43
1:N:3043:TYR:HD1	1:N:3048:PHE:CE1	2.36	0.43
1:H:7009:LEU:CD2	1:H:7121:PRO:HB2	2.48	0.43
1:K:157:GLN:HG3	1:P:5122:ARG:HH21	1.84	0.43
1:L:1043:TYR:HD2	1:L:1048:PHE:CE1	2.36	0.43
1:A:40:MET:HE2	1:A:133:LEU:CD2	2.46	0.43
1:I:8074:SER:O	1:I:8122:ARG:NH2	2.50	0.43
1:K:103:LEU:HG	1:K:183:ILE:HG13	1.99	0.43
1:E:4041:LEU:HB2	1:E:4050:GLN:NE2	2.34	0.43
2:F:5201:FMN:H9	2:F:5201:FMN:H1'1	1.77	0.43
1:G:6008:PHE:CZ	1:G:6050:GLN:NE2	2.86	0.43
1:R:7009:LEU:HD12	1:R:7009:LEU:C	2.38	0.43
1:P:5003:LEU:HG	1:P:5083:ILE:HG13	2.01	0.43
1:E:4003:LEU:HD21	1:E:4086:ARG:HG3	2.01	0.43
1:L:1025:MET:HG2	1:L:1095:LEU:HD22	2.01	0.43
1:L:1074:SER:HB3	1:L:1122:ARG:HH22	1.83	0.43
1:O:4091:TRP:CH2	1:O:4140:SER:HB2	2.33	0.43
1:A:25:MET:HA	1:A:25:MET:CE	2.48	0.43
1:K:193:MET:HA	1:K:193:MET:CE	2.49	0.43
1:L:1006:LEU:HB2	1:L:1080:PHE:CD1	2.53	0.43
1:N:3009:LEU:CD2	1:N:3121:PRO:HB2	2.47	0.43
1:R:7066:ILE:HG22	1:R:7072:HIS:HE1	1.84	0.43
1:A:76:GLU:OE2	1:A:122:ARG:HD3	2.18	0.43
1:C:2009:LEU:HD22	1:C:2121:PRO:HB2	1.99	0.43
1:D:3025:MET:SD	1:D:3095:LEU:HB2	2.58	0.43
1:E:4042:CYS:SG	1:E:4098:LEU:HD21	2.59	0.43
1:L:1088:PHE:CD1	1:L:1088:PHE:N	2.87	0.43
1:O:4023:ASP:O	1:O:4026:ALA:HB3	2.18	0.43
1:O:4069:ASP:OD1	1:O:4070:PRO:HD2	2.18	0.43
1:P:5006:LEU:HG	1:P:5007:ILE:N	2.34	0.43
1:R:7040:MET:O	1:R:7050:GLN:HG3	2.19	0.43
1:S:8055:ASP:HB3	1:S:8058:LYS:HG3	2.01	0.43
1:D:3093:MET:HA	1:D:3093:MET:HE2	2.00	0.43
1:Q:6017:SER:HB2	1:Q:6019:PRO:HD2	2.00	0.43
1:A:37:ILE:CG2	1:A:52:LEU:HD22	2.49	0.42



Atom 1 Atom 2		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:L:1122:ARG:O	1:Q:6001:MET:CE	2.67	0.42
1:N:3017:SER:CB	1:N:3019:PRO:HD2	2.42	0.42
1:N:3024:ILE:HG13	1:N:3071:ARG:NH1	2.34	0.42
1:N:3025:MET:CE	1:N:3093:MET:HG3	2.49	0.42
1:O:4025:MET:CE	1:O:4094:ARG:HA	2.40	0.42
1:O:4034:ARG:HE	1:O:4034:ARG:HB2	1.59	0.42
1:P:5010:SER:OG	1:P:5048:PHE:HB2	2.19	0.42
1:P:5041:LEU:HD13	1:P:5050:GLN:HB2	2.00	0.42
1:T:9009:LEU:HD22	1:T:9121:PRO:HB2	2.00	0.42
1:T:9024:ILE:HD11	2:T:9201:FMN:C8M	2.49	0.42
1:A:76:GLU:HG2	1:F:5057:GLN:HG3	2.00	0.42
1:N:3043:TYR:CD1	1:N:3048:PHE:CE1	3.07	0.42
1:N:3044:GLY:HA3	1:N:3098:LEU:HD12	2.00	0.42
1:S:8006:LEU:O	1:S:8051:THR:HA	2.20	0.42
1:A:57:GLN:HA	1:F:5076:GLU:HG2	2.02	0.42
1:A:102:ASP:C	1:A:104:ASP:H	2.22	0.42
1:C:2006:LEU:HB2	1:C:2080:PHE:HD1	1.85	0.42
1:E:4066:ILE:HA	2:E:4201:FMN:O2'	2.19	0.42
1:M:2044:GLY:HA3	1:M:2098:LEU:HD12	2.01	0.42
1:O:4033:LEU:HA	1:O:4033:LEU:HD12	1.47	0.42
1:F:5063:TYR:CE2	1:F:5067:LEU:HD11	2.54	0.42
1:H:7050:GLN:NE2	2:H:7201:FMN:H6	2.35	0.42
1:D:3109:LEU:HA	1:D:3109:LEU:HD12	1.74	0.42
1:K:231:ARG:HE	1:K:231:ARG:HB3	1.31	0.42
1:M:2043:TYR:CD1	1:M:2048:PHE:CE1	3.07	0.42
1:P:5072:HIS:CD2	1:P:5072:HIS:C	2.93	0.42
1:Q:6109:LEU:CD1	1:Q:6135:GLU:OE1	2.68	0.42
1:T:9050:GLN:HG2	1:T:9052:LEU:HD22	1.99	0.42
1:T:9083:ILE:HD12	1:T:9085:GLU:O	2.20	0.42
1:C:2050:GLN:HE21	1:C:2052:LEU:HD21	1.83	0.42
1:F:5018:TYR:N	1:F:5019:PRO:HD2	2.35	0.42
1:F:5026:ALA:O	1:F:5030:VAL:HG23	2.19	0.42
1:J:9003:LEU:HD21	1:J:9086:ARG:HG3	2.01	0.42
1:M:2017:SER:C	1:M:2021:LEU:HD12	2.40	0.42
1:H:7066:ILE:HD11	2:H:7201:FMN:C4A	2.49	0.42
1:O:4008:PHE:CZ	1:O:4050:GLN:NE2	2.85	0.42
1:P:5101:MET:O	1:P:5102:ASP:C	2.58	0.42
1:Q:6069:ASP:HB2	2:Q:6201:FMN:O2'	2.20	0.42
1:L:1044:GLY:HA3	1:L:1098:LEU:HD12	2.00	0.42
1:M:2018:TYR:HA	1:M:2021:LEU:HB2	2.02	0.42
1:N:3050:GLN:NE2	1:N:3052:LEU:HD21	2.34	0.42



