

Full wwPDB X-ray Structure Validation Report (i)

Aug 8, 2023 – 05:49 PM EDT

PDB ID	:	10WR					
Title	:	CRYSTAL STRUCTURE	OF	HUMAN	NFAT1	BOUND	MONOMERI-
		CALLY TO DNA					
Authors	:	Stroud, J.C.; Chen, L.					
Deposited on	:	2003-03-29					
Resolution	:	3.00 Å(reported)					

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

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

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

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
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 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive	Similar resolution
	$(\# { m Entries})$	$(\# { m Entries}, { m resolution} { m range}({ m \AA}))$
R _{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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	А	15	7% 13% 87%	
1	С	15	100%	
1	Е	15	80%	20%
1	G	15	7% 7% 93%	
2	В	15	93%	7%



Mol	Chain	Length	Quality of chain	L	
2	D	15	93%		7%
2	F	15	7% 87%		7%
2	Н	15	93%		7%
3	М	284	51%	48%	.
3	Ν	284	15%	44%	5%
3	Р	284	2% 56%	41%	•
3	Q	284	% 50%	49%	•



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2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 11436 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Δ	15	Total	С	Ν	0	Р	0	0	0
1	A	10	310	149	61	86	14	0	0	0
1	C	15	Total	С	Ν	0	Р	0	0	0
1		10	310	149	61	86	14	0	0	0
1	F	15	Total	С	Ν	0	Р	0	0	0
1		10	310	149	61	86	14	0	0	0
1	C	15	Total	С	Ν	Ο	Р	0	0	0
1	I G	61	310	149	61	86	14	0	0	0

• Molecule 1 is a DNA chain called NFAT1 Monomeric Binding Site, Plus Strand.

• Molecule 2 is a DNA chain called NFAT1 Monomeric Binding Site, Minus Strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
0	р	15	Total	С	Ν	0	Р	0	0	0
	D	10	299	146	49	90	14	0	0	0
0	П	15	Total	С	Ν	0	Р	0	0	0
	D	10	299	146	49	90	14	0	0	0
0	Б	15	Total	С	Ν	Ο	Р	0	0	0
	Г	10	299	146	49	90	14	0	0	0
0	ц	15	Total	С	Ν	Ο	Р	0	0	0
	п	10	299	146	49	90	14	0	U	

• Molecule 3 is a protein called Nuclear factor of activated T-cells, cytoplasmic 2.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
9	м	201	Total	С	Ν	0	\mathbf{S}	0	0	0
3	1/1	204	2250	1414	411	416	9	0	0	0
9	N	201	Total	С	Ν	0	S	0	0	0
5	IN	204	2250	1414	411	416	9	0	0	0
9	D	201	Total	С	Ν	0	S	0	0	0
3	Г	204	2250	1414	411	416	9	0	0	0
9	0	201	Total	С	Ν	0	S	0	0	0
5	Q	204	2250	1414	411	416	9	0	0	0



Chain	Residue	Modelled	Actual	Comment	Reference
М	395	VAL	-	cloning artifact	UNP Q13469
N	395	VAL	-	cloning artifact	UNP Q13469
Р	395	VAL	-	cloning artifact	UNP Q13469
Q	395	VAL	-	cloning artifact	UNP Q13469

There are 4 discrepancies between the modelled and reference sequences:



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: NFAT1 Monomeric Binding Site, Plus Strand



• Molecule 2: NFAT1 Monomeric Binding Site, Minus Strand



Chain D: 93% 7% 75003 75004 75005 75006 75006 75008 75008 500 • Molecule 2: NFAT1 Monomeric Binding Site, Minus Strand Chain F: 7% 87% 7% 5005 5006 5007 5008 5008 5009 5010 • Molecule 2: NFAT1 Monomeric Binding Site, Minus Strand Chain H: 93% 7% • Molecule 3: Nuclear factor of activated T-cells, cytoplasmic 2 Chain M: 51% 48% 000 001 001 • Molecule 3: Nuclear factor of activated T-cells, cytoplasmic 2 15% Chain N: 51% 44% 5%

S633 S633 N635 N635 N635 P635 N635 P635 P635 P635 P635 P643 F639 F645 P645 P645 P645 P645 P645 P645 P645 P653 P654 P655 P655 P656 P657 P658 P659 P650 P650 P651 P657

 \bullet Molecule 3: Nuclear factor of activated T-cells, cytoplasmic 2





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	100.65Å 94.85Å 112.79Å	Depositor
a, b, c, α , β , γ	90.00° 104.34° 90.00°	Depositor
Bosolution (Å)	20.00 - 3.00	Depositor
Resolution (A)	20.01 - 2.98	EDS
% Data completeness	(Not available) (20.00-3.00)	Depositor
(in resolution range)	91.5 (20.01-2.98)	EDS
R _{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.42 (at 2.98 \text{\AA})$	Xtriage
Refinement program	CNS	Depositor
D D	0.241 , 0.273	Depositor
$\mathbf{n}, \mathbf{n}_{free}$	0.251 , 0.276	DCC
R_{free} test set	3538 reflections $(8.91%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	59.5	Xtriage
Anisotropy	0.697	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.31,60.6	EDS
L-test for twinning ²	$ \langle L \rangle = 0.49, \langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	11436	wwPDB-VP
Average B, all atoms $(Å^2)$	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 7.43% 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)

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

Mol	Chain	Bo	nd lengths	Bo	ond angles	
	Ullaili	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.71	0/349	0.89	0/538	
1	С	0.63	0/349	0.78	0/538	
1	Е	0.78	0/349	1.10	3/538~(0.6%)	
1	G	0.55	0/349	0.78	0/538	
2	В	0.79	0/333	0.99	1/511~(0.2%)	
2	D	0.88	1/333~(0.3%)	1.02	1/511~(0.2%)	
2	F	0.70	0/333	0.87	0/511	
2	Н	0.64	0/333	0.81	1/511~(0.2%)	
3	М	0.52	0/2300	0.76	0/3115	
3	Ν	0.51	0/2300	0.79	0/3115	
3	Р	0.49	0/2300	0.74	0/3115	
3	Q	0.47	0/2300	0.72	1/3115~(0.0%)	
All	All	0.55	1/11928~(0.0%)	0.79	$7/16656 \ (0.0\%)$	

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	Ε	0	1
2	F	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
2	D	5001	DA	N9-C4	-7.20	1.33	1.37

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	Ε	4004	DC	O5'-P-OP2	-6.38	99.96	105.70



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	В	5004	DT	OP2-P-O3'	6.15	118.73	105.20
1	Ε	4004	DC	O4'-C4'-C3'	-5.32	102.37	104.50
2	Н	5008	DT	N1-C1'-C2'	5.16	122.40	112.60
2	D	5003	DC	O5'-P-OP2	5.12	116.85	110.70
3	Q	494	GLY	N-CA-C	-5.12	100.30	113.10
1	Ε	4003	DG	O5'-P-OP1	-5.12	101.09	105.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	Е	4001	DT	Sidechain
2	F	5002	DA	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	310	0	171	33	0
1	С	310	0	171	36	0
1	Е	310	0	171	24	0
1	G	310	0	171	36	0
2	В	299	0	173	23	0
2	D	299	0	173	16	0
2	F	299	0	173	23	0
2	Н	299	0	173	17	0
3	М	2250	0	2238	142	0
3	Ν	2250	0	2238	135	0
3	Р	2250	0	2238	121	0
3	Q	2250	0	2238	143	0
All	All	11436	0	10328	724	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 33.

All (724) 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:A:4008:DA:OP1	3:M:665:ARG:HB3	1.37	1.17
1:C:4003:DG:H2"	1:C:4004:DC:H5'	1.20	1.16
3:M:421:ARG:HD2	3:M:571:GLN:HB2	1.27	1.12
1:G:4003:DG:H2"	1:G:4004:DC:H5'	1.21	1.11
1:A:4004:DC:H2"	1:A:4005:DT:H5"	1.16	1.09
1:E:4004:DC:H2"	1:E:4005:DT:H5"	1.10	1.09
1:C:4003:DG:H2"	1:C:4004:DC:C5'	1.84	1.07
1:A:4003:DG:H2"	1:A:4004:DC:C5'	1.83	1.07
1:A:4003:DG:H2"	1:A:4004:DC:H5'	1.09	1.07
2:B:5003:DC:H1'	2:B:5004:DT:H5'	1.38	1.06
1:G:4004:DC:H2"	1:G:4005:DT:H5"	1.07	1.03
1:C:4004:DC:C2'	1:C:4005:DT:H5"	1.87	1.03
1:G:4004:DC:C2'	1:G:4005:DT:H5"	1.87	1.03
2:D:5015:DC:H4'	2:D:5015:DC:OP1	1.59	1.02
1:A:4002:DT:H2"	1:A:4003:DG:O4'	1.59	1.02
1:C:4003:DG:H4'	1:C:4003:DG:OP1	1.59	1.01
1:C:4004:DC:H2"	1:C:4005:DT:H5"	1.04	1.01
3:N:577:LEU:HB2	3:N:578:PRO:HD3	1.43	1.00
3:M:457:GLN:HG2	3:M:500:GLU:OE1	1.62	1.00
3:P:432:ALA:HB2	3:P:479:ILE:HD12	1.43	0.99
3:N:617:ASP:OD2	3:N:619:GLN:HG2	1.66	0.96
1:G:4003:DG:H2"	1:G:4004:DC:C5'	1.95	0.95
1:A:4003:DG:H4'	1:A:4003:DG:OP1	1.63	0.95
1:C:4001:DT:H2'	1:C:4002:DT:H72	1.49	0.95
1:A:4003:DG:C2'	1:A:4004:DC:H5'	1.96	0.95
2:F:5015:DC:H4'	2:F:5015:DC:OP1	1.63	0.95
2:F:5002:DA:H4'	2:F:5003:DC:OP1	1.68	0.93
3:Q:413:GLU:HG2	3:Q:510:ARG:NH2	1.83	0.93
2:H:5015:DC:H4'	2:H:5015:DC:OP1	1.67	0.91
3:Q:644:GLU:OE1	3:Q:648:LYS:HD3	1.70	0.91
1:E:4004:DC:H2"	1:E:4005:DT:C5'	2.00	0.91
2:B:5015:DC:H4'	2:B:5015:DC:OP1	1.70	0.91
1:A:4004:DC:C2'	1:A:4005:DT:H5"	2.01	0.89
1:G:4004:DC:H2"	1:G:4005:DT:C5'	2.00	0.89
3:P:581:GLU:HG2	3:P:600:GLY:HA2	1.54	0.88
1:E:4004:DC:C2'	1:E:4005:DT:H5"	2.03	0.87
1:C:4003:DG:C2'	1:C:4004:DC:H5'	2.03	0.87
3:M:418:PRO:HB3	3:P:411:ARG:NH2	1.89	0.87
1:G:4003:DG:H4'	1:G:4003:DG:OP1	1.74	0.85
3:P:596:MET:HB2	3:P:642:ILE:HD11	1.58	0.85
1:E:4012:DA:H2"	1:E:4013:DT:H5'	1.55	0.85
3:M:547:ARG:NH2	3:M:561:GLN:OE1	2.11	0.84



