



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 09:05 pm GMT

PDB ID : 1OWR
Title : CRYSTAL STRUCTURE OF HUMAN NFAT1 BOUND MONOMERICALLY 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

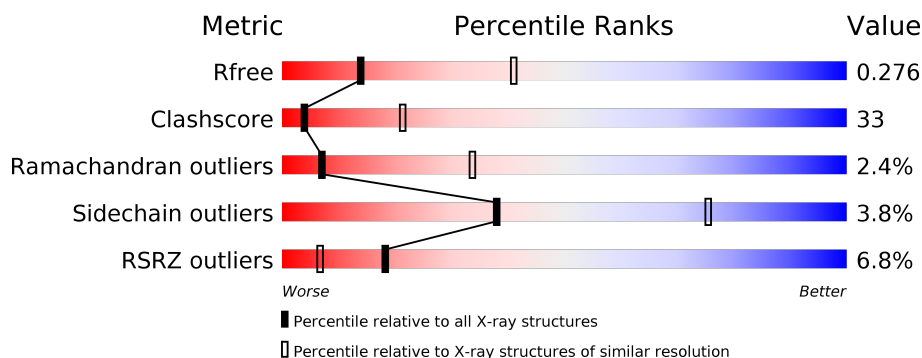
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-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 (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1692 (3.00-3.00)
Clashscore	112137	2037 (3.00-3.00)
Ramachandran outliers	110173	1973 (3.00-3.00)
Sidechain outliers	110143	1976 (3.00-3.00)
RSRZ outliers	101464	1716 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	15	<div> <div>7%</div> <div>13%</div> <div>87%</div> </div>
1	C	15	<div> <div>100%</div> </div>
1	E	15	<div> <div>80%</div> <div>20%</div> </div>
1	G	15	<div> <div>7%</div> <div>7%</div> <div>93%</div> </div>
2	B	15	<div> <div>93%</div> <div>7%</div> </div>
2	D	15	<div> <div>93%</div> <div>7%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	F	15	<div><div></div><div>7%87%7%</div></div>
2	H	15	<div><div></div><div>93%7%</div></div>
3	M	284	<div><div></div><div>11%51%48%. </div></div>
3	N	284	<div><div></div><div>15%51%44%5% </div></div>
3	P	284	<div><div></div><div>2%56%41%. </div></div>
3	Q	284	<div><div></div><div>%50%49%. </div></div>

2 Entry composition

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.

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	15	Total	C	N	O	P	0	0	0
			310	149	61	86	14			
1	C	15	Total	C	N	O	P	0	0	0
			310	149	61	86	14			
1	E	15	Total	C	N	O	P	0	0	0
			310	149	61	86	14			
1	G	15	Total	C	N	O	P	0	0	0
			310	149	61	86	14			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	15	Total	C	N	O	P	0	0	0
			299	146	49	90	14			
2	D	15	Total	C	N	O	P	0	0	0
			299	146	49	90	14			
2	F	15	Total	C	N	O	P	0	0	0
			299	146	49	90	14			
2	H	15	Total	C	N	O	P	0	0	0
			299	146	49	90	14			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	284	Total	C	N	O	S	0	0	0
			2250	1414	411	416	9			
3	N	284	Total	C	N	O	S	0	0	0
			2250	1414	411	416	9			
3	P	284	Total	C	N	O	S	0	0	0
			2250	1414	411	416	9			
3	Q	284	Total	C	N	O	S	0	0	0
			2250	1414	411	416	9			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	395	VAL	-	CLONING ARTIFACT	UNP Q13469
N	395	VAL	-	CLONING ARTIFACT	UNP Q13469
P	395	VAL	-	CLONING ARTIFACT	UNP Q13469
Q	395	VAL	-	CLONING ARTIFACT	UNP Q13469

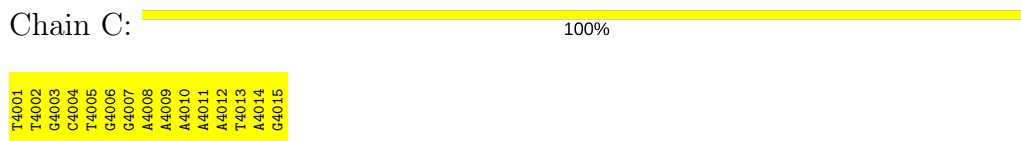
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