Atom-1	Atom-2	Interatomic	Clash
	110000-2	distance (Å)	overlap (Å)
1:R:7041:LEU:O	1:R:7095:LEU:HA	2.19	0.42
1:S:8017:SER:O	1:S:8020:ASP:HB2	2.20	0.42
1:T:9042:CYS:HA	1:T:9096:VAL:O	2.20	0.42
2:A:201:FMN:H9	2:A:201:FMN:H1'1	1.81	0.42
1:L:1005:ARG:HB2	1:L:1053:GLU:HG2	2.01	0.42
1:L:1041:LEU:HB2	1:L:1093:MET:CE	2.49	0.42
1:O:4139:MET:HE2	1:O:4139:MET:HB2	1.83	0.42
1:S:8013:THR:HG23	1:S:8072:HIS:N	2.35	0.42
1:T:9127:GLU:OE1	1:T:9127:GLU:HA	2.20	0.42
1:A:127:GLU:HG2	1:G:6084:GLU:CD	2.40	0.41
1:E:4125:THR:CG2	1:J:9001:MET:HE1	2.48	0.41
1:K:145:ASN:O	1:K:147:MET:HG2	2.20	0.41
1:P:5031:ASN:O	1:P:5034:ARG:HG2	2.19	0.41
1:A:16:LEU:HD21	1:A:21:LEU:CD2	2.45	0.41
1:D:3041:LEU:HD13	1:D:3050:GLN:HB2	2.02	0.41
1:K:156:ARG:HG2	1:P:5077:ILE:O	2.19	0.41
1:M:2016:LEU:HD21	1:M:2048:PHE:HZ	1.84	0.41
1:C:2009:LEU:HD12	1:C:2009:LEU:C	2.40	0.41
1:C:2098:LEU:HD23	1:C:2098:LEU:HA	1.75	0.41
1:S:8041:LEU:HD23	1:S:8042:CYS:N	2.35	0.41
1:C:2001:MET:CE	1:H:7125:THR:HG22	2.51	0.41
1:M:2001:MET:HB3	1:S:8001:MET:HE2	2.00	0.41
1:Q:6112:LYS:HD3	1:Q:6113:TYR:CZ	2.56	0.41
1:S:8115:PRO:HA	1:T:9086:ARG:HH21	1.85	0.41
1:A:91:TRP:CE2	1:A:94:ARG:HD3	2.55	0.41
1:B:1041:LEU:HD13	1:B:1050:GLN:HB2	2.03	0.41
1:I:8076:GLU:OE2	1:I:8122:ARG:NH1	2.45	0.41
1:J:9017:SER:CB	1:J:9019:PRO:HD2	2.48	0.41
1:K:198:LEU:O	1:K:201:MET:HG3	2.19	0.41
1:L:1041:LEU:HB3	1:L:1094:ARG:O	2.20	0.41
1:O:4040:MET:HE1	1:O:4137:TYR:CA	2.50	0.41
1:P:5090:ASN:HB3	1:P:5091:TRP:CD1	2.55	0.41
1:Q:6101:MET:HE1	1:Q:6136:LEU:HD22	2.02	0.41
1:S:8038:THR:HB	1:S:8088:PHE:O	2.20	0.41
1:T:9057:GLN:HG2	1:T:9061:GLU:OE2	2.20	0.41
1:B:1004:HIS:CE1	1:B:1056:ARG:HB2	2.56	0.41
1:D:3006:LEU:O	1:D:3051:THR:HA	2.21	0.41
1:L:1021:LEU:HD12	1:L:1021:LEU:HA	1.75	0.41
1:O:4019:PRO:O	1:O:4020:ASP:C	2.59	0.41
1:R:7079:GLU:OE2	1:R:7081:LYS:HE2	2.21	0.41
1:C:2055:ASP:HB3	1:C:2058:LYS:HB2	2.02	0.41



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:H:7017:SER:O	1:H:7020:ASP:HB2	2.20	0.41
1:L:1028:SER:HB3	1:L:1093:MET:HG2	2.03	0.41
1:O:4011:CYS:HB2	1:O:4073:HIS:CE1	2.56	0.41
1:S:8042:CYS:SG	1:S:8098:LEU:CD2	3.09	0.41
2:H:7201:FMN:H4'	2:H:7201:FMN:H1'2	1.85	0.41
1:O:4027:LYS:HB3	1:O:4027:LYS:HE3	1.73	0.41
1:P:5119:PHE:CZ	1:P:5121:PRO:HG3	2.56	0.41
1:T:9028:SER:OG	2:T:9201:FMN:C4A	2.69	0.41
1:P:5018:TYR:N	1:P:5019:PRO:CD	2.85	0.40
1:N:3031:ASN:O	1:N:3034:ARG:HB3	2.21	0.40
1:O:4009:LEU:HD11	1:O:4076:GLU:HB2	2.02	0.40
1:A:109:LEU:HG	1:A:132:PHE:CD1	2.57	0.40
1:F:5025:MET:HE2	1:F:5025:MET:HA	2.03	0.40
1:H:7011:CYS:HB2	1:H:7073:HIS:CE1	2.56	0.40
1:H:7031:ASN:OD1	1:H:7034:ARG:NH1	2.54	0.40
1:O:4072:HIS:O	1:O:4072:HIS:HD2	2.04	0.40
1:R:7006:LEU:HD12	1:R:7007:ILE:N	2.36	0.40
1:T:9062:THR:HA	1:T:9065:ARG:NH1	2.37	0.40
1:T:9098:LEU:HD23	1:T:9098:LEU:HA	1.81	0.40
2:G:6201:FMN:H9	2:G:6201:FMN:H1'1	1.87	0.40
1:L:1043:TYR:CD1	1:L:1044:GLY:N	2.89	0.40
1:L:1050:GLN:HE21	1:L:1052:LEU:CD2	2.34	0.40
1:N:3093:MET:HA	1:N:3093:MET:CE	2.43	0.40
1:F:5104:ASP:O	1:F:5108:ARG:HG2	2.22	0.40
1:H:7103:SER:O	1:H:7107:ARG:CB	2.70	0.40
1:I:8112:LYS:HE3	1:J:9085:GLU:OE1	2.22	0.40
1:J:9013:THR:HG22	1:J:9073:HIS:CD2	2.49	0.40
1:N:3025:MET:HE2	1:N:3095:LEU:N	2.37	0.40
1:T:9028:SER:OG	2:T:9201:FMN:C10	2.70	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
1	А	138/163~(85%)	133 (96%)	5 (4%)	0	100	100
1	В	139/163~(85%)	136 (98%)	3(2%)	0	100	100
1	С	138/163~(85%)	138 (100%)	0	0	100	100
1	D	139/163~(85%)	134 (96%)	4 (3%)	1 (1%)	22	30
1	Е	140/163~(86%)	137 (98%)	3 (2%)	0	100	100
1	F	141/163 (86%)	140 (99%)	1 (1%)	0	100	100
1	G	138/163~(85%)	136 (99%)	2 (1%)	0	100	100
1	Н	139/163~(85%)	135 (97%)	4 (3%)	0	100	100
1	Ι	139/163~(85%)	137 (99%)	2 (1%)	0	100	100
1	J	139/163~(85%)	136 (98%)	3 (2%)	0	100	100
1	K	138/163~(85%)	137 (99%)	1 (1%)	0	100	100
1	L	139/163~(85%)	133 (96%)	6 (4%)	0	100	100
1	М	138/163~(85%)	133 (96%)	5 (4%)	0	100	100
1	Ν	138/163~(85%)	134 (97%)	4 (3%)	0	100	100
1	Ο	138/163~(85%)	131 (95%)	7 (5%)	0	100	100
1	Р	139/163~(85%)	134 (96%)	5 (4%)	0	100	100
1	Q	138/163~(85%)	133 (96%)	5 (4%)	0	100	100
1	R	138/163~(85%)	134 (97%)	4 (3%)	0	100	100
1	S	139/163~(85%)	134 (96%)	5 (4%)	0	100	100
1	Т	138/163~(85%)	135 (98%)	3 (2%)	0	100	100
All	All	2773/3260~(85%)	2700 (97%)	72 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	3001	MET