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:G:4012:DA:H2"	1:G:4013:DT:H5'	1.58	0.84
3:N:620:GLN:O	3:N:620:GLN:HG3	1.77	0.84
3:P:485:THR:HG22	3:P:514:ASP:OD1	1.76	0.84
1:C:4004:DC:H2"	1:C:4005:DT:C5'	1.99	0.84
1:G:4001:DT:H2'	1:G:4002:DT:H72	1.58	0.83
3:Q:578:PRO:HA	3:Q:602:ASN:HB2	1.59	0.83
1:G:4008:DA:H2"	1:G:4009:DA:C8	2.13	0.83
1:G:4003:DG:C2'	1:G:4004:DC:H5'	2.06	0.82
3:M:415:GLN:HE22	3:M:565:ASN:H	1.28	0.82
3:N:578:PRO:HG3	3:N:662:ASN:ND2	1.93	0.82
3:N:633:SER:O	3:Q:554:SER:HB3	1.80	0.82
1:A:4007:DG:H1'	1:A:4008:DA:H5"	1.62	0.81
1:A:4008:DA:H2"	1:A:4009:DA:C8	2.16	0.81
3:P:421:ARG:HD2	3:P:571:GLN:HG3	1.60	0.81
2:B:5002:DA:H2"	2:B:5003:DC:OP2	1.81	0.81
3:N:421:ARG:HD2	3:N:571:GLN:HB2	1.63	0.80
1:C:4002:DT:H2"	1:C:4003:DG:O4'	1.82	0.80
3:M:418:PRO:HB3	3:P:411:ARG:HH22	1.45	0.80
3:Q:488:SER:HB2	3:Q:499:LEU:HD11	1.65	0.79
3:M:413:GLU:HG2	3:M:510:ARG:HH22	1.47	0.79
1:G:4001:DT:H2'	1:G:4002:DT:C7	2.11	0.79
3:N:653:PRO:HG3	3:N:677:PRO:HD2	1.66	0.78
1:A:4008:DA:OP1	3:M:665:ARG:CB	2.28	0.78
3:P:520:LYS:HZ1	3:P:523:ASN:HD21	1.28	0.78
3:M:460:ILE:HD13	3:M:518:ILE:HG23	1.66	0.77
3:M:614:LYS:HA	3:M:619:GLN:O	1.83	0.77
2:B:5005:DA:H1'	2:B:5006:DT:H5"	1.67	0.77
3:N:468:LEU:HD23	3:N:561:GLN:NE2	2.00	0.76
1:C:4012:DA:H2"	1:C:4013:DT:H5'	1.67	0.76
3:M:415:GLN:NE2	3:M:565:ASN:H	1.83	0.76
3:Q:596:MET:HB2	3:Q:642:ILE:HD11	1.68	0.76
3:N:467:ILE:HG13	3:Q:583:GLN:O	1.85	0.76
2:B:5009:DT:H1'	2:B:5010:DT:H5'	1.68	0.75
3:M:414:VAL:HG23	3:M:442:VAL:HB	1.67	0.75
3:Q:415:GLN:HE22	3:Q:565:ASN:H	1.31	0.75
3:M:479:ILE:HG22	3:M:484:VAL:HG21	1.68	0.75
2:H:5005:DA:H1'	2:H:5006:DT:H5"	1.69	0.74
3:Q:581:GLU:HG2	3:Q:600:GLY:HA2	1.69	0.74
3:P:488:SER:HB2	3:P:499:LEU:HD11	1.69	0.74
3:P:644:GLU:OE1	3:P:648:LYS:HD3	1.87	0.74
3:M:604:THR:HG22	3:M:605:SER:H	1.52	0.74



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:4006:DG:H2"	1:A:4007:DG:H5'	1.68	0.74
1:E:4008:DA:H2"	1:E:4009:DA:C8	2.24	0.73
1:C:4001:DT:H2'	1:C:4002:DT:C7	2.19	0.73
1:G:4002:DT:H2"	1:G:4003:DG:O4'	1.89	0.73
2:H:5004:DT:H2"	2:H:5005:DA:OP2	1.89	0.73
3:N:403:SER:O	3:N:560:LEU:HD13	1.89	0.73
3:Q:485:THR:HG22	3:Q:514:ASP:OD1	1.88	0.72
1:C:4008:DA:H2"	1:C:4009:DA:C8	2.24	0.72
3:N:457:GLN:NE2	3:N:500:GLU:OE2	2.20	0.72
3:P:524:ALA:O	3:P:528:LEU:HD13	1.89	0.72
3:Q:432:ALA:HB2	3:Q:479:ILE:HD12	1.71	0.72
3:M:485:THR:HG22	3:M:514:ASP:OD1	1.89	0.72
2:F:5005:DA:H1'	2:F:5006:DT:H5"	1.70	0.72
1:E:4012:DA:H2"	1:E:4013:DT:C5'	2.19	0.71
1:G:4011:DA:H1'	1:G:4012:DA:H5"	1.73	0.71
1:G:4012:DA:H2"	1:G:4013:DT:C5'	2.21	0.71
1:E:4007:DG:H2"	1:E:4008:DA:H5"	1.73	0.71
3:M:413:GLU:HG2	3:M:510:ARG:NH2	2.04	0.71
1:E:4007:DG:H2"	1:E:4008:DA:C5'	2.20	0.70
3:Q:617:ASP:OD2	3:Q:619:GLN:HG2	1.90	0.70
3:P:647:ASN:O	3:P:650:ILE:HG23	1.91	0.70
3:M:604:THR:HG22	3:M:605:SER:N	2.05	0.70
3:N:581:GLU:O	3:N:582:ARG:HG3	1.91	0.70
3:N:489:TYR:CE2	3:N:500:GLU:HB2	2.26	0.70
3:P:415:GLN:NE2	3:P:416:PRO:HD2	2.06	0.70
3:M:596:MET:HB2	3:M:642:ILE:HD11	1.72	0.69
2:H:5001:DA:H2"	2:H:5002:DA:C8	2.27	0.69
3:N:489:TYR:CE1	3:N:500:GLU:HG3	2.27	0.69
3:M:574:ALA:HB2	3:M:577:LEU:HD12	1.74	0.69
3:M:471:HIS:HE1	3:M:473:PHE:HB2	1.57	0.69
1:A:4005:DT:H2"	1:A:4006:DG:C8	2.29	0.68
3:M:664:LYS:HG3	3:M:665:ARG:HG3	1.75	0.68
3:P:415:GLN:HE21	3:P:416:PRO:HD2	1.56	0.68
3:P:471:HIS:CD2	3:P:474:TYR:HD2	2.11	0.68
3:N:524:ALA:O	3:N:528:LEU:HD13	1.93	0.68
3:P:573:SER:HB2	3:P:577:LEU:CD1	2.24	0.68
3:M:471:HIS:CE1	3:M:473:PHE:HB2	2.29	0.67
1:C:4011:DA:H1'	1:C:4012:DA:H5"	1.77	0.67
3:N:432:ALA:HB2	3:N:479:ILE:HD12	1.74	0.67
3:Q:413:GLU:HG2	3:Q:510:ARG:HH22	1.56	0.67
2:F:5003:DC:H2"	2:F:5004:DT:OP2	1.93	0.67