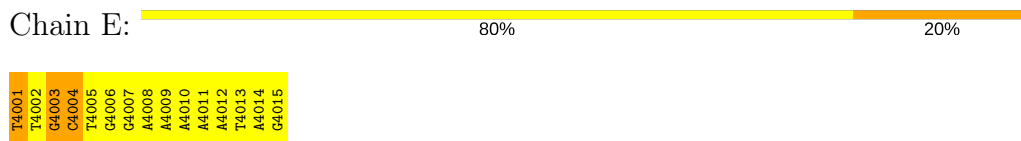
- Molecule 1: NFAT1 Monomeric Binding Site, Plus Strand



- Molecule 1: NFAT1 Monomeric Binding Site, Plus Strand



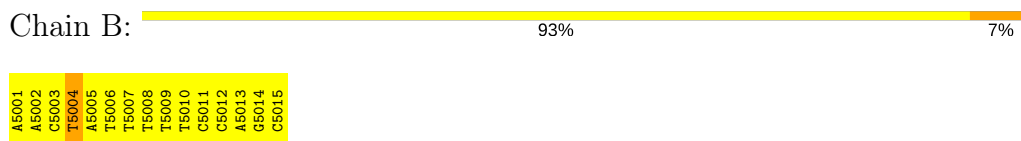
- Molecule 1: NFAT1 Monomeric Binding Site, Plus Strand



- Molecule 1: NFAT1 Monomeric Binding Site, Plus Strand



- Molecule 2: NFAT1 Monomeric Binding Site, Minus Strand



- Molecule 2: NFAT1 Monomeric Binding Site, Minus Strand

Chain D:  93% 7%

A5001
A5002
C5003
T5004
A5005
T5006
T5007
T5008
T5009
T5010
C5011
C5012
A5013
G5014
C5015

- Molecule 2: NFAT1 Monomeric Binding Site, Minus Strand

Chain F:  7% 87% 7%

A5001
A5002
C5003
T5004
A5005
T5006
T5007
T5008
T5009
T5010
C5011
C5012
A5013
G5014
C5015

- Molecule 2: NFAT1 Monomeric Binding Site, Minus Strand

Chain H:  93% 7%

A5001
A5002
C5003
T5004
A5005
T5006
T5007
T5008
T5009
T5010
C5011
C5012
A5013
G5014
C5015

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

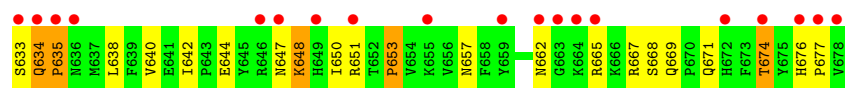
Chain M:  11% 51% 48% •

V995 P996 L997 E998 W999 S403 Q404 S405 R411 I412 E413 V414 Q415 P416 K417 P418 H419 H420 R421 A422 H423 Y424 E425 T426 E427 G428 S429 R430 R431 A432 V433 K434 A435 P436 T437 G438 H440 P441 V442 V443 Q444 E450 N451 G455 L456 Q457 I458 F459 I460 G461 T462 A463 D464 E465 R466
I467 L468 K469 P470 H471 A472 F473 F474 Q475 I479 V484 T485 T487 S488 Y489 V493 L499 E500 E501 P502 L503 E504 P505 M509 R510 D514 C515 I518 L519 K520 L521 R522 N523 A524 D525 V526 E527 L528 R529 E532 T533 D534 I535 G536 R539 R543 L544 V545 F546
R547 E552 S553 S554 G555 R556 I557 L560 Q561 N565 C569 S570 R571 R572 S573 A574 H575 E576 L577 P578 M579 V580 E581 R582 Q583 D584 S587 G588 Y591 G594 Q595 M596 L597 T598 T599 G600 Q601 N602 F603 T604 S605 E606 S607 T612 E613 K614 T615 T616 D617 G618 Q619 Q620
I621 W622 T627 D628 K630 D631 K632 S633 Q634 P635 E636 M637 L638 I642 P643 E644 Y645 E646 N647 E648 H649 I650 R651 V656 Y659 V660 I661 G662 G663 K664 R665 Q671 T674 V678