5.3.2 Protein sidechains (i)

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

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



Mol	Chain	Analysed	Rotameric	Outliers	Perce	entiles
1	А	120/143~(84%)	116~(97%)	4 (3%)	38	51
1	В	123/143~(86%)	118 (96%)	5 (4%)	30	41
1	С	121/143~(85%)	113~(93%)	8 (7%)	16	22
1	D	122/143~(85%)	119 (98%)	3(2%)	47	62
1	Ε	126/143~(88%)	122~(97%)	4 (3%)	39	53
1	F	124/143~(87%)	121 (98%)	3 (2%)	49	64
1	G	121/143 (85%)	118 (98%)	3 (2%)	47	62
1	Н	122/143~(85%)	117 (96%)	5 (4%)	30	41
1	Ι	119/143 (83%)	115 (97%)	4 (3%)	37	50
1	J	122/143~(85%)	121 (99%)	1 (1%)	81	88
1	K	117/143 (82%)	112 (96%)	5 (4%)	29	39
1	L	120/143 (84%)	113 (94%)	7~(6%)	20	26
1	М	120/143 (84%)	113 (94%)	7 (6%)	20	26
1	Ν	118/143 (82%)	115 (98%)	3 (2%)	47	62
1	О	118/143 (82%)	104 (88%)	14 (12%)	5	5
1	Р	112/143~(78%)	107 (96%)	5 (4%)	27	37
1	Q	122/143~(85%)	120 (98%)	2 (2%)	62	77
1	R	118/143 (82%)	110 (93%)	8 (7%)	16	20
1	S	120/143 (84%)	112 (93%)	8 (7%)	16	21
1	Т	121/143 (85%)	118 (98%)	3 (2%)	47	62
All	All	2406/2860~(84%)	2304 (96%)	102 (4%)	30	40

All (102) residues with a non-rotameric side chain are listed below:

Mol	Chain	Res	Type
1	А	71	ARG
1	А	72	HIS
1	А	98	LEU
1	А	114	SER
1	В	1022	ARG
1	В	1072	HIS
1	В	1107	ARG
1	В	1114	SER
1	В	1118	THR
1	С	2017	SER
1	С	2027	LYS



Mol	Chain	Res	Type
1	С	2057	GLN
1	С	2072	HIS
1	С	2093	MET
1	С	2094	ARG
1	С	2103	SER
1	С	2106	ILE
1	D	3001	MET
1	D	3072	HIS
1	D	3122	ARG
1	Е	4072	HIS
1	Е	4079	GLU
1	Е	4094	ARG
1	E	4114	SER
1	F	5072	HIS
1	F	5108	ARG
1	F	5114	SER
1	G	6072	HIS
1	G	6084	GLU
1	G	6114	SER
1	Н	7027	LYS
1	Н	7072	HIS
1	Н	7093	MET
1	Н	7102	ASP
1	Н	7104	ASP
1	Ι	8072	HIS
1	Ι	8101	MET
1	Ι	8104	ASP
1	Ι	8114	SER
1	J	9072	HIS
1	Κ	140	MET
1	Κ	145	ASN
1	Κ	172	HIS
1	K	179	GLU
1	K	201	MET
1	L	1014	ASP
1	L	1021	LEU
1	L	1072	HIS
1	L	1093	MET
1	L	1094	ARG
1	L	1101	MET
1	L	1104	ASP
1	М	2014	ASP



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Mol	Chain	Res	Type
1	М	2021	LEU
1	М	2023	ASP
1	М	2042	CYS
1	М	2072	HIS
1	М	2101	MET
1	М	2104	ASP
1	Ν	3027	LYS
1	Ν	3072	HIS
1	Ν	3124	MET
1	0	4001	MET
1	0	4016	LEU
1	0	4027	LYS
1	0	4035	ASP
1	0	4040	MET
1	0	4055	ASP
1	0	4072	HIS
1	0	4093	MET
1	0	4097	GLN
1	0	4098	LEU
1	0	4105	THR
1	0	4106	ILE
1	0	4109	LEU
1	0	4140	SER
1	Р	5017	SER
1	Р	5071	ARG
1	Р	5091	TRP
1	Р	5136	LEU
1	Р	5141	GLN
1	Q	6001	MET
1	Q	6072	HIS
1	R	7014	ASP
1	R	7027	LYS
1	R	7045	ASN
1	R	7072	HIS
1	R	7092	SER
1	R	7095	LEU
1	R	7104	ASP
1	R	7131	ARG
1	S	8014	ASP
1	S	8033	LEU
1	S	8065	ARG
1	S	8068	LYS



Continued from previous page...

Mol	Chain	Res	Type
1	S	8072	HIS
1	S	8101	MET
1	S	8103	SER
1	S	8108	ARG
1	Т	9016	LEU
1	Т	9042	CYS
1	Т	9068	LYS

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such side chains are listed below:

Mol	Chain	Res	Type
1	В	1045	ASN
1	В	1120	GLN
1	В	1128	GLN
1	D	3090	ASN
1	D	3120	GLN
1	Е	4050	GLN
1	F	5141	GLN
1	Н	7050	GLN
1	Н	7141	GLN
1	J	9050	GLN
1	K	150	GLN
1	Κ	173	HIS
1	L	1050	GLN
1	0	4072	HIS
1	0	4073	HIS
1	0	4090	ASN
1	Р	5031	ASN
1	Р	5072	HIS
1	Р	5090	ASN
1	Р	5141	GLN
1	Q	6057	GLN
1	Q	6128	GLN
1	R	7004	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.



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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

20 ligands are modelled in this entry.