	• • • • • • •	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:G:4007:DG:H1'	1:G:4008:DA:H5"	1.75	0.67
2:D:5005:DA:H1'	2:D:5006:DT:H5"	1.76	0.67
3:M:557:ILE:HD12	3:M:557:ILE:N	2.09	0.67
3:P:520:LYS:NZ	3:P:523:ASN:HD21	1.93	0.67
3:M:468:LEU:HD23	3:M:561:GLN:NE2	2.08	0.67
3:M:580:VAL:HB	3:M:671:GLN:NE2	2.10	0.66
3:Q:580:VAL:HB	3:Q:671:GLN:NE2	2.09	0.66
1:E:4007:DG:C2'	1:E:4008:DA:H5"	2.26	0.66
3:P:603:PHE:CD1	3:P:638:LEU:HG	2.30	0.66
3:M:581:GLU:HG2	3:M:600:GLY:HA2	1.78	0.66
3:P:492:ILE:HG21	3:Q:492:ILE:HD11	1.77	0.66
3:Q:468:LEU:HD21	3:Q:543:ARG:HH11	1.61	0.66
3:M:578:PRO:HB3	3:M:602:ASN:O	1.96	0.66
3:N:421:ARG:NH2	3:N:430:ARG:NH2	2.44	0.66
3:Q:464:ASP:CG	3:Q:541:ARG:HE	1.98	0.65
2:B:5006:DT:H2"	2:B:5007:DT:H5'	1.79	0.65
1:G:4005:DT:H2"	1:G:4006:DG:C8	2.31	0.65
1:C:4007:DG:H1'	1:C:4008:DA:H5"	1.79	0.65
2:H:5006:DT:H2"	2:H:5007:DT:H5'	1.78	0.65
3:N:481:GLY:O	3:N:483:THR:N	2.30	0.65
3:N:489:TYR:CZ	3:N:500:GLU:HG3	2.31	0.64
3:Q:524:ALA:O	3:Q:528:LEU:HD13	1.96	0.64
2:B:5014:DG:H2"	2:B:5015:DC:O5'	1.98	0.64
1:C:4005:DT:H2"	1:C:4006:DG:C8	2.33	0.64
3:P:520:LYS:HZ1	3:P:523:ASN:ND2	1.94	0.64
1:A:4004:DC:H2"	1:A:4005:DT:C5'	2.10	0.64
1:C:4003:DG:H2"	1:C:4004:DC:H5"	1.79	0.64
2:F:5006:DT:H2"	2:F:5007:DT:H5'	1.78	0.64
3:M:489:TYR:CE2	3:M:500:GLU:HB3	2.32	0.64
3:P:580:VAL:HB	3:P:671:GLN:NE2	2.12	0.64
1:A:4012:DA:H2"	1:A:4013:DT:H5'	1.79	0.64
3:M:644:GLU:OE1	3:M:648:LYS:HD3	1.98	0.64
3:P:421:ARG:HD2	3:P:571:GLN:CG	2.27	0.64
3:Q:463:ALA:HB2	3:Q:542:VAL:C	2.18	0.64
3:Q:584:ASP:HB2	3:Q:597:ILE:HB	1.79	0.64
1:G:4007:DG:C2'	1:G:4008:DA:H5"	2.28	0.64
3:N:647:ASN:O	3:N:650:ILE:HG23	1.98	0.64
3:M:423:HIS:O	3:M:519:LEU:HD12	1.97	0.64
3:M:520:LYS:HZ1	3:M:523:ASN:HD21	1.46	0.63
3:N:577:LEU:HB2	3:N:578:PRO:CD	2.24	0.63
3:Q:612:THR:O	3:Q:656:VAL:HG22	1.98	0.63



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
3:Q:614:LYS:HA	3:Q:619:GLN:O	1.97	0.63
2:D:5003:DC:H2"	2:D:5004:DT:OP2	1.98	0.63
3:N:414:VAL:HG23	3:N:442:VAL:HB	1.81	0.63
1:G:4007:DG:H2"	1:G:4008:DA:C5'	2.28	0.63
3:Q:415:GLN:NE2	3:Q:565:ASN:H	1.95	0.63
3:Q:463:ALA:HA	3:Q:543:ARG:HD2	1.81	0.63
1:E:4011:DA:H1'	1:E:4012:DA:H5"	1.79	0.63
1:E:4005:DT:H2"	1:E:4006:DG:C8	2.33	0.63
3:Q:484:VAL:HG13	3:Q:515:CYS:HB3	1.81	0.62
2:F:5015:DC:H5"	2:F:5015:DC:H6	1.64	0.62
1:G:4007:DG:H2"	1:G:4008:DA:H5"	1.81	0.62
2:H:5014:DG:H2"	2:H:5015:DC:O5'	1.99	0.62
3:P:651:ARG:HH11	3:P:651:ARG:HG3	1.63	0.62
1:A:4003:DG:C2'	1:A:4004:DC:C5'	2.69	0.62
3:M:461:GLY:HA2	3:M:471:HIS:H	1.64	0.62
1:E:4014:DA:H1'	1:E:4015:DG:H5'	1.80	0.62
1:C:4007:DG:H2"	1:C:4008:DA:C5'	2.30	0.61
3:M:612:THR:O	3:M:656:VAL:HG22	2.01	0.61
1:C:4001:DT:H6	1:C:4001:DT:H5'	1.65	0.61
3:N:415:GLN:NE2	3:N:565:ASN:H	1.98	0.61
3:Q:588:CYS:SG	3:Q:589:LEU:N	2.74	0.61
1:C:4007:DG:C2'	1:C:4008:DA:H5"	2.30	0.61
3:P:614:LYS:HA	3:P:619:GLN:O	2.01	0.61
2:B:5009:DT:OP2	3:M:424:TYR:OH	2.12	0.61
2:H:5002:DA:H1'	2:H:5003:DC:H5'	1.83	0.61
3:N:471:HIS:CE1	3:N:473:PHE:HB2	2.35	0.61
3:M:416:PRO:HG3	3:M:544:LEU:HD12	1.83	0.61
3:P:580:VAL:CG2	3:P:671:GLN:HE21	2.14	0.60
3:M:450:GLU:CD	3:M:451:ASN:H	2.04	0.60
3:Q:421:ARG:HD2	3:Q:571:GLN:HB2	1.82	0.60
3:M:578:PRO:HA	3:M:601:GLN:O	2.01	0.60
3:M:432:ALA:HB2	3:M:479:ILE:HD12	1.82	0.60
1:A:4007:DG:C1'	1:A:4008:DA:H5"	2.32	0.60
1:G:4010:DA:H1'	1:G:4011:DA:H5'	1.82	0.60
3:P:431:GLY:O	3:P:479:ILE:HD11	2.02	0.60
3:N:471:HIS:HE1	3:N:473:PHE:HB2	1.64	0.60
3:P:464:ASP:OD1	3:P:465:GLU:N	2.35	0.60
1:A:4002:DT:H2'	1:A:4003:DG:C8	2.37	0.60
2:B:5003:DC:C1'	2:B:5004:DT:H5'	2.24	0.60
3:P:596:MET:CB	3:P:642:ILE:HD11	2.31	0.59
1:E:4006:DG:H2"	1:E:4007:DG:H5'	1.85	0.59



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
3:P:612:THR:O	3:P:656:VAL:HG22	2.01	0.59
3:M:460:ILE:CD1	3:M:518:ILE:HG23	2.33	0.59
3:Q:582:ARG:HB2	3:Q:599:THR:OG1	2.03	0.59
3:N:423:HIS:HB3	3:N:430:ARG:HD2	1.84	0.59
1:C:4006:DG:H2"	1:C:4007:DG:H5'	1.85	0.59
3:M:489:TYR:CZ	3:M:500:GLU:HB3	2.38	0.59
1:G:4006:DG:H2"	1:G:4007:DG:H5'	1.83	0.59
3:N:400:PRO:HB2	3:Q:582:ARG:NH2	2.18	0.59
2:B:5003:DC:H1'	2:B:5004:DT:C5'	2.23	0.59
3:Q:484:VAL:CG1	3:Q:515:CYS:HB3	2.33	0.59
3:Q:603:PHE:CD1	3:Q:638:LEU:HG	2.38	0.59
2:D:5013:DA:H2"	2:D:5014:DG:OP2	2.02	0.59
3:N:415:GLN:HE21	3:N:416:PRO:HD2	1.68	0.59
3:P:615:THR:HB	3:P:617:ASP:OD2	2.03	0.59
3:P:421:ARG:HD2	3:P:571:GLN:HB2	1.84	0.58
3:P:557:ILE:N	3:P:557:ILE:HD12	2.17	0.58
3:N:669:GLN:OE1	3:N:669:GLN:HA	2.03	0.58
1:C:4007:DG:H2"	1:C:4008:DA:H5"	1.85	0.58
2:F:5007:DT:OP1	3:P:665:ARG:NH1	2.36	0.58
2:F:5002:DA:C4'	2:F:5003:DC:OP1	2.50	0.58
3:N:578:PRO:HB2	3:N:668:SER:HB3	1.84	0.58
3:P:488:SER:HB3	3:P:501:ILE:HD11	1.84	0.58
2:F:5013:DA:H2"	2:F:5014:DG:OP2	2.04	0.58
3:N:487:THR:HG22	3:N:488:SER:N	2.19	0.58
3:N:635:PRO:HB3	3:Q:552:GLU:OE1	2.04	0.58
2:D:5006:DT:H2"	2:D:5007:DT:H5'	1.84	0.58
2:F:5001:DA:H2"	2:F:5002:DA:H8	1.69	0.58
1:G:4012:DA:H1'	1:G:4013:DT:H5"	1.85	0.57
3:P:455:GLY:HA3	3:P:500:GLU:OE1	2.04	0.57
1:E:4007:DG:H1'	1:E:4008:DA:H5"	1.86	0.57
3:M:524:ALA:O	3:M:528:LEU:HD13	2.05	0.57
3:Q:557:ILE:HD12	3:Q:557:ILE:N	2.20	0.57
3:Q:580:VAL:CG1	3:Q:671:GLN:HE21	2.17	0.57
3:Q:554:SER:OG	3:Q:556:ARG:HD2	2.05	0.57
1:C:4003:DG:C2'	1:C:4004:DC:C5'	2.70	0.57
3:N:537:ARG:O	3:N:538:LYS:HB2	2.03	0.57
1:C:4010:DA:H1'	1:C:4011:DA:H5'	1.87	0.56
3:M:417:LYS:HG3	3:M:434:LYS:O	2.05	0.56
3:Q:547:ARG:NH2	3:Q:561:GLN:OE1	2.34	0.56
3:N:501:ILE:HG23	3:N:502:PRO:HD2	1.87	0.56
3:P:578:PRO:HA	3:P:602:ASN:HB2	1.87	0.56