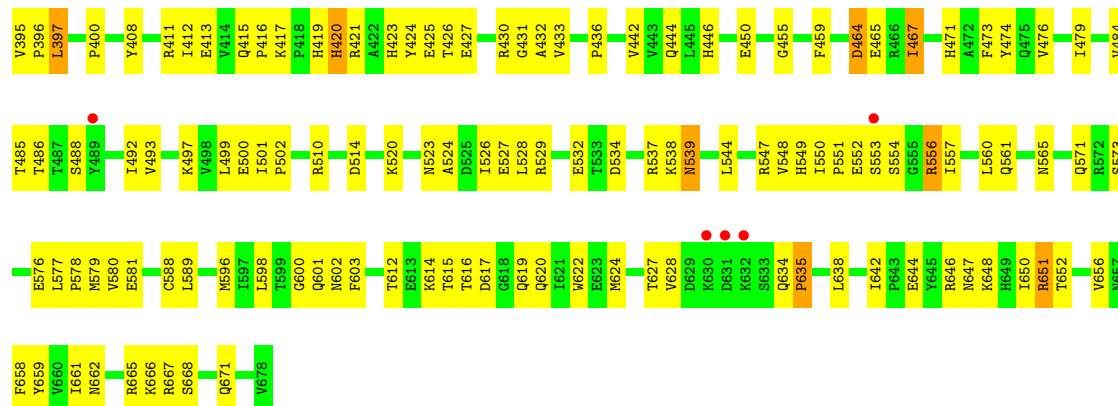
- Molecule 3: Nuclear factor of activated T-cells, cytoplasmic 2

Chain N:  15% 51% 44% 5%

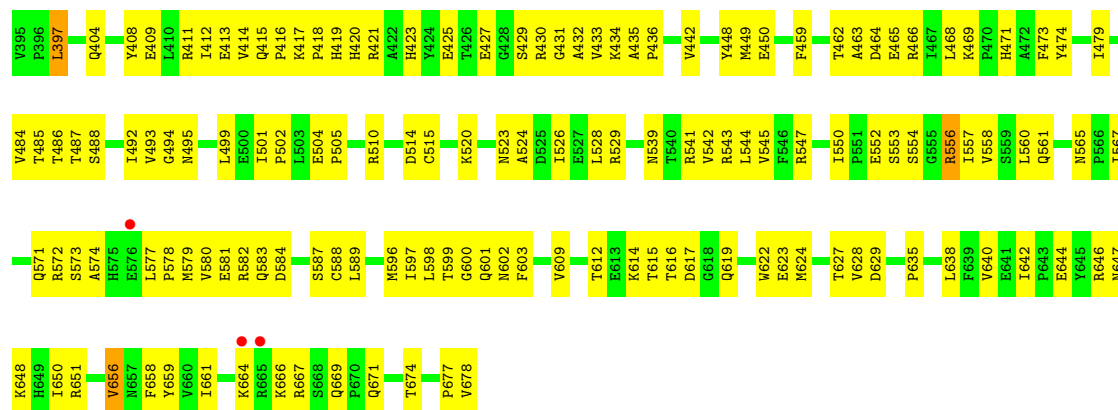
V995 P996 L997 P400 S403 Y408 R411 I412 E413 V414 Q415 P416 K417 P418 H419 H420 R421 A422 H423 Y424 E425 T426 E427 G430 R431 A432 V433 K434 A435 P436 H440 P441 V442 Y448 E450 L456 Q457 I458 F459 I460 A463 L468 H471 A472 F473 I479
T480 G481 K482 T483 V484 T486 T487 S488 Y489 I492 V493 L499 E500 E501 P502 L503 E504 P505 M509 R510 D514 C515 I518 L519 K520 L521 R522 N523 A524 D525 V526 E527 L528 R529 E532 T533 D534 I535 G536 R539 R543 L544 V545 F546 R547 G548 Y549 I550 P551 E552 S553 S554 G555 R556 I557 V558 S559
L560 Q561 N565 P566 S570 Q571 R572 A574 V576 E577 P578 M579 V580 E581 R582 Q583 D584 S587 C588 Y591 G594 Q595 M596 L597 T598 T599 G600 Q601 N602 F603 T604 S605 E606 S607 T612 E613 K614 T615 T616 D617 G618 Q619 Q620 I621 W622 E623 T627 D628 K629 K630 D631 K632



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	100.65Å 94.85Å 112.79Å 90.00° 104.34° 90.00°	Depositor
Resolution (Å)	20.00 – 3.00 20.01 – 2.98	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-3.00) 91.5 (20.01-2.98)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.42 (at 2.98Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.241 , 0.273 0.251 , 0.276	Depositor DCC
R_{free} test set	3420 reflections (9.05%)	DCC
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.*

¹Intensities estimated from amplitudes.