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

Mal	Type	Chain	Dog	Link	Bo	ond leng	ths	Bond angles		
IVIOI	туре	Ullalli	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
2	FMN	R	7201	-	33,33,33	1.12	2 (6%)	$48,\!50,\!50$	1.39	8 (16%)
2	FMN	Н	7201	-	33,33,33	1.03	2 (6%)	48,50,50	1.62	11 (22%)
2	FMN	L	1201	-	33,33,33	1.05	2 (6%)	48,50,50	1.52	13 (27%)
2	FMN	G	6201	-	33,33,33	1.14	2 (6%)	48,50,50	1.48	8 (16%)
2	FMN	Р	5201	-	33,33,33	1.07	2 (6%)	48,50,50	1.69	12 (25%)
2	FMN	Ι	8201	-	33,33,33	1.15	2 (6%)	48,50,50	1.36	7 (14%)
2	FMN	Т	9201	-	33,33,33	1.11	2 (6%)	48,50,50	1.38	7 (14%)
2	FMN	Е	4201	-	33,33,33	1.08	2 (6%)	48,50,50	1.56	10 (20%)
2	FMN	F	5201	-	33,33,33	1.12	2 (6%)	48,50,50	1.42	10 (20%)
2	FMN	J	9201	-	33,33,33	1.20	3 (9%)	48,50,50	1.73	11 (22%)
2	FMN	Ο	4201	-	33,33,33	1.08	2 (6%)	48,50,50	1.52	9 (18%)
2	FMN	В	1201	-	33,33,33	1.03	1 (3%)	48,50,50	1.71	13 (27%)
2	FMN	Ν	3201	-	33,33,33	1.14	3 (9%)	48,50,50	1.59	12 (25%)
2	FMN	Q	6201	-	33,33,33	1.13	2 (6%)	$48,\!50,\!50$	1.54	9 (18%)
2	FMN	D	3201	-	33,33,33	1.13	2 (6%)	48,50,50	1.50	9 (18%)
2	FMN	S	8201	-	33,33,33	1.05	2 (6%)	48,50,50	1.81	11 (22%)
2	FMN	М	2201	-	33,33,33	1.08	2 (6%)	48,50,50	1.36	7 (14%)
2	FMN	K	301	-	33,33,33	1.03	2 (6%)	48,50,50	1.37	8 (16%)



Mal	Turne	Chain	Dec	Tinle	Bo	Bond lengths			Bond angles		
MOI	туре	Chain	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2	
2	FMN	C	2201	-	33,33,33	1.12	2 (6%)	48,50,50	1.41	8 (16%)	
2	FMN	А	201	-	33,33,33	1.22	4 (12%)	48,50,50	1.34	8 (16%)	

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
2	FMN	R	7201	-	-	4/18/18/18	0/3/3/3
2	FMN	Н	7201	-	-	6/18/18/18	0/3/3/3
2	FMN	L	1201	-	-	6/18/18/18	0/3/3/3
2	FMN	G	6201	-	-	2/18/18/18	0/3/3/3
2	FMN	Р	5201	-	-	4/18/18/18	0/3/3/3
2	FMN	Ι	8201	-	-	2/18/18/18	0/3/3/3
2	FMN	Т	9201	-	-	3/18/18/18	0/3/3/3
2	FMN	Е	4201	-	-	4/18/18/18	0/3/3/3
2	FMN	F	5201	-	-	6/18/18/18	0/3/3/3
2	FMN	J	9201	-	-	4/18/18/18	0/3/3/3
2	FMN	0	4201	-	-	1/18/18/18	0/3/3/3
2	FMN	В	1201	-	-	4/18/18/18	0/3/3/3
2	FMN	Ν	3201	-	-	2/18/18/18	0/3/3/3
2	FMN	Q	6201	-	-	2/18/18/18	0/3/3/3
2	FMN	D	3201	-	-	6/18/18/18	0/3/3/3
2	FMN	S	8201	-	-	5/18/18/18	0/3/3/3
2	FMN	М	2201	-	-	1/18/18/18	0/3/3/3
2	FMN	К	301	-	-	3/18/18/18	0/3/3/3
2	FMN	С	2201	-	-	5/18/18/18	0/3/3/3
2	FMN	А	201	-	-	0/18/18/18	0/3/3/3

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	$\operatorname{Observed}(\operatorname{\AA})$	$\mathrm{Ideal}(\mathrm{\AA})$
2	Q	6201	FMN	C4A-N5	4.21	1.38	1.30
2	D	3201	FMN	C4A-N5	4.11	1.38	1.30
2	В	1201	FMN	C4A-N5	4.07	1.38	1.30
2	С	2201	FMN	C4A-N5	3.98	1.38	1.30
2	Ν	3201	FMN	C4A-N5	3.92	1.38	1.30



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	5201	FMN	C4A-N5	3.90	1.38	1.30
2	Ι	8201	FMN	C4A-N5	3.89	1.38	1.30
2	А	201	FMN	C4A-N5	3.88	1.38	1.30
2	Р	5201	FMN	C4A-N5	3.83	1.38	1.30
2	J	9201	FMN	C4A-N5	3.75	1.38	1.30
2	0	4201	FMN	C4A-N5	3.68	1.37	1.30
2	Е	4201	FMN	C4A-N5	3.66	1.37	1.30
2	S	8201	FMN	C4A-N5	3.61	1.37	1.30
2	Κ	301	FMN	C4A-N5	3.59	1.37	1.30
2	L	1201	FMN	C4A-N5	3.52	1.37	1.30
2	М	2201	FMN	C4A-N5	3.52	1.37	1.30
2	G	6201	FMN	C4A-N5	3.50	1.37	1.30
2	Т	9201	FMN	C4A-N5	3.49	1.37	1.30
2	R	7201	FMN	C4A-N5	3.36	1.37	1.30
2	Н	7201	FMN	C4A-N5	3.24	1.37	1.30
2	0	4201	FMN	C10-N1	3.23	1.39	1.33
2	R	7201	FMN	C10-N1	3.13	1.39	1.33
2	F	5201	FMN	C10-N1	3.11	1.39	1.33
2	С	2201	FMN	C10-N1	2.93	1.39	1.33
2	А	201	FMN	C10-N1	2.85	1.39	1.33
2	D	3201	FMN	C10-N1	2.82	1.39	1.33
2	Ν	3201	FMN	C10-N1	2.82	1.39	1.33
2	Т	9201	FMN	C10-N1	2.78	1.38	1.33
2	Q	6201	FMN	C10-N1	2.68	1.38	1.33
2	Ι	8201	FMN	C10-N1	2.67	1.38	1.33
2	Р	5201	FMN	C10-N1	2.62	1.38	1.33
2	Κ	301	FMN	C10-N1	2.51	1.38	1.33
2	J	9201	FMN	C4A-C10	-2.47	1.36	1.44
2	G	6201	FMN	C10-N1	2.44	1.38	1.33
2	Ε	4201	FMN	C10-N1	2.30	1.37	1.33
2	М	2201	FMN	C10-N1	2.28	1.37	1.33
2	Н	7201	FMN	C10-N1	2.26	1.37	1.33
2	S	8201	FMN	C10-N1	2.16	1.37	1.33
2	А	201	FMN	C9A-C5A	-2.15	1.37	1.41
2	L	1201	FMN	C10-N1	2.14	1.37	1.33
2	J	9201	FMN	C5'-C4'	2.09	1.54	1.51
2	N	3201	FMN	C4A-C10	-2.08	1.38	1.44
2	А	201	FMN	C4A-C10	-2.01	1.38	1.44