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
3:Q:413:GLU:CG	3:Q:510:ARG:HH22	2.19	0.56
2:B:5011:DC:H1'	2:B:5012:DC:H5'	1.87	0.56
3:N:634:GLN:CB	3:N:635:PRO:HD2	2.36	0.56
3:P:520:LYS:NZ	3:P:523:ASN:ND2	2.53	0.56
3:N:425:GLU:O	3:N:427:GLU:N	2.38	0.56
3:N:580:VAL:HB	3:N:671:GLN:NE2	2.20	0.56
3:P:427:GLU:OE1	3:P:430:ARG:NH2	2.34	0.56
3:P:651:ARG:HG3	3:P:651:ARG:NH1	2.19	0.56
1:A:4012:DA:H2"	1:A:4013:DT:C5'	2.36	0.56
3:M:467:ILE:O	3:M:467:ILE:HG22	2.06	0.56
1:G:4007:DG:C1'	1:G:4008:DA:H5"	2.36	0.56
3:P:421:ARG:HD2	3:P:571:GLN:CB	2.36	0.56
3:M:615:THR:OG1	3:M:619:GLN:HB2	2.06	0.55
3:P:423:HIS:HB3	3:P:430:ARG:HB2	1.87	0.55
3:P:552:GLU:O	3:P:554:SER:N	2.39	0.55
3:P:578:PRO:HG2	3:P:668:SER:HB3	1.87	0.55
3:Q:615:THR:HG22	3:Q:616:THR:H	1.71	0.55
1:G:4002:DT:C2'	1:G:4003:DG:C8	2.90	0.55
2:F:5006:DT:H2"	2:F:5007:DT:C5'	2.36	0.55
2:F:5014:DG:H2"	2:F:5015:DC:H5"	1.87	0.55
3:M:488:SER:HB3	3:M:501:ILE:HD11	1.89	0.55
3:Q:415:GLN:NE2	3:Q:416:PRO:HD2	2.22	0.55
3:N:423:HIS:CB	3:N:430:ARG:HD2	2.37	0.55
3:N:584:ASP:HB3	3:N:597:ILE:H	1.71	0.55
3:Q:419:HIS:HB3	3:Q:579:MET:SD	2.46	0.55
3:M:420:HIS:O	3:M:569:CYS:HA	2.06	0.55
3:M:604:THR:CG2	3:M:605:SER:H	2.18	0.55
3:N:583:GLN:HA	3:N:598:LEU:HD12	1.89	0.55
3:Q:419:HIS:HE1	3:Q:601:GLN:HG3	1.72	0.55
3:P:529:ARG:HG3	3:Q:495:ASN:OD1	2.07	0.54
1:G:4008:DA:H2"	1:G:4009:DA:N7	2.22	0.54
1:G:4004:DC:C3'	1:G:4005:DT:H5"	2.38	0.54
3:P:552:GLU:C	3:P:554:SER:H	2.10	0.54
3:Q:615:THR:HG22	3:Q:616:THR:N	2.23	0.54
2:B:5007:DT:C6	2:B:5008:DT:H72	2.43	0.54
3:Q:415:GLN:HE21	3:Q:416:PRO:HD2	1.73	0.54
3:N:633:SER:C	3:Q:554:SER:HB3	2.27	0.54
3:P:573:SER:HB2	3:P:577:LEU:HD11	1.90	0.54
2:D:5014:DG:H2"	2:D:5015:DC:O5'	2.08	0.54
1:C:4002:DT:H2'	1:C:4003:DG:H8	1.73	0.54
2:D:5011:DC:H1'	2:D:5012:DC:H5'	1.90	0.54



		Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
3:M:423:HIS:HB3	3:M:430:ARG:HD2	1.89	0.53	
3:P:628:VAL:HG23	3:P:628:VAL:O 2.08		0.53	
3:Q:462:THR:HB	3:Q:465:GLU:HB2	1.90	0.53	
3:Q:464:ASP:OD2	3:Q:541:ARG:NE	2.39	0.53	
1:A:4002:DT:H2'	1:A:4003:DG:H8	1.73	0.53	
3:N:425:GLU:C	3:N:427:GLU:H	2.11	0.53	
3:Q:659:TYR:CE1	3:Q:661:ILE:HD11	2.43	0.53	
3:P:432:ALA:CB	3:P:479:ILE:HD12	2.28	0.53	
3:N:500:GLU:O	3:N:501:ILE:HD12	2.09	0.53	
1:A:4002:DT:C2'	1:A:4003:DG:C8	2.91	0.53	
3:N:644:GLU:OE1	3:N:648:LYS:HD3	2.08	0.53	
3:Q:423:HIS:HA	3:Q:430:ARG:HD2	1.89	0.53	
3:M:520:LYS:NZ	3:M:523:ASN:HD21	2.06	0.53	
3:P:425:GLU:C	3:P:427:GLU:H	2.12	0.53	
1:A:4011:DA:H1'	1:A:4012:DA:H5"	1.91	0.53	
2:H:5001:DA:H8	2:H:5001:DA:HO5'	1.54	0.53	
3:M:520:LYS:HZ1	3:M:523:ASN:ND2	2.06	0.53	
3:N:557:ILE:N	3:N:557:ILE:HD12	2.23	0.53	
3:N:577:LEU:O	3:N:602:ASN:HB2	2.08	0.53	
3:M:415:GLN:NE2	3:M:416:PRO:HD2	2.24	0.52	
3:N:412:ILE:HG22	3:N:412:ILE:O	2.09	0.52	
3:Q:423:HIS:CA	3:Q:430:ARG:HD2	2.39	0.52	
3:Q:552:GLU:C	3:Q:554:SER:H	2.12	0.52	
3:M:431:GLY:O	3:M:479:ILE:HD11	$\overline{)11}$ 2.08 (
3:M:423:HIS:CB	3:M:430:ARG:HD2	2.40	0.52	
3:M:425:GLU:C	3:M:427:GLU:H	2.12	0.52	
3:N:440:HIS:CD2	3:N:514:ASP:HB3	2.44	0.52	
3:M:418:PRO:HG2	3:P:446:HIS:CD2	2.44	0.52	
3:N:488:SER:HB3	3:N:501:ILE:HD11	1.91	0.52	
3:P:471:HIS:CD2	3:P:473:PHE:H	2.27	0.52	
3:Q:678:VAL:HG13	3:Q:678:VAL:OXT	2.09	0.52	
1:A:4013:DT:H2"	1:A:4014:DA:C8	2.45	0.52	
3:M:467:ILE:CG2	3:M:469:LYS:HE3	2.39	0.52	
3:N:415:GLN:NE2	3:N:416:PRO:HD2	2.24	0.52	
3:Q:571:GLN:O	3:Q:574:ALA:HB3	2.10	0.52	
1:C:4002:DT:C2'	1:C:4003:DG:C8	2.93	0.52	
3:N:397:LEU:HD11	3:N:493:VAL:HB	1.90	0.52	
3:Q:552:GLU:O	3:Q:554:SER:N	2.43	0.52	
3:N:448:TYR:CE1	3:N:450:GLU:HB3	2.44	0.52	
3:P:580:VAL:HG13	3:P:598:LEU:HG	1.91	0.52	
1:C:4007:DG:OP1	3:N:665:ARG:NH2	2.42	0.52	



		Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
2:H:5006:DT:H2"	2:H:5007:DT:C5'	:5007:DT:C5' 2.40		
3:N:485:THR:HG22	3:N:485:THR:O	2.10	0.52	
3:N:417:LYS:HG3	3:N:434:LYS:O	2.10	0.52	
3:N:614:LYS:HA	3:N:619:GLN:O	2.09	0.52	
3:P:421:ARG:CD	3:P:571:GLN:HG3	2.35	0.52	
3:P:492:ILE:N	3:P:492:ILE:HD12	2.25	0.52	
3:P:432:ALA:HB2	3:P:479:ILE:CD1	2.31	0.51	
3:P:617:ASP:OD2	3:P:619:GLN:HG2	2.10	0.51	
3:Q:628:VAL:O	3:Q:628:VAL:HG23	2.10	0.51	
3:M:574:ALA:CB	3:M:577:LEU:HD12	2.41	0.51	
3:M:587:SER:HA	3:M:674:THR:O	2.10	0.51	
3:N:552:GLU:C	3:N:554:SER:H	2.13	0.51	
1:C:4007:DG:C1'	1:C:4008:DA:H5"	2.40	0.51	
3:M:418:PRO:CB	3:P:411:ARG:HH22	2.21	0.51	
1:A:4003:DG:OP1	1:A:4003:DG:C4'	2.46	0.51	
3:M:607:SER:OG	3:M:662:ASN:ND2	2.44	0.51	
3:Q:488:SER:HB3	3:Q:501:ILE:HD11	1.93	0.51	
3:M:661:ILE:HG23	3:M:663:GLY:O	2.11	0.51	
3:N:411:ARG:HG3	411:ARG:HG3 3:N:412:ILE:N		0.51	
3:P:421:ARG:NH1	3:P:571:GLN:HG3	2.26	0.51	
3:P:430:ARG:HG2	3:P:430:ARG:HH11	1.76	0.51	
2:D:5002:DA:H1'	002:DA:H1' 2:D:5003:DC:O5'		0.50	
3:N:457:GLN:HG2	3:N:500:GLU:OE1	3:N:500:GLU:OE1 2.11		
3:P:573:SER:HA	3:P:576:GLU:HB3	LU:HB3 1.92		
3:Q:423:HIS:HB3	3:Q:430:ARG:CG	2.41	0.50	
1:E:4002:DT:H2"	1:E:4003:DG:O5'	2.10	0.50	
3:M:479:ILE:HG22	3:M:484:VAL:CG2	2.40	0.50	
3:N:523:ASN:O	3:N:527:GLU:HG3	2.11	0.50	
3:N:565:ASN:HB3	3:N:566:PRO:HD2	1.93	0.50	
3:P:671:GLN:OE1	3:P:671:GLN:HA	2.12	0.50	
3:M:423:HIS:HB3	3:M:430:ARG:CG	2.41	0.50	
3:N:548:VAL:HG22	3:N:549:HIS:N	2.26	0.50	
3:P:479:ILE:HG22	3:P:484:VAL:HG21	1.94	0.50	
3:P:552:GLU:C	3:P:554:SER:N	2.65	0.50	
3:M:413:GLU:CG	3:M:510:ARG:HH22	2.20	0.50	
3:M:467:ILE:HG22	3:M:469:LYS:HG3	1.94	0.50	
3:P:413:GLU:HG2	3:P:510:ARG:HH22	1.77	0.50	
3:P:421:ARG:HH11	3:P:571:GLN:HG3	1.77	0.50	
2:F:5001:DA:H2"	2:F:5002:DA:C8	2.47	0.50	
3:Q:584:ASP:HB3	3:Q:597:ILE:H	1.77	0.50	
1:C:4003:DG:OP1	1:C:4003:DG:C4'	2.42	0.50	



		Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
3:M:578:PRO:HA	3:M:602:ASN:HB3	1.93	0.50	
3:N:463:ALA:HB2	3:N:543:ARG:HG3	1.93	0.50	
3:Q:659:TYR:HE1	3:Q:661:ILE:HD11	1.77	0.50	
3:M:412:ILE:O	3:M:412:ILE:HG22	2.12	0.49	
3:N:467:ILE:CG1	3:Q:583:GLN:O	2.56	0.49	
3:N:481:GLY:C	3:N:483:THR:H	2.15	0.49	
3:P:421:ARG:NH2	3:P:430:ARG:NH2	2.59	0.49	
3:P:486:THR:HG22	3:P:501:ILE:HG13	1.94	0.49	
2:H:5013:DA:H2"	2:H:5014:DG:OP2	2.12	0.49	
3:M:576:GLU:O	3:M:602:ASN:ND2	2.45	0.49	
1:E:4012:DA:H1'	1:E:4013:DT:H5"	1.93	0.49	
3:M:488:SER:HB2	3:M:499:LEU:HD11	1.93	0.49	
3:M:520:LYS:NZ	3:M:521:LEU:O	2.44	0.49	
3:N:603:PHE:HD1	3:N:638:LEU:HG	1.77	0.49	
3:P:634:GLN:CB	3:P:635:PRO:HD2	2.42	0.49	
3:N:594:GLN:O	3:N:642:ILE:HD12	2.11	0.49	
3:Q:572:ARG:HG2	3:Q:572:ARG:HH11	1.76	0.49	
3:M:459:PHE:CZ	3:M:545:VAL:HG11	2.47	0.49	
3:M:500:GLU:HG3	3:M:501:ILE:N	2.27	0.49	
3:N:584:ASP:HB2	3:N:597:ILE:HB	1.95	0.49	
3:Q:541:ARG:HH12	3:Q:669:GLN:CD	2.16	0.49	
1:G:4002:DT:H2'	1:G:4003:DG:H8	1.78	0.49	
3:M:583:GLN:HA	3:M:598:LEU:HD12	1.93	0.49	
2:H:5010:DT:H1'	2:H:5011:DC:H5"	1:DC:H5" 1.95		
3:N:459:PHE:CZ	3:N:545:VAL:HG11	2.47	0.49	
3:N:628:VAL:HG12	3:N:640:VAL:HG22	1.94	0.49	
3:N:653:PRO:CG	3:N:677:PRO:HD2	2.40	0.49	
3:Q:520:LYS:HZ1	3:Q:523:ASN:HD21	1.60	0.49	
1:A:4006:DG:C2'	1:A:4007:DG:H5'	2.39	0.49	
2:H:5011:DC:H1'	2:H:5012:DC:H5'	1.94	0.49	
3:M:411:ARG:HH11	3:M:411:ARG:HG2	1.78	0.49	
3:N:415:GLN:HE22	3:N:565:ASN:H	1.60	0.49	
3:Q:423:HIS:HB3	3:Q:430:ARG:HB2	1.93	0.49	
3:M:411:ARG:HG3	3:M:412:ILE:N	2.27	0.48	
3:N:603:PHE:CD1	3:N:638:LEU:HG	2.48	0.48	
3:P:423:HIS:HB3	3:P:430:ARG:HD2	1.95	0.48	
1:C:4008:DA:H2"	1:C:4009:DA:N7	2.28	0.48	
3:M:465:GLU:CA	3:M:543:ARG:HH12	2.26	0.48	
3:M:468:LEU:HD23	3:M:561:GLN:HE21	1.77	0.48	
3:N:467:ILE:CD1	3:Q:583:GLN:O	2.61	0.48	
3:N:489:TYR:O	3:N:499:LEU:HD12	2.13	0.48	



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
3:P:433:VAL:HG21	3:P:544:LEU:HD21	1.95	0.48	
1:A:4007:DG:C2'	1:A:4008:DA:H5"	2.43	0.48	
3:P:532:GLU:OE1	3:P:534:ASP:HB2	84:ASP:HB2 2.14		
2:B:5001:DA:HO5'	2:B:5001:DA:H8	1.60	0.48	
3:M:489:TYR:CE2	3:M:500:GLU:HG2	2.49	0.48	
3:Q:411:ARG:HG2	3:Q:411:ARG:HH11	1.79	0.48	
3:Q:418:PRO:O	3:Q:567:ILE:HA	2.14	0.48	
3:Q:550:ILE:HB	3:Q:558:VAL:HB	1.95	0.48	
3:Q:584:ASP:CB	3:Q:597:ILE:HB	2.44	0.48	
3:M:576:GLU:O	3:M:576:GLU:HG3	2.14	0.48	
3:N:602:ASN:HD22	3:Q:449:MET:HG3	1.78	0.48	
3:P:580:VAL:CG1	3:P:598:LEU:HG	2.44	0.48	
2:B:5007:DT:H1'	2:B:5008:DT:H5'	1.95	0.48	
2:H:5009:DT:H2'	2:H:5010:DT:H72	1.96	0.48	
3:N:492:ILE:N	3:N:492:ILE:HD12	2.29	0.48	
3:N:547:ARG:HB2	3:N:560:LEU:O	2.13	0.48	
3:P:411:ARG:HG3	3:P:412:ILE:N	2.28	0.48	
1:C:4004:DC:C3'	1:C:4005:DT:H5"	2.42	0.48	
3:M:488:SER:HB3	3:M:501:ILE:CD1	2.43	0.48	
3:N:628:VAL:HG23	3:N:628:VAL:O	2.13	0.48	
3:P:419:HIS:O	3:P:420:HIS:HB2	2.14	0.48	
3:P:471:HIS:HE1	3:P:539:ASN:ND2	2.12	0.48	
1:G:4013:DT:H2"	1:G:4014:DA:C8	2.49	0.47	
3:M:532:GLU:OE1	3:M:534:ASP:HB2	2.14	0.47	
3:N:400:PRO:HG3	3:Q:599:THR:HG21	1.96	0.47	
1:C:4002:DT:H2'	1:C:4003:DG:C8	2.49	0.47	
3:N:468:LEU:HD21	3:N:545:VAL:HG13	1.96	0.47	
3:P:474:TYR:CZ	3:P:520:LYS:HD3	2.49	0.47	
1:C:4002:DT:C2'	1:C:4003:DG:H8	2.26	0.47	
3:P:579:MET:O	3:P:600:GLY:HA3	2.13	0.47	
3:Q:448:TYR:CE1	3:Q:450:GLU:HB3	2.50	0.47	
1:C:4014:DA:H1'	1:C:4015:DG:H5'	1.95	0.47	
3:N:577:LEU:CB	3:N:578:PRO:HD3	2.31	0.47	
3:N:580:VAL:HB	3:N:671:GLN:HE21	1.78	0.47	
3:P:423:HIS:CB	3:P:430:ARG:HD2	2.44	0.47	
1:G:4002:DT:H2'	1:G:4003:DG:C8	2.49	0.47	
3:M:547:ARG:CZ	3:M:561:GLN:OE1	2.63	0.47	
3:N:423:HIS:HA	3:N:430:ARG:HD2	1.97	0.47	
3:N:584:ASP:O	3:N:584:ASP:OD2	2.32	0.47	
3:P:556:ARG:HG2	3:P:556:ARG:HH11	1.80	0.47	
3:P:615:THR:OG1	3:P:619:GLN:HB2	2.15	0.47	



		Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
3:Q:420:HIS:CD2	3:Q:433:VAL:HA	2.50	0.47	
3:Q:474:TYR:CE1	3:Q:520:LYS:HD3	2.49	0.47	
2:H:5007:DT:C6	2:H:5008:DT:H72	2.50	0.47	
3:M:617:ASP:O	3:M:619:GLN:NE2	2.44	0.47	
3:N:440:HIS:CD2	3:N:514:ASP:CB	2.97	0.47	
3:N:489:TYR:CZ	3:N:500:GLU:CB	2.98	0.47	
3:P:444:GLN:OE1	3:P:510:ARG:NH1	2.48	0.47	
3:Q:552:GLU:C	3:Q:554:SER:N	2.68	0.47	
3:Q:579:MET:O	3:Q:600:GLY:HA3	2.14	0.47	
1:G:4005:DT:OP2	3:Q:431:GLY:HA3	2.15	0.47	
3:P:588:CYS:SG	3:P:589:LEU:N	2.88	0.47	
1:E:4007:DG:C1'	1:E:4008:DA:H5"	2.45	0.47	
3:M:431:GLY:C	3:M:479:ILE:HD11	2.35	0.47	
3:N:413:GLU:HG2	3:N:510:ARG:HH22	1.80	0.47	
3:N:556:ARG:HG2	3:N:556:ARG:HH11	1.80	0.47	
1:G:4003:DG:C2'	1:G:4004:DC:C5'	2.79	0.46	
3:M:397:LEU:HD11	3:M:493:VAL:HB	1.97	0.46	
3:M:552:GLU:C	3:M:554:SER:H	2.18	0.46	
3:Q:615:THR:HB	3:Q:617:ASP:OD2	2.15	0.46	
3:Q:647:ASN:O	3:Q:650:ILE:HG23	2.15	0.46	
1:A:4001:DT:H2'	1:A:4002:DT:C7	2.45	0.46	
2:F:5008:DT:H1'	2:F:5009:DT:H5"	1.97	0.46	
3:N:397:LEU:CD1	3:N:493:VAL:HB	2.45	0.46	
3:P:476:VAL:HG12	3:P:497:LYS:O	2.15	0.46	
1:A:4003:DG:H2"	1:A:4004:DC:H5"	1.89	0.46	
3:M:628:VAL:HG23	3:M:628:VAL:O	2.16	0.46	
3:N:460:ILE:CG2	3:N:542:VAL:HB	2.46	0.46	
3:Q:463:ALA:CB	3:Q:543:ARG:HG3	2.45	0.46	
3:Q:464:ASP:OD1	3:Q:541:ARG:NH2	2.45	0.46	
3:Q:609:VAL:HG21	3:Q:640:VAL:HG21	1.97	0.46	
2:B:5010:DT:H2"	2:B:5011:DC:H5'	1.96	0.46	
3:N:411:ARG:HG2	3:N:411:ARG:HH11	1.79	0.46	
3:N:489:TYR:CZ	3:N:500:GLU:HB2	2.50	0.46	
3:N:674:THR:HG23	3:N:676:HIS:CD2	2.49	0.46	
2:B:5003:DC:H2"	2:B:5004:DT:OP2	2.15	0.46	
3:N:423:HIS:CA	3:N:430:ARG:HD2	2.45	0.46	
3:N:596:MET:HB2	3:N:642:ILE:HD11	1.97	0.46	
3:Q:465:GLU:CD	3:Q:469:LYS:HE2	2.35	0.46	
3:M:462:THR:HG22	3:M:463:ALA:N	2.30	0.46	
3:P:622:TRP:CG	3:P:646:ARG:HD3	2.50	0.46	
3:Q:411:ARG:HG3	3:Q:412:ILE:N	2.30	0.46	



		Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
3:Q:520:LYS:NZ	3:Q:523:ASN:HD21	2.13	0.46	
1:A:4001:DT:H2'	1:A:4002:DT:H72	1.98	0.46	
3:P:408:TYR:HB3	3:P:560:LEU:HD11	1.96	0.46	
3:P:431:GLY:C	3:P:479:ILE:HD11	2.36	0.46	
3:Q:414:VAL:HG23	3:Q:442:VAL:HB	1.98	0.46	
2:F:5007:DT:C6	2:F:5008:DT:H72	2.51	0.45	
3:M:403:SER:O	3:M:560:LEU:HD13	2.17	0.45	
3:M:547:ARG:NE	3:M:561:GLN:OE1	2.50	0.45	
3:M:604:THR:CG2	3:M:605:SER:N	2.73	0.45	
3:P:501:ILE:HG23	3:P:502:PRO:HD2	1.97	0.45	
3:Q:462:THR:CB	3:Q:465:GLU:HB2	2.45	0.45	
2:F:5005:DA:C1'	2:F:5006:DT:H5"	2.43	0.45	
3:M:460:ILE:HD12	3:M:475:GLN:C	2.37	0.45	
3:N:480:THR:O	3:N:480:THR:HG22	2.16	0.45	
3:N:550:ILE:HB	3:N:558:VAL:HB	1.97	0.45	
3:N:552:GLU:O	3:N:554:SER:N	2.49	0.45	
2:B:5013:DA:H2"	2:B:5014:DG:OP2	2.16	0.45	
2:F:5002:DA:H1'	2:F:5003:DC:C6	2.51	0.45	
2:B:5003:DC:H2"	2:B:5004:DT:O5'	2.16	0.45	
2:D:5006:DT:H2"	2:D:5007:DT:C5'	2.46	0.45	
1:A:4007:DG:H2"	1:A:4008:DA:C5'	2.47	0.45	
1:E:4008:DA:H2"	1:E:4009:DA:N7	2.30	0.45	
2:H:5003:DC:H2"	2:H:5004:DT:OP2	2.15	0.45	
3:N:552:GLU:C	3:N:554:SER:N	N 2.70 (
3:Q:404:GLN:HB3	3:Q:409:GLU:HG3	1.98	0.45	
3:M:467:ILE:HG23	3:M:469:LYS:HE3	1.99	0.45	
3:P:526:ILE:O	3:P:529:ARG:HB3	2.17	0.45	
3:Q:412:ILE:HG22	3:Q:412:ILE:O	2.17	0.45	
3:Q:661:ILE:HA	3:Q:666:LYS:O	2.16	0.45	
3:N:442:VAL:HG13	3:N:511:ALA:O	2.16	0.45	
2:D:5008:DT:H1'	2:D:5009:DT:H5"	1.99	0.45	
1:G:4002:DT:H2"	1:G:4003:DG:C8	2.52	0.45	
3:M:582:ARG:HB2	3:M:599:THR:OG1	2.17	0.45	
3:Q:397:LEU:HD23	3:Q:459:PHE:CE1	2.52	0.45	
2:H:5002:DA:H1'	2:H:5003:DC:C5'	2.46	0.45	
3:Q:504:GLU:HA	3:Q:505:PRO:HD3	1.86	0.45	
3:Q:587:SER:HA	3:Q:674:THR:O	2.17	0.45	
1:E:4006:DG:H1'	1:E:4007:DG:H5"	1.98	0.44	
3:M:615:THR:CB	3:M:619:GLN:HB2	2.47	0.44	
3:P:548:VAL:HG22	3:P:549:HIS:N	2.32	0.44	
3:Q:459:PHE:CZ	3:Q:545:VAL:HG11	2.53	0.44	



		Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
3:M:415:GLN:HE22	3:M:565:ASN:N	2.03	0.44	
3:M:552:GLU:C	3:M:554:SER:N	2.71	0.44	
3:P:547:ARG:NH2	3:P:561:GLN:OE1	2.39	0.44	
3:Q:419:HIS:CE1	3:Q:601:GLN:HG3	2.51	0.44	
3:Q:609:VAL:HG21	3:Q:640:VAL:CG2	2.48	0.44	
3:P:486:THR:CG2	3:P:501:ILE:HG13	2.47	0.44	
3:M:450:GLU:CG	3:M:451:ASN:N	2.80	0.44	
3:M:584:ASP:HB3	3:M:597:ILE:H	1.82	0.44	
3:N:417:LYS:HG2	3:N:436:PRO:HA	1.99	0.44	
2:B:5001:DA:H2"	2:B:5002:DA:C8	2.53	0.44	
3:M:440:HIS:CD2	3:M:514:ASP:HB3	2.52	0.44	
3:M:465:GLU:HA	3:M:543:ARG:HH12	1.82	0.44	
3:M:552:GLU:O	3:M:554:SER:N	2.50	0.44	
3:N:581:GLU:HG2	3:N:599:THR:O	2.18	0.44	
3:P:424:TYR:CE2	3:P:520:LYS:HG3	2.53	0.44	
3:Q:622:TRP:CG	3:Q:646:ARG:HD3	2.53	0.44	
2:B:5001:DA:H8	2:B:5001:DA:O5'	2.01	0.44	
3:N:613:GLU:HB2	3:N:622:TRP:HB3	1.99	0.44	
3:P:578:PRO:HA	3:P:601:GLN:O	2.17	0.44	
3:P:661:ILE:HA	3:P:666:LYS:O	2.18	0.44	
2:F:5004:DT:H2"	2:F:5005:DA:OP2	2.17	0.44	
1:G:4002:DT:C2'	1:G:4003:DG:H8	2.28	0.44	
3:P:662:ASN:HB2	3:P:666:LYS:CB	2.48	0.44	
3:Q:584:ASP:CB	3:Q:597:ILE:H	2.31	0.44	
3:M:461:GLY:HA2	3:M:470:PRO:HA	2.00	0.44	
3:Q:408:TYR:HB3	3:Q:560:LEU:HD11	2.00	0.44	
3:Q:448:TYR:CZ	3:Q:450:GLU:HB3	2.52	0.44	
1:A:4012:DA:H1'	1:A:4013:DT:H5"	1.99	0.44	
3:M:489:TYR:CZ	3:M:500:GLU:CB	3.01	0.44	
3:M:520:LYS:NZ	3:M:523:ASN:ND2	2.66	0.44	
3:N:570:SER:OG	3:N:572:ARG:HB2	2.18	0.44	
3:N:584:ASP:OD2	3:N:584:ASP:C	2.56	0.44	
3:Q:413:GLU:HG2	3:Q:510:ARG:CZ	2.46	0.43	
3:Q:416:PRO:HG3	3:Q:544:LEU:HD12	1.99	0.43	
1:A:4008:DA:H2"	1:A:4009:DA:N7	2.33	0.43	
3:M:615:THR:HG22	3:M:616:THR:N	2.33	0.43	
3:M:618:GLY:C	3:M:619:GLN:NE2	2.72	0.43	
3:P:397:LEU:HD11	3:P:493:VAL:HB	1.99	0.43	
3:Q:435:ALA:HB1	3:Q:436:PRO:HD2	1.99	0.43	
3:Q:471:HIS:CE1	3:Q:474:TYR:HD2	2.36	0.43	
1:E:4007:DG:H2"	1:E:4008:DA:H5'	1.96	0.43	



	h h	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
2:F:5009:DT:OP2	3:P:520:LYS:NZ	2.50	0.43
3:M:468:LEU:CD2	3:M:561:GLN:NE2	2.78	0.43
3:M:556:ARG:HH11	3:M:556:ARG:HG2	1.82	0.43
2:F:5006:DT:H2'	2:F:5007:DT:H71	2.01	0.43
3:M:622:TRP:CG	3:M:646:ARG:HD3	2.53	0.43
3:P:420:HIS:CD2	3:P:433:VAL:HA	2.53	0.43
3:P:556:ARG:HG2	3:P:556:ARG:NH1	2.33	0.43
3:M:484:VAL:CG1	3:M:515:CYS:HB3	2.49	0.43
3:M:489:TYR:O	3:M:499:LEU:HD12	2.19	0.43
3:N:650:ILE:O	3:N:677:PRO:HB3	2.18	0.43
3:Q:465:GLU:HG3	3:Q:466:ARG:N	2.34	0.43
3:Q:601:GLN:OE1	3:Q:601:GLN:HA	2.19	0.43
3:Q:650:ILE:HG13	3:Q:677:PRO:HB3	2.01	0.43
3:Q:659:TYR:HE1	3:Q:661:ILE:CD1	2.31	0.43
1:C:4012:DA:H2"	1:C:4013:DT:C5'	2.44	0.43
1:G:4003:DG:OP1	1:G:4003:DG:C4'	2.56	0.43
3:M:584:ASP:HB2	3:M:597:ILE:HB	2.00	0.43
3:P:537:ARG:O	3:P:538:LYS:HB2	2.19	0.43
3:Q:471:HIS:CE1	3:Q:473:PHE:HB2	2.53	0.43
3:N:635:PRO:HD3	3:Q:552:GLU:OE2	2.19	0.43
3:P:550:ILE:C	3:P:557:ILE:HG23	2.39	0.43
1:E:4001:DT:HO5'	1:E:4001:DT:H6	1.65	0.43
3:P:580:VAL:HB	3:P:671:GLN:HE21	1.84	0.43
3:Q:408:TYR:CE1	3:Q:558:VAL:HG21	2.54	0.43
3:Q:423:HIS:CB	3:Q:430:ARG:HD2	2.49	0.43
3:P:413:GLU:HG2	3:P:510:ARG:NH2	2.34	0.42
3:P:430:ARG:HG2	3:P:430:ARG:NH1	2.33	0.42
3:Q:471:HIS:HE1	3:Q:473:PHE:HB2	1.84	0.42
3:Q:547:ARG:HB2	3:Q:560:LEU:O	2.18	0.42
2:B:5005:DA:C1'	2:B:5006:DT:H5"	2.45	0.42
3:M:423:HIS:CA	3:M:430:ARG:HD2	2.49	0.42
3:M:557:ILE:HD12	3:M:557:ILE:H	1.84	0.42
3:N:520:LYS:NZ	3:N:523:ASN:HD21	2.17	0.42
3:N:651:ARG:NE	3:N:651:ARG:HA	2.34	0.42
3:Q:474:TYR:CZ	3:Q:520:LYS:HD3	2.54	0.42
3:M:526:ILE:O	3:M:529:ARG:HB3	2.20	0.42
3:M:584:ASP:CB	3:M:597:ILE:H	2.32	0.42
3:M:603:PHE:CD1	3:M:638:LEU:HG	2.55	0.42
3:P:523:ASN:O	3:P:527:GLU:HG3	2.19	0.42
3:Q:411:ARG:HG2	3:Q:411:ARG:NH1	2.33	0.42
3:Q:450:GLU:OE2	3:Q:450:GLU:HA	2.19	0.42