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.

5 Model quality

5.1 Standard geometry

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	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.71	0/349	0.89	0/538
1	C	0.63	0/349	0.78	0/538
1	E	0.78	0/349	1.10	3/538 (0.6%)
1	G	0.55	0/349	0.78	0/538
2	B	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	H	0.64	0/333	0.81	1/511 (0.2%)
3	M	0.52	0/2300	0.76	0/3115
3	N	0.51	0/2300	0.79	0/3115
3	P	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	E	0	1
2	F	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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(°)	Ideal(°)
1	E	4004	DC	O5'-P-OP2	-6.38	99.96	105.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	5004	DT	OP2-P-O3'	6.15	118.73	105.20
1	E	4004	DC	O4'-C4'-C3'	-5.32	102.37	104.50
2	H	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	E	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	E	4001	DT	Sidechain
2	F	5002	DA	Sidechain

5.2 Too-close contacts

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	A	310	0	171	33	0
1	C	310	0	171	36	0
1	E	310	0	171	24	0
1	G	310	0	171	36	0
2	B	299	0	173	23	0
2	D	299	0	173	16	0
2	F	299	0	173	23	0
2	H	299	0	173	17	0
3	M	2250	0	2238	142	0
3	N	2250	0	2238	135	0
3	P	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 distance (Å)	Clash 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:OP1	2:H:5015:DC:H4'	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:OP1	2:B:5015:DC:H4'	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash 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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash 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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash 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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash 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:463:ALA:HA	3:Q:543:ARG:HD2	1.81	0.63
3:Q:415:GLN:NE2	3:Q:565:ASN:H	1.95	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:HG3	3:P:651:ARG:HH11	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash 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:HD12	3:P:557:ILE:N	2.17	0.58
3:N:669:GLN:HA	3:N:669:GLN:OE1	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:P:578:PRO:HA	3:P:602:ASN:HB2	1.87	0.56
3:N:501:ILE:HG23	3:N:502:PRO:HD2	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash 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:NH1	3:P:651:ARG:HG3	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:P:573:SER:HB2	3:P:577:LEU:HD11	1.90	0.54
3:N:633:SER:C	3:Q:554:SER:HB3	2.27	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash 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:HD12	3:N:557:ILE:N	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	2.08	0.52
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:N:488:SER:HB3	3:N:501:ILE:HD11	1.91	0.52
3:M:418:PRO:HG2	3:P:446:HIS:CD2	2.44	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:5006:DT:H2''	2:H:5007:DT:C5'	2.40	0.52
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:492:ILE:N	3:P:492:ILE:HD12	2.25	0.52
3:P:421:ARG:CD	3:P:571:GLN:HG3	2.35	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:C4'	1:A:4003:DG:OP1	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	3:N:412:ILE:N	2.25	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'	2:D:5003:DC:O5'	2.11	0.50
3:N:457:GLN:HG2	3:N:500:GLU:OE1	2.11	0.50
3:P:573:SER:HA	3:P:576:GLU:HB3	1.92	0.50
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:HA	3:P:671:GLN:OE1	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:467:ILE:HG22	3:M:469:LYS:HG3	1.94	0.50
3:M:413:GLU:CG	3:M:510:ARG:HH22	2.20	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:C4'	1:C:4003:DG:OP1	2.42	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash 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:HG22	3:M:412:ILE:O	2.12	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
3:N:467:ILE:CG1	3:Q:583:GLN:O	2.56	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:500:GLU:HG3	3:M:501:ILE:N	2.27	0.49
3:M:459:PHE:CZ	3:M:545:VAL:HG11	2.47	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''	1.95	0.49
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:HG2	3:M:411:ARG:HH11	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash 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	2.14	0.48