All (191) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
Mol	Chain	Res	Type	Atoms	Ζ	Observed(°)	Ideal(°)
2	S	8201	FMN	C5'-C4'-C3'	5.58	122.98	112.20
2	0	4201	FMN	C5'-C4'-C3'	-5.31	101.95	112.20
2	Q	6201	FMN	C5'-C4'-C3'	-4.98	102.58	112.20
2	J	9201	FMN	C5'-C4'-C3'	-4.69	103.15	112.20
2	D	3201	FMN	C5'-C4'-C3'	-4.54	103.42	112.20
2	Е	4201	FMN	C5'-C4'-C3'	-4.46	103.59	112.20
2	Р	5201	FMN	C5'-C4'-C3'	4.38	120.66	112.20
2	В	1201	FMN	C5'-C4'-C3'	-4.29	103.92	112.20
2	S	8201	FMN	C4'-C3'-C2'	-4.14	104.74	113.36
2	R	7201	FMN	C5'-C4'-C3'	-4.11	104.26	112.20
2	J	9201	FMN	C4A-C10-N10	3.91	122.19	116.48
2	S	8201	FMN	C4-N3-C2	-3.89	118.45	125.64
2	В	1201	FMN	C4A-C10-N10	3.86	122.12	116.48
2	Ν	3201	FMN	C5'-C4'-C3'	-3.84	104.79	112.20
2	Р	5201	FMN	C4'-C3'-C2'	-3.82	105.42	113.36
2	С	2201	FMN	C5'-C4'-C3'	-3.70	105.05	112.20
2	Р	5201	FMN	C4-N3-C2	-3.69	118.83	125.64
2	Q	6201	FMN	O4'-C4'-C3'	3.61	117.89	109.10
2	Н	7201	FMN	C4A-C10-N10	3.47	121.56	116.48
2	Н	7201	FMN	C5'-C4'-C3'	3.43	118.83	112.20
2	G	6201	FMN	C4-N3-C2	-3.43	119.30	125.64
2	Q	6201	FMN	C4-N3-C2	-3.43	119.31	125.64
2	J	9201	FMN	C4-C4A-N5	3.36	123.02	118.23
2	Ν	3201	FMN	O3P-P-O5'	3.33	115.59	106.73
2	Ε	4201	FMN	C4-N3-C2	-3.33	119.49	125.64
2	J	9201	FMN	C4-N3-C2	-3.33	119.50	125.64
2	Ι	8201	FMN	C4-N3-C2	-3.25	119.64	125.64
2	Т	9201	FMN	C4-N3-C2	-3.23	119.68	125.64
2	S	8201	FMN	C4A-C10-N1	-3.21	117.28	124.73
2	В	1201	FMN	C10-C4A-N5	-3.18	118.10	124.86
2	R	7201	FMN	O4-C4-C4A	-3.18	118.16	126.60
2	А	201	FMN	C5'-C4'-C3'	-3.18	106.07	112.20
2	Ν	3201	FMN	C4-N3-C2	-3.17	119.78	125.64
2	0	4201	FMN	C4-N3-C2	-3.17	119.78	125.64
2	В	1201	FMN	C4-N3-C2	-3.17	119.79	125.64
2	P	5201	FMN	C4A-C10-N1	-3.16	117.39	124.73
2	J	9201	FMN	C4A-C4-N3	3.16	121.21	113.19
2	F	5201	FMN	O3'-C3'-C2'	3.15	116.42	108.81
2	Ι	8201	FMN	C4A-C4-N3	3.13	121.15	113.19
2	L	1201	FMN	C4A-C10-N10	3.13	121.06	116.48
2	С	2201	FMN	C4-N3-C2	-3.11	119.89	125.64



Mol	Chain	\mathbf{Res}	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	D	3201	FMN	O4'-C4'-C3'	3.11	116.65	109.10
2	F	5201	FMN	C4-N3-C2	-3.10	119.91	125.64
2	G	6201	FMN	C4A-C10-N10	3.07	120.97	116.48
2	J	9201	FMN	C10-C4A-N5	-3.06	118.37	124.86
2	Ν	3201	FMN	C9A-C5A-N5	-3.05	119.12	122.43
2	S	8201	FMN	C4A-C4-N3	3.05	120.92	113.19
2	М	2201	FMN	C4-N3-C2	-3.04	120.02	125.64
2	L	1201	FMN	C4-N3-C2	-3.03	120.04	125.64
2	D	3201	FMN	C10-C4A-N5	-3.03	118.43	124.86
2	R	7201	FMN	C4-N3-C2	-3.01	120.07	125.64
2	Т	9201	FMN	C5A-C9A-N10	3.01	121.06	117.95
2	Н	7201	FMN	C4-N3-C2	-3.01	120.09	125.64
2	М	2201	FMN	C4A-C10-N10	3.00	120.87	116.48
2	С	2201	FMN	C4A-C4-N3	3.00	120.81	113.19
2	Н	7201	FMN	C4'-C3'-C2'	-2.99	107.14	113.36
2	А	201	FMN	C4-N3-C2	-2.98	120.13	125.64
2	А	201	FMN	C4A-C4-N3	2.98	120.76	113.19
2	Н	7201	FMN	C10-N1-C2	2.98	122.85	116.90
2	L	1201	FMN	C4'-C3'-C2'	-2.96	107.20	113.36
2	G	6201	FMN	C4A-C4-N3	2.93	120.63	113.19
2	Ι	8201	FMN	O4-C4-C4A	-2.92	118.85	126.60
2	Р	5201	FMN	C4A-C4-N3	2.91	120.59	113.19
2	М	2201	FMN	C4A-C4-N3	2.91	120.59	113.19
2	Н	7201	FMN	C10-C4A-N5	-2.91	118.69	124.86
2	Е	4201	FMN	C10-C4A-N5	-2.87	118.77	124.86
2	G	6201	FMN	C10-C4A-N5	-2.86	118.80	124.86
2	G	6201	FMN	O2'-C2'-C1'	-2.85	102.91	109.80
2	Е	4201	FMN	O4'-C4'-C3'	2.83	115.98	109.10
2	Н	7201	FMN	C4A-C4-N3	2.83	120.37	113.19
2	0	4201	FMN	C4A-C4-N3	2.82	120.36	113.19
2	D	3201	FMN	C4A-C10-N10	2.81	120.59	116.48
2	В	1201	FMN	O2'-C2'-C1'	-2.81	103.02	109.80
2	Κ	301	FMN	C4A-C10-N10	2.80	120.57	116.48
2	J	9201	FMN	C10-N1-C2	2.80	122.50	116.90
2	K	301	FMN	C4-N3-C2	-2.79	120.48	125.64
2	Q	6201	FMN	C4A-C4-N3	2.79	120.27	113.19
2	S	8201	FMN	C4A-C10-N10	2.78	120.55	116.48
2	F	5201	FMN	C4A-C4-N3	2.76	120.21	113.19
2	D	3201	FMN	C4A-C4-N3	2.75	120.18	113.19
2	Т	9201	FMN	C4-C4A-C10	2.75	121.41	116.79
2	С	2201	FMN	O4'-C4'-C3'	2.75	115.79	109.10
2	J	9201	FMN	O4'-C4'-C5'	2.75	116.10	109.92

Continued from previous page...