	A 4 O	Interatomic	Clash	
Atom-1	$\begin{array}{c c} \text{Atom-2} \\ \text{distance } (A \\ A $		overlap (Å)	
3:M:440:HIS:CD2	3:M:514:ASP:CB	3.02	0.42	
3:N:556:ARG:HG2	3:N:556:ARG:NH1	2.34	0.42	
3:N:520:LYS:HZ3	3:N:523:ASN:ND2	2.17	0.42	
3:N:526:ILE:O	3:N:529:ARG:HB3	2.19	0.42	
3:P:415:GLN:NE2	3:P:565:ASN:H	2.18	0.42	
3:P:450:GLU:OE2	3:P:450:GLU:HA	2.19	0.42	
3:P:651:ARG:NE	3:P:651:ARG:HA	2.33	0.42	
3:M:484:VAL:HG13	3:M:515:CYS:HB3	2.01	0.42	
3:M:504:GLU:HA	3:M:505:PRO:HD3	1.78	0.42	
3:M:526:ILE:HD13	3:M:526:ILE:HA	1.85	0.42	
3:N:413:GLU:HG2	3:N:510:ARG:NH2	2.34	0.42	
3:P:397:LEU:HD23	3:P:459:PHE:CE1	2.54	0.42	
3:P:615:THR:HG22	3:P:616:THR:N	2.35	0.42	
2:D:5009:DT:H2"	2:D:5010:DT:H71	2.02	0.42	
1:C:4012:DA:H1'	1:C:4013:DT:H5"	2.02	0.42	
1:E:4010:DA:H1'	1:E:4011:DA:H5'	2.02	0.42	
3:Q:526:ILE:O	3:Q:529:ARG:HB3	2.20	0.42	
3:M:425:GLU:O	3:M:427:GLU:N	2.50	0.42	
3:N:489:TYR:CE2	3:N:500:GLU:CB	2.99	0.42	
3:N:657:ASN:HA	3:N:671:GLN:O	2.19	0.42	
3:P:415:GLN:HE22	3:P:565:ASN:H	1.68	0.42	
3:Q:615:THR:OG1	3:Q:619:GLN:HB2	2.20	0.42	
3:M:500:GLU:O	3:M:501:ILE:HD12	2.20	0.41	
3:M:501:ILE:HG23	3:M:502:PRO:HD2	2.02	0.41	
3:P:400:PRO:HB3	3:P:467:ILE:HD11	2.01	0.41	
3:P:488:SER:HB3	3:P:501:ILE:CD1	2.48	0.41	
2:D:5009:DT:H1'	2:D:5010:DT:H5'	2.03	0.41	
3:P:551:PRO:HG2	3:P:551:PRO:O	2.20	0.41	
3:M:486:THR:HG22	3:M:487:THR:O	2.19	0.41	
3:N:504:GLU:HA	3:N:505:PRO:HD3	1.85	0.41	
3:N:571:GLN:O	3:N:572:ARG:C	2.58	0.41	
3:P:650:ILE:HD12	3:P:652:THR:O	2.19	0.41	
3:Q:423:HIS:HB3	3:Q:430:ARG:CB	2.49	0.41	
3:Q:488:SER:HB3	3:Q:501:ILE:CD1	2.51	0.41	
2:D:5004:DT:H2"	2:D:5005:DA:OP2	2.20	0.41	
3:M:423:HIS:HA	3:M:430:ARG:HD2	2.02	0.41	
3:N:615:THR:C	3:N:617:ASP:N	2.72	0.41	
3:Q:423:HIS:HB3	3:Q:430:ARG:HD2	2.01	0.41	
3:Q:486:THR:HG22	3:Q:501:ILE:HG13	2.03	0.41	
2:B:5001:DA:H2"	2:B:5002:DA:H8	1.85	0.41	
1:G:4007:DG:H2"	1:G:4008:DA:H5'	2.02	0.41	



	• • • • • • •	Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
3:N:487:THR:CG2	3:N:488:SER:N	2.83	0.41	
3:P:395:VAL:HA	3:P:396:PRO:HD3	1.79	0.41	
3:Q:479:ILE:HG22	3:Q:484:VAL:HG21	2.02	0.41	
2:D:5009:DT:C2'	2:D:5010:DT:H71	2.51	0.41	
3:M:435:ALA:HB1	3:M:436:PRO:HD2	2.03	0.41	
3:M:536:GLY:O	3:M:539:ASN:HB3	2.20	0.41	
3:Q:418:PRO:CD	3:Q:581:GLU:HB3	2.50	0.41	
3:Q:520:LYS:NZ	3:Q:523:ASN:ND2	2.68	0.41	
3:Q:550:ILE:C	3:Q:557:ILE:HG23	2.41	0.41	
3:M:423:HIS:HB3	3:M:430:ARG:CD	2.50	0.41	
3:M:433:VAL:HG11	3:M:544:LEU:HD11	2.01	0.41	
3:M:444:GLN:HA	3:M:509:MET:O	2.21	0.41	
3:M:581:GLU:HG2	3:M:599:THR:O	2.20	0.41	
3:M:612:THR:HA	3:M:622:TRP:O	2.21	0.41	
3:M:628:VAL:O	3:M:630:LYS:N	2.54	0.41	
3:N:467:ILE:O	3:N:468:LEU:C	2.58	0.41	
3:N:488:SER:HB3	3:N:501:ILE:CD1	2.50	0.41	
3:Q:623:GLU:O	3:Q:624:MET:HB2	2.21	0.41	
3:Q:650:ILE:O	3:Q:677:PRO:HB3	2.21	0.41	
1:E:4012:DA:C2'	1:E:4013:DT:C5'	2.95	0.41	
3:M:450:GLU:CG	3:M:451:ASN:H	2.34	0.41	
3:P:417:LYS:HG2	3:P:436:PRO:HA	2.03	0.41	
3:P:427:GLU:CD	3:P:430:ARG:HE	2.24	0.41	
3:Q:486:THR:CG2	3:Q:501:ILE:HG13	:ILE:HG13 2.51		
1:A:4004:DC:H2'	3:M:429:SER:O	2.21	0.41	
1:C:4006:DG:H1'	1:C:4007:DG:C5'	2.51	0.41	
2:D:5010:DT:H1'	2:D:5011:DC:H5'	2.03	0.41	
2:F:5001:DA:H2"	2:F:5002:DA:O5'	2.21	0.41	
2:F:5009:DT:H1'	2:F:5010:DT:H5'	2.01	0.41	
2:F:5010:DT:H1'	2:F:5011:DC:H5"	2.03	0.41	
1:G:4004:DC:H2'	3:Q:429:SER:O	2.20	0.41	
3:N:579:MET:HG3	3:N:579:MET:O	2.20	0.41	
3:P:659:TYR:CE1	3:P:661:ILE:HD11	2.55	0.41	
3:Q:408:TYR:HE1	3:Q:558:VAL:HG21	1.86	0.41	
3:Q:417:LYS:HG3	3:Q:434:LYS:O	2.21	0.41	
3:Q:425:GLU:C	3:Q:427:GLU:H	2.24	0.41	
3:Q:501:ILE:HG23	3:Q:502:PRO:HD2	2.02	0.41	
3:Q:577:LEU:O	3:Q:602:ASN:ND2	2.48	0.41	
3:Q:580:VAL:HG11	3:Q:671:GLN:HE21	1.85	0.41	
1:E:4002:DT:C2'	1:E:4003:DG:O5'	2.66	0.41	
3:N:500:GLU:C	3:N:501:ILE:HD12	2.41	0.41	