2:B:5001:DA:H8	2:B:5001:DA:HO5'	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:HG3	3:M:576:GLU:O	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:HD12	3:N:492:ILE:N	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: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:615:THR:OG1	3:P:619:GLN:HB2	2.15	0.47
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:547:ARG:CZ	3:M:561:GLN:OE1	2.63	0.47
3:P:556:ARG:HH11	3:P:556:ARG:HG2	1.80	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
3:P:588:CYS:SG	3:P:589:LEU:N	2.88	0.47
1:G:4005:DT:OP2	3:Q:431:GLY:HA3	2.15	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:464:ASP:OD1	3:Q:541:ARG:NH2	2.45	0.46
3:Q:463:ALA:CB	3:Q:543:ARG:HG3	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash 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	2.70	0.45
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:O	3:Q:412:ILE:HG22	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash 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:448:TYR:CZ	3:Q:450:GLU:HB3	2.52	0.44
3:Q:408:TYR:HB3	3:Q:560:LEU:HD11	2.00	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:C	3:N:584:ASP:OD2	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash 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:NH1	3:P:556:ARG:HG2	2.33	0.43
3:M:489:TYR:O	3:M:499:LEU:HD12	2.19	0.43
3:M:484:VAL:CG1	3:M:515:CYS:HB3	2.49	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:C4'	1:G:4003:DG:OP1	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:H6	1:E:4001:DT:HO5'	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:430:ARG:HG2	3:P:430:ARG:NH1	2.33	0.42
3:P:413:GLU:HG2	3:P:510:ARG:NH2	2.34	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:HA	3:N:651:ARG:NE	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:HA	3:Q:450:GLU:OE2	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:440:HIS:CD2	3:M:514:ASP:CB	3.02	0.42
3:N:556:ARG:NH1	3:N:556:ARG:HG2	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:HA	3:P:450:GLU:OE2	2.19	0.42
3:P:651:ARG:HA	3:P:651:ARG:NE	2.33	0.42
3:M:504:GLU:HA	3:M:505:PRO:HD3	1.78	0.42
3:M:484:VAL:HG13	3:M:515:CYS:HB3	2.01	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash 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: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:Q:418:PRO:CD	3:Q:581:GLU:HB3	2.50	0.41
3:M:423:HIS:HB3	3:M:430:ARG:CD	2.50	0.41
3:M:444:GLN:HA	3:M:509:MET:O	2.21	0.41
3:M:433:VAL:HG11	3:M:544:LEU:HD11	2.01	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:427:GLU:CD	3:P:430:ARG:HE	2.24	0.41
3:P:417:LYS:HG2	3:P:436:PRO:HA	2.03	0.41
3:Q:486:THR:CG2	3:Q:501:ILE:HG13	2.51	0.41
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: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
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: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:408:TYR:HE1	3:Q:558:VAL:HG21	1.86	0.41
3:Q:577:LEU:O	3:Q:602:ASN:ND2	2.48	0.41
2:D:5010:DT:H1'	2:D:5011:DC:H5'	2.03	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:Q:417:LYS:HG3	3:Q:434:LYS:O	2.21	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:587:SER:HB3	3:N:674:THR:HG22	2.03	0.41
3:Q:486:THR:HG22	3:Q:487:THR:O	2.21	0.41
3:Q:397:LEU:HD11	3:Q:493:VAL:HB	2.03	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:H6	2:D:5007:DT:H5'	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:HD12	3:N:456:LEU:HA	1.84	0.40
3:P:413:GLU:N	3:P:442:VAL:O	2.55	0.40
3:P:658:PHE:C	3:P:658:PHE:CD1	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

5.3.1 Protein backbone

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	Percentiles	
3	M	282/284 (99%)	252 (89%)	24 (8%)	6 (2%)	8	38
3	N	282/284 (99%)	251 (89%)	21 (7%)	10 (4%)	4	23
3	P	282/284 (99%)	254 (90%)	21 (7%)	7 (2%)	6	32
3	Q	282/284 (99%)	251 (89%)	27 (10%)	4 (1%)	13	49
All	All	1128/1136 (99%)	1008 (89%)	93 (8%)	27 (2%)	7	34

All (27) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains ⓘ

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	Percentiles	
3	M	247/254 (97%)	240 (97%)	7 (3%)	49	82
3	N	247/254 (97%)	230 (93%)	17 (7%)	18	53
3	P	247/254 (97%)	240 (97%)	7 (3%)	49	82
3	Q	247/254 (97%)	240 (97%)	7 (3%)	49	82
All	All	988/1016 (97%)	950 (96%)	38 (4%)	38	75

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

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	P	627	THR
3	P	651	ARG
3	P	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