Mol	Chain	Res	Type	Atoms	Ζ	$Observed(^{o})$	$Ideal(^{o})$
2	D	3201	FMN	C4-N3-C2	-2.74	120.57	125.64
2	Р	5201	FMN	C4-C4A-C10	2.74	121.39	116.79
2	Ν	3201	FMN	O4-C4-C4A	-2.73	119.36	126.60
2	Е	4201	FMN	C4A-C10-N10	2.72	120.45	116.48
2	Н	7201	FMN	C4-C4A-N5	2.71	122.09	118.23
2	Q	6201	FMN	O4-C4-C4A	-2.70	119.43	126.60
2	G	6201	FMN	C4A-C10-N1	-2.69	118.50	124.73
2	0	4201	FMN	C4A-C10-N10	2.67	120.39	116.48
2	0	4201	FMN	C10-C4A-N5	-2.66	119.21	124.86
2	J	9201	FMN	O5'-P-O1P	2.66	113.93	106.47
2	Ν	3201	FMN	C4A-C4-N3	2.65	119.92	113.19
2	R	7201	FMN	C4A-C4-N3	2.64	119.90	113.19
2	Κ	301	FMN	C5'-C4'-C3'	2.63	117.28	112.20
2	Т	9201	FMN	C4A-C10-N1	-2.63	118.63	124.73
2	Κ	301	FMN	C4A-C10-N1	-2.62	118.64	124.73
2	Ι	8201	FMN	C5A-C9A-N10	2.61	120.65	117.95
2	Е	4201	FMN	C4A-C10-N1	-2.61	118.68	124.73
2	Р	5201	FMN	O3'-C3'-C2'	2.61	115.11	108.81
2	S	8201	FMN	C10-N1-C2	2.60	122.11	116.90
2	Е	4201	FMN	C4A-C4-N3	2.60	119.78	113.19
2	D	3201	FMN	C4A-C10-N1	-2.59	118.71	124.73
2	S	8201	FMN	C10-C4A-N5	-2.58	119.39	124.86
2	Р	5201	FMN	C4A-C10-N10	2.56	120.22	116.48
2	Q	6201	FMN	C4A-C10-N10	2.56	120.22	116.48
2	В	1201	FMN	C4-C4A-N5	2.53	121.83	118.23
2	Т	9201	FMN	C4A-C10-N10	2.52	120.16	116.48
2	Κ	301	FMN	C4'-C3'-C2'	-2.52	108.13	113.36
2	Κ	301	FMN	C10-C4A-N5	-2.50	119.55	124.86
2	Н	7201	FMN	C4A-C10-N1	-2.49	118.94	124.73
2	Р	5201	FMN	O2'-C2'-C1'	-2.49	103.77	109.80
2	L	1201	FMN	C4A-C4-N3	2.49	119.52	113.19
2	М	2201	FMN	C4A-C10-N1	-2.49	118.95	124.73
2	В	1201	FMN	O4'-C4'-C5'	2.49	115.50	109.92
2	0	4201	FMN	C4A-C10-N1	-2.46	119.03	124.73
2	А	201	FMN	C10-C4A-N5	-2.46	119.65	124.86
2	Κ	301	FMN	C4A-C4-N3	2.44	119.39	113.19
2	F	5201	FMN	C10-C4A-N5	-2.44	119.68	124.86
2	A	201	FMN	C4A-C10-N1	-2.43	119.09	124.73
2	I	8201	FMN	$P-O5'-\overline{C5'}$	$2.4\overline{3}$	124.99	118.30
2	L	1201	FMN	C4A-C10-N1	-2.43	119.09	124.73
2	В	1201	FMN	C4A-C4-N3	2.41	119.31	113.19
2	Т	9201	FMN	O4-C4-C4A	-2.41	120.22	126.60



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	Р	5201	FMN	O4-C4-C4A	-2.41	120.22	126.60
2	В	1201	FMN	O2-C2-N1	-2.40	117.85	121.83
2	Н	7201	FMN	O2'-C2'-C1'	-2.40	103.99	109.80
2	G	6201	FMN	C5'-C4'-C3'	2.39	116.83	112.20
2	М	2201	FMN	C10-N1-C2	2.39	121.69	116.90
2	Ι	8201	FMN	O3'-C3'-C2'	2.39	114.58	108.81
2	0	4201	FMN	O4-C4-C4A	-2.39	120.26	126.60
2	Ν	3201	FMN	C4A-C10-N1	-2.39	119.19	124.73
2	D	3201	FMN	C4-C4A-N5	2.38	121.63	118.23
2	А	201	FMN	O4-C4-C4A	-2.38	120.30	126.60
2	Е	4201	FMN	C4-C4A-C10	2.38	120.78	116.79
2	Ν	3201	FMN	O5'-C5'-C4'	2.36	115.67	109.36
2	С	2201	FMN	C10-C4A-N5	-2.35	119.87	124.86
2	L	1201	FMN	C5'-C4'-C3'	2.35	116.73	112.20
2	F	5201	FMN	C4A-C10-N1	-2.34	119.29	124.73
2	Т	9201	FMN	C4A-C4-N3	2.34	119.13	113.19
2	F	5201	FMN	C4A-C10-N10	2.34	119.90	116.48
2	Ν	3201	FMN	C4-C4A-C10	2.33	120.71	116.79
2	R	7201	FMN	C4A-C10-N1	-2.33	119.33	124.73
2	М	2201	FMN	C10-C4A-N5	-2.32	119.92	124.86
2	R	7201	FMN	P-O5'-C5'	2.32	124.69	118.30
2	Е	4201	FMN	O3'-C3'-C4'	2.32	114.41	108.81
2	L	1201	FMN	C6-C5A-C9A	2.31	122.21	118.94
2	S	8201	FMN	C9A-C5A-N5	-2.31	119.92	122.43
2	F	5201	FMN	O3'-C3'-C4'	-2.31	103.24	108.81
2	С	2201	FMN	C4A-C10-N10	2.30	119.84	116.48
2	В	1201	FMN	C4'-C3'-C2'	2.29	118.12	113.36
2	J	9201	FMN	C4A-C10-N1	-2.27	119.45	124.73
2	Κ	301	FMN	C4-C4A-C10	2.27	120.60	116.79
2	F	5201	FMN	C10-N1-C2	2.25	121.41	116.90
2	Ν	3201	FMN	C10-C4A-N5	-2.25	120.09	124.86
2	М	2201	FMN	O4-C4-C4A	-2.24	120.66	126.60
2	В	1201	FMN	C4A-C10-N1	-2.24	$119.5\overline{4}$	124.73
2	G	6201	FMN	$C4-C4A-\overline{C10}$	$2.2\overline{2}$	$120.5\overline{3}$	116.79
2	Р	5201	FMN	C10-C4A-N5	-2.21	120.16	124.86
2	Н	7201	FMN	O4-C4-C4A	-2.21	120.75	126.60
2	R	7201	FMN	C4-C4A-C10	2.20	120.49	116.79
2	R	7201	FMN	C4A-C10-N10	2.19	119.69	116.48
2	В	1201	FMN	P-O5'-C5'	2.17	124.28	118.30
2	L	1201	FMN	C4-C4A-C10	2.17	120.44	116.79
2	Ι	8201	FMN	O2'-C2'-C1'	-2.17	104.56	109.80
2	Q	6201	FMN	C4A-C10-N1	-2.17	119.70	124.73