A 4 amo 1	A + 2	Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
3:N:587:SER:HB3	3:N:674:THR:HG22	2.03	0.41	
3:Q:397:LEU:HD11	3:Q:493:VAL:HB	2.03	0.41	
3:Q:486:THR:HG22	3:Q:487:THR:O	2.21	0.41	
2:B:5006:DT:H2"	2:B:5007:DT:C5'	2.49	0.40	
3:N:419:HIS:O	3:N:420:HIS:HB2	2.21	0.40	
3:N:501:ILE:HG23	3:N:502:PRO:CD	2.49	0.40	
3:N:548:VAL:CG2	3:N:549:HIS:N	2.84	0.40	
3:N:647:ASN:HD22	3:N:650:ILE:HG22	1.87	0.40	
3:Q:541:ARG:NH1	3:Q:669:GLN:OE1	2.54	0.40	
3:Q:573:SER:O	3:Q:577:LEU:HB2	2.21	0.40	
3:M:457:GLN:CG	3:M:500:GLU:OE1	2.51	0.40	
3:N:448:TYR:CZ	3:N:450:GLU:HB3	2.57	0.40	
3:N:520:LYS:NZ	3:N:521:LEU:O	2.52	0.40	
2:H:5001:DA:C2'	2:H:5002:DA:C8	3.00	0.40	
3:M:455:GLY:HA3	3:M:500:GLU:OE2	2.22	0.40	
3:M:556:ARG:HG2	3:M:556:ARG:NH1	2.36	0.40	
3:N:408:TYR:HD1	3:N:558:VAL:HG11	1.86	0.40	
3:N:650:ILE:HG13	3:N:677:PRO:HB3	2.02	0.40	
3:Q:598:LEU:HD21	3:Q:658:PHE:HE1	1.86	0.40	
2:D:5007:DT:H5'	2:D:5007:DT:H6	1.87	0.40	
3:M:411:ARG:HG2	3:M:411:ARG:NH1	2.36	0.40	
3:N:628:VAL:O	3:N:630:LYS:N	2.54	0.40	
3:N:456:LEU:HA	3:N:456:LEU:HD12	1.84	0.40	
3:P:413:GLU:N	3:P:442:VAL:O	2.55	0.40	
3:P:658:PHE:CD1	3:P:658:PHE:C	2.94	0.40	
3:Q:463:ALA:HA	3:Q:543:ARG:CD	2.48	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	entiles
3	М	282/284~(99%)	252~(89%)	24 (8%)	6(2%)	7	33
3	Ν	282/284~(99%)	251 (89%)	21 (7%)	10 (4%)	3	20
3	Р	282/284~(99%)	254 (90%)	21 (7%)	7~(2%)	5	28
3	Q	282/284~(99%)	251 (89%)	27~(10%)	4 (1%)	11	43
All	All	1128/1136 (99%)	1008 (89%)	93~(8%)	27(2%)	6	29

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	М	635	PRO
3	N	426	THR
3	N	482	LYS
3	Р	635	PRO
3	Q	635	PRO
3	М	629	ASP
3	N	629	ASP
3	N	635	PRO
3	Р	420	HIS
3	Р	553	SER
3	Q	553	SER
3	М	426	THR
3	М	553	SER
3	N	553	SER
3	N	574	ALA
3	N	577	LEU
3	Р	624	MET
3	Q	664	LYS
3	N	572	ARG
3	Р	426	THR
3	Q	629	ASP
3	М	405	SER
3	N	573	SER
3	Р	620	GLN
3	Ν	634	GLN
3	М	438	GLY
3	Р	467	ILE

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.

	<i></i>		1001dddobr			
Mol	Chain	Analysed	Rotameric	Outliers	Perce	entiles
3	М	247/254~(97%)	240~(97%)	7 (3%)	43	77
3	Ν	247/254~(97%)	230~(93%)	17 (7%)	15	48
3	Р	247/254~(97%)	240~(97%)	7 (3%)	43	77
3	Q	247/254~(97%)	240 (97%)	7(3%)	43	77
All	All	988/1016~(97%)	950~(96%)	38 (4%)	33	69

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

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	М	397	LEU
3	М	539	ASN
3	М	556	ARG
3	М	557	ILE
3	М	571	GLN
3	М	627	THR
3	М	651	ARG
3	Ν	397	LEU
3	Ν	539	ASN
3	Ν	556	ARG
3	Ν	572	ARG
3	Ν	583	GLN
3	N	588	CYS
3	Ν	599	THR
3	Ν	605	SER
3	Ν	613	GLU
3	N	617	ASP
3	N	620	GLN
3	Ν	621	ILE
3	N	627	THR
3	Ν	648	LYS
3	Ν	653	PRO
3	Ν	667	ARG
3	Ν	674	THR
3	Р	397	LEU
3	Р	464	ASP
3	Р	539	ASN
3	Р	556	ARG



Mol	Chain	Res	Type
3	Р	627	THR
3	Р	651	ARG
3	Р	667	ARG
3	Q	397	LEU
3	Q	539	ASN
3	Q	556	ARG
3	Q	627	THR
3	Q	651	ARG
3	Q	656	VAL
3	Q	667	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
3	М	415	GLN
3	М	440	HIS
3	М	507	ASN
3	М	523	ASN
3	М	539	ASN
3	М	565	ASN
3	М	583	GLN
3	М	602	ASN
3	М	662	ASN
3	М	669	GLN
3	М	671	GLN
3	Ν	415	GLN
3	Ν	440	HIS
3	Ν	507	ASN
3	Ν	523	ASN
3	Ν	539	ASN
3	Ν	565	ASN
3	N	575	HIS
3	Ν	602	ASN
3	Р	415	GLN
3	Р	446	HIS
3	Р	471	HIS
3	Р	507	ASN
3	Р	523	ASN
3	Р	539	ASN
3	Р	565	ASN
3	Р	583	GLN
3	Р	662	ASN



Mol	Chain	\mathbf{Res}	Type
3	Р	671	GLN
3	Q	415	GLN
3	Q	419	HIS
3	Q	507	ASN
3	Q	508	ASN
3	Q	523	ASN
3	Q	539	ASN
3	Q	565	ASN
3	Q	647	ASN
3	Q	657	ASN
3	Q	662	ASN
3	Q	671	GLN
3	Q	672	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)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



6 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	$\langle RSRZ \rangle$	#RSRZ>2	$\mathbf{OWAB}(\mathbf{\AA}^2)$	Q < 0.9
1	А	15/15~(100%)	-0.32	1 (6%) 17 5	34, 44, 84, 95	0
1	С	15/15~(100%)	-0.47	0 100 100	33, 42, 77, 87	0
1	Ε	15/15~(100%)	-0.11	0 100 100	47, 57, 103, 112	0
1	G	15/15~(100%)	0.09	1 (6%) 17 5	44,55,96,103	0
2	В	15/15~(100%)	-0.22	0 100 100	18, 48, 79, 80	0
2	D	15/15~(100%)	-0.39	0 100 100	27, 45, 62, 63	0
2	F	15/15~(100%)	-0.19	0 100 100	35, 67, 101, 117	0
2	Н	15/15~(100%)	-0.17	0 100 100	38, 62, 83, 96	0
3	М	284/284~(100%)	0.35	31 (10%) 5 2	16, 65, 120, 142	0
3	Ν	284/284~(100%)	0.52	44 (15%) 2 1	17, 76, 124, 141	0
3	Р	284/284~(100%)	-0.19	5 (1%) 68 40	22, 54, 94, 130	0
3	Q	284/284~(100%)	-0.12	4 (1%) 75 49	25, 62, 101, 126	0
All	All	1256/1256~(100%)	0.11	86 (6%) 17 5	$16, \overline{62, 114, 142}$	0

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	Ν	576	GLU	6.0
3	М	664	LYS	6.0
3	М	633	SER	5.9
3	М	637	MET	5.3
3	М	665	ARG	5.2
3	М	635	PRO	5.1
3	Р	631	ASP	4.9
3	М	618	GLY	4.9
3	М	631	ASP	4.8
3	М	627	THR	4.8
3	Ν	586	ASP	4.8



Mol	Chain	Res	Type	RSRZ
3	N	619	GLN	4.6
3	Ν	575	HIS	4.4
3	М	605	SER	4.4
3	N	636	ASN	4.4
3	N	672	HIS	4.3
3	Ν	635	PRO	4.1
3	Ν	555	GLY	4.0
3	Ν	631	ASP	4.0
3	Р	630	LYS	4.0
3	М	634	GLN	3.9
3	М	591	TYR	3.9
3	Ν	616	THR	3.9
3	Ν	677	PRO	3.9
3	Ν	651	ARG	3.8
3	M	606	GLU	3.8
3	N	574	ALA	3.7
3	Ν	663	GLY	3.7
3	N	592	GLY	3.6
3	N	591	TYR	3.6
3	М	576	GLU	3.5
3	N	585	THR	3.5
3	М	604	THR	3.4
3	N	617	ASP	3.4
3	N	602	ASN	3.4
3	М	651	ARG	3.2
3	N	634	GLN	3.2
3	N	665	ARG	3.1
3	М	399	TRP	3.1
3	М	649	HIS	3.1
3	М	595	GLN	3.1
3	M	588	CYS	3.0
3	N	633	SER	2.9
3	N	595	GLN	2.9
3	Р	632	LYS	2.9
3	N	678	VAL	2.9
3	Q	665	ARG	2.8
3	М	628	VAL	2.8
3	N	655	LYS	2.8
3	М	620	GLN	2.8
3	N	659	TYR	2.8
3	М	587	SER	2.8
3	Р	489	TYR	2.8



Mol	Chain	\mathbf{Res}	Type	RSRZ
3	N	649	HIS	2.7
3	N	664	LYS	2.7
3	М	617	ASP	2.7
3	N	594	GLN	2.7
3	N	674	THR	2.6
3	N	662	ASN	2.6
3	Q	664	LYS	2.6
3	N	676	HIS	2.6
3	N	647	ASN	2.6
3	М	573	SER	2.6
3	М	594	GLN	2.5
3	Р	553	SER	2.5
3	Q	576	GLU	2.5
3	М	584	ASP	2.5
3	N	593	GLY	2.4
3	М	659	TYR	2.4
3	М	619	GLN	2.3
3	Ν	599	THR	2.3
3	N	621	ILE	2.3
1	А	4001	DT	2.2
3	М	577	LEU	2.2
3	N	597	ILE	2.2
3	N	627	THR	2.2
3	N	646	ARG	2.2
3	М	615	THR	2.2
3	N	614	LYS	2.2
3	Ν	615	THR	2.2
3	N	623	GLU	2.1
3	М	582	ARG	2.1
3	Ν	601	GLN	2.1
1	G	4001	DT	2.0
3	Q	633	SER	2.0
3	Ν	451	ASN	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.



6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.