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

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	P	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 carbohydrates 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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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, 95th 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	OWAB(Å ²)	Q<0.9
1	A	15/15 (100%)	-0.32	1 (6%) 19 7	34, 44, 84, 95	0
1	C	15/15 (100%)	-0.47	0 100 100	33, 42, 77, 87	0
1	E	15/15 (100%)	-0.12	0 100 100	47, 57, 103, 112	0
1	G	15/15 (100%)	0.08	1 (6%) 19 7	44, 55, 96, 103	0
2	B	15/15 (100%)	-0.22	0 100 100	18, 48, 79, 80	0
2	D	15/15 (100%)	-0.40	0 100 100	27, 45, 62, 63	0
2	F	15/15 (100%)	-0.19	0 100 100	35, 67, 101, 117	0
2	H	15/15 (100%)	-0.17	0 100 100	38, 62, 83, 96	0
3	M	284/284 (100%)	0.35	32 (11%) 6 2	16, 65, 120, 142	0
3	N	284/284 (100%)	0.52	43 (15%) 3 1	17, 76, 124, 141	0
3	P	284/284 (100%)	-0.19	5 (1%) 69 40	22, 54, 94, 130	0
3	Q	284/284 (100%)	-0.12	3 (1%) 80 55	25, 62, 101, 126	0
All	All	1256/1256 (100%)	0.11	85 (6%) 18 7	16, 62, 114, 142	0

All (85) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	N	576	GLU	6.0
3	M	633	SER	6.0
3	M	664	LYS	6.0
3	M	665	ARG	5.3
3	M	637	MET	5.3
3	M	635	PRO	5.1
3	P	631	ASP	4.9
3	N	586	ASP	4.9
3	M	618	GLY	4.8
3	M	627	THR	4.7
3	M	631	ASP	4.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	N	619	GLN	4.6
3	N	575	HIS	4.4
3	M	605	SER	4.4
3	N	636	ASN	4.3
3	N	672	HIS	4.2
3	N	635	PRO	4.0
3	N	555	GLY	4.0
3	P	630	LYS	4.0
3	M	591	TYR	4.0
3	N	631	ASP	3.9
3	N	677	PRO	3.9
3	M	634	GLN	3.9
3	N	616	THR	3.9
3	M	606	GLU	3.8
3	N	651	ARG	3.8
3	N	592	GLY	3.7
3	N	663	GLY	3.7
3	N	574	ALA	3.7
3	N	591	TYR	3.6
3	M	576	GLU	3.5
3	N	585	THR	3.5
3	M	604	THR	3.4
3	N	602	ASN	3.3
3	N	617	ASP	3.3
3	M	651	ARG	3.2
3	N	634	GLN	3.2
3	N	665	ARG	3.2
3	M	649	HIS	3.1
3	M	399	TRP	3.1
3	M	595	GLN	3.1
3	M	588	CYS	3.1
3	N	633	SER	2.9
3	P	632	LYS	2.9
3	N	595	GLN	2.9
3	Q	665	ARG	2.9
3	N	678	VAL	2.9
3	M	587	SER	2.8
3	N	655	LYS	2.8
3	N	659	TYR	2.8
3	P	489	TYR	2.8
3	M	620	GLN	2.8
3	M	628	VAL	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	N	664	LYS	2.8
3	N	649	HIS	2.8
3	N	594	GLN	2.7
3	Q	664	LYS	2.7
3	N	676	HIS	2.6
3	M	617	ASP	2.6
3	N	674	THR	2.6
3	N	662	ASN	2.6
3	N	647	ASN	2.6
3	M	573	SER	2.6
3	M	594	GLN	2.5
3	P	553	SER	2.5
3	M	584	ASP	2.5
3	Q	576	GLU	2.5
3	N	593	GLY	2.4
3	M	659	TYR	2.4
3	M	619	GLN	2.3
3	N	621	ILE	2.3
3	N	599	THR	2.3
1	A	4001	DT	2.2
3	M	577	LEU	2.2
3	M	582	ARG	2.2
3	N	646	ARG	2.2
3	M	615	THR	2.2
3	N	597	ILE	2.2
3	N	627	THR	2.2
3	N	614	LYS	2.1
3	N	623	GLU	2.1
3	N	615	THR	2.1
3	N	601	GLN	2.1
1	G	4001	DT	2.1
3	M	556	ARG	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 carbohydrates 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.