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	F	5201	FMN	C4'-C3'-C2'	-2.16	108.86	113.36
2	N	3201	FMN	C5A-N5-C4A	2.16	121.67	118.07
2	L	1201	FMN	P-O5'-C5'	2.16	124.25	118.30
2	С	2201	FMN	C4A-C10-N1	-2.15	119.74	124.73
2	S	8201	FMN	C4-C4A-C10	2.15	120.40	116.79
2	N	3201	FMN	O2'-C2'-C1'	-2.15	104.61	109.80
2	А	201	FMN	C4'-C3'-C2'	-2.14	108.90	113.36
2	L	1201	FMN	C10-C4A-N5	-2.14	120.32	124.86
2	L	1201	FMN	C5A-C9A-N10	2.13	120.16	117.95
2	0	4201	FMN	O5'-C5'-C4'	2.13	115.05	109.36
2	S	8201	FMN	O4'-C4'-C5'	-2.13	105.14	109.92
2	С	2201	FMN	C9A-C5A-N5	-2.13	120.12	122.43
2	D	3201	FMN	C10-N1-C2	2.12	121.13	116.90
2	В	1201	FMN	C10-N1-C2	2.11	121.12	116.90
2	Р	5201	FMN	C10-N1-C2	2.10	121.11	116.90
2	F	5201	FMN	O4-C4-C4A	-2.10	121.03	126.60
2	Q	6201	FMN	C10-C4A-N5	-2.07	120.47	124.86
2	J	9201	FMN	O2'-C2'-C3'	2.07	114.12	109.10
2	0	4201	FMN	C10-N1-C2	2.06	121.03	116.90
2	A	201	FMN	C10-N1-C2	2.06	121.02	116.90
2	L	1201	FMN	C1'-C2'-C3'	2.05	115.52	109.79
2	Е	4201	FMN	C9A-C5A-N5	-2.04	120.21	122.43
2	L	1201	FMN	O4-C4-C4A	-2.04	121.19	126.60
2	Q	6201	FMN	C5A-C9A-N10	2.01	120.03	117.95

There are no chirality outliers.

All (70) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	В	1201	FMN	C5'-O5'-P-O2P
2	В	1201	FMN	C5'-O5'-P-O3P
2	С	2201	FMN	O4'-C4'-C5'-O5'
2	С	2201	FMN	C5'-O5'-P-O1P
2	С	2201	FMN	C5'-O5'-P-O2P
2	С	2201	FMN	C5'-O5'-P-O3P
2	D	3201	FMN	O4'-C4'-C5'-O5'
2	D	3201	FMN	C5'-O5'-P-O1P
2	D	3201	FMN	C5'-O5'-P-O2P
2	D	3201	FMN	C5'-O5'-P-O3P
2	Е	4201	FMN	C5'-O5'-P-O2P
2	Е	4201	FMN	C5'-O5'-P-O3P
2	F	5201	FMN	O4'-C4'-C5'-O5'



Mol	Chain	Res	Type	Atoms
2	F	5201	FMN	C5'-O5'-P-O2P
2	F	5201	FMN	C5'-O5'-P-O3P
2	Н	7201	FMN	C3'-C4'-C5'-O5'
2	Н	7201	FMN	O4'-C4'-C5'-O5'
2	Н	7201	FMN	C5'-O5'-P-O1P
2	Н	7201	FMN	C5'-O5'-P-O2P
2	Н	7201	FMN	C5'-O5'-P-O3P
2	Ι	8201	FMN	C3'-C4'-C5'-O5'
2	Ι	8201	FMN	O4'-C4'-C5'-O5'
2	J	9201	FMN	O4'-C4'-C5'-O5'
2	J	9201	FMN	C5'-O5'-P-O2P
2	J	9201	FMN	C5'-O5'-P-O3P
2	K	301	FMN	C5'-O5'-P-O1P
2	К	301	FMN	C5'-O5'-P-O2P
2	K	301	FMN	C5'-O5'-P-O3P
2	L	1201	FMN	O3'-C3'-C4'-O4'
2	L	1201	FMN	O3'-C3'-C4'-C5'
2	L	1201	FMN	C3'-C4'-C5'-O5'
2	L	1201	FMN	O4'-C4'-C5'-O5'
2	М	2201	FMN	O4'-C4'-C5'-O5'
2	Ν	3201	FMN	N10-C1'-C2'-O2'
2	Р	5201	FMN	C5'-O5'-P-O2P
2	Р	5201	FMN	C5'-O5'-P-O3P
2	Q	6201	FMN	N10-C1'-C2'-O2'
2	Q	6201	FMN	O4'-C4'-C5'-O5'
2	R	7201	FMN	C5'-O5'-P-O1P
2	R	7201	FMN	C5'-O5'-P-O2P
2	R	7201	FMN	C5'-O5'-P-O3P
2	S	8201	FMN	C3'-C4'-C5'-O5'
2	S	8201	FMN	O4'-C4'-C5'-O5'
2	S	8201	FMN	C5'-O5'-P-O1P
2	S	8201	FMN	C5'-O5'-P-O2P
2	S	8201	FMN	C5'-O5'-P-O3P
2	T	9201	FMN	C5'-O5'-P-O1P
2	Т	9201	FMN	C5'-O5'-P-O2P
2	Т	9201	FMN	C5'-O5'-P-O3P
2	L	1201	FMN	C2'-C3'-C4'-O4'
2	L	1201	FMN	C2'-C3'-C4'-C5'
2	N	3201	FMN	O4'-C4'-C5'-O5'
2	B	1201	FMN	C5'-O5'-P-O1P
2	Е	4201	FMN	C5'-O5'-P-O1P
2	F	5201	FMN	C5'-O5'-P-O1P

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Mol	Chain	Res	Type	Atoms
2	G	6201	FMN	C5'-O5'-P-O1P
2	J	9201	FMN	C5'-O5'-P-O1P
2	Р	5201	FMN	C5'-O5'-P-O1P
2	Р	5201	FMN	C3'-C4'-C5'-O5'
2	D	3201	FMN	N10-C1'-C2'-O2'
2	F	5201	FMN	N10-C1'-C2'-O2'
2	R	7201	FMN	N10-C1'-C2'-O2'
2	F	5201	FMN	C3'-C4'-C5'-O5'
2	D	3201	FMN	C3'-C4'-C5'-O5'
2	В	1201	FMN	N10-C1'-C2'-O2'
2	С	2201	FMN	N10-C1'-C2'-O2'
2	Ε	4201	FMN	N10-C1'-C2'-O2'
2	G	6201	FMN	N10-C1'-C2'-O2'
2	Н	7201	FMN	N10-C1'-C2'-O2'
2	0	4201	FMN	N10-C1'-C2'-O2'

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There are no ring outliers.

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	R	7201	FMN	1	0
2	Н	7201	FMN	4	0
2	L	1201	FMN	2	0
2	G	6201	FMN	2	0
2	Р	5201	FMN	4	0
2	Ι	8201	FMN	2	0
2	Т	9201	FMN	9	0
2	Е	4201	FMN	1	0
2	F	5201	FMN	2	0
2	J	9201	FMN	3	0
2	0	4201	FMN	4	0
2	N	3201	FMN	2	0
2	Q	6201	FMN	1	0
2	D	3201	FMN	1	0
2	М	2201	FMN	1	0
2	С	2201	FMN	4	0
2	А	201	FMN	2	0

17 monomers are involved in 45 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)

There are no chain breaks in this entry.



6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ $>$	#RSRZ>2	$\mathbf{OWAB}(\mathrm{\AA}^2)$	Q < 0.9
1	А	140/163~(85%)	0.08	2 (1%) 75 81	32, 48, 76, 93	0
1	В	141/163~(86%)	-0.04	1 (0%) 87 90	32, 44, 62, 79	0
1	С	140/163~(85%)	-0.01	0 100 100	35, 48, 72, 87	0
1	D	141/163~(86%)	0.00	2 (1%) 75 81	33, 42, 64, 84	0
1	Ε	142/163~(87%)	-0.06	2 (1%) 75 81	29, 41, 59, 73	0
1	F	143/163~(87%)	-0.01	1 (0%) 87 90	32, 45, 65, 96	0
1	G	140/163~(85%)	0.01	0 100 100	33, 45, 66, 73	0
1	Н	141/163~(86%)	-0.02	0 100 100	35, 47, 62, 80	0
1	Ι	141/163~(86%)	-0.10	0 100 100	34, 44, 62, 73	0
1	J	141/163~(86%)	-0.02	0 100 100	30, 43, 66, 84	0
1	Κ	140/163~(85%)	0.12	1 (0%) 87 90	37, 56, 75, 82	0
1	L	141/163~(86%)	0.27	6 (4%) 35 42	45,60,83,95	0
1	М	140/163~(85%)	0.25	4 (2%) 51 59	45,65,88,97	0
1	Ν	140/163~(85%)	0.01	1 (0%) 87 90	40, 55, 73, 85	0
1	Ο	140/163~(85%)	0.39	5 (3%) 42 49	46, 66, 88, 99	0
1	Р	141/163~(86%)	0.32	6 (4%) 35 42	43, 66, 85, 118	0
1	Q	140/163~(85%)	-0.06	1 (0%) 87 90	38, 49, 62, 74	0
1	R	140/163~(85%)	0.03	0 100 100	41, 57, 79, 87	0
1	S	141/163~(86%)	0.04	1 (0%) 87 90	38, 56, 83, 106	0
1	Т	140/163~(85%)	0.06	2 (1%) 75 81	42, 57, 82, 101	0
All	All	2813/3260 (86%)	0.06	35 (1%) 79 84	29, 51, 79, 118	0

All (35) RSRZ outliers are listed below:



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Mol	Chain	Res	Type	RSRZ	
1	L	1094	ARG	4.1	
1	L	1000	HIS	4.1	
1	0	4018	TYR	4.0	
1	D	3018	TYR	3.8	
1	0	4001	MET	3.6	
1	L	1018	TYR	3.5	
1	F	5142	GLY	3.3	
1	L	1095	LEU	3.1	
1	Т	9018	TYR	3.1	
1	Р	5098	LEU	3.0	
1	Р	5043	TYR	3.0	
1	0	4014	ASP	3.0	
1	А	18	TYR	3.0	
1	D	3140	SER	2.8	
1	S	8018	TYR	2.8	
1	Т	9016	LEU	2.8	
1	Р	5141	GLN	2.8	
1	Е	4018	TYR	2.7	
1	Ε	4000	HIS	2.7	
1	М	2024	ILE	2.7	
1	А	109	LEU	2.6	
1	0	4024	ILE	2.5	
1	М	2091	TRP	2.4	
1	Q	6100	GLU	2.3	
1	Р	5099	GLY	2.3	
1	М	2018	TYR	2.2	
1	L	1021	LEU	2.1	
1	В	1022	ARG	2.1	
1	0	4027	LYS	2.1	
1	Κ	201	MET	2.1	
1	М	2015	GLY	2.1	
1	Р	5136	LEU	2.0	
1	Р	5016	LEU	2.0	
1	N	3109	LEU	2.0	
1	L	1101	MET	2.0	

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

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



6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B -factors($Å^2$)	Q<0.9
2	FMN	0	4201	31/31	0.83	0.20	74,79,106,118	0
2	FMN	Р	5201	31/31	0.86	0.23	69,75,111,119	0
2	FMN	М	2201	31/31	0.89	0.20	60,68,104,115	0
2	FMN	R	7201	31/31	0.91	0.17	49,59,89,100	0
2	FMN	Т	9201	31/31	0.91	0.16	62,76,90,93	0
2	FMN	S	8201	31/31	0.92	0.16	43,55,94,101	0
2	FMN	K	301	31/31	0.92	0.20	57,67,112,121	0
2	FMN	G	6201	31/31	0.93	0.19	40,45,92,97	0
2	FMN	Ι	8201	31/31	0.93	0.16	35,44,92,108	0
2	FMN	С	2201	31/31	0.93	0.15	44,52,85,95	0
2	FMN	L	1201	31/31	0.93	0.17	48,58,95,115	0
2	FMN	F	5201	31/31	0.93	0.15	36,49,88,98	0
2	FMN	Н	7201	31/31	0.94	0.14	38,49,86,99	0
2	FMN	Q	6201	31/31	0.94	0.16	41,45,76,79	0
2	FMN	D	3201	31/31	0.94	0.14	40,48,87,93	0
2	FMN	Ν	3201	31/31	0.94	0.14	44,51,71,74	0
2	FMN	Е	4201	31/31	0.94	0.14	31,41,79,86	0
2	FMN	A	201	31/31	0.95	0.14	44,52,87,90	0
2	FMN	J	9201	31/31	0.95	0.18	36,42,68,70	0
2	FMN	В	1201	31/31	0.95	0.15	35,43,86,103	0

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















































6.5 Other polymers (i)

There are no such residues in this entry.

