



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:27 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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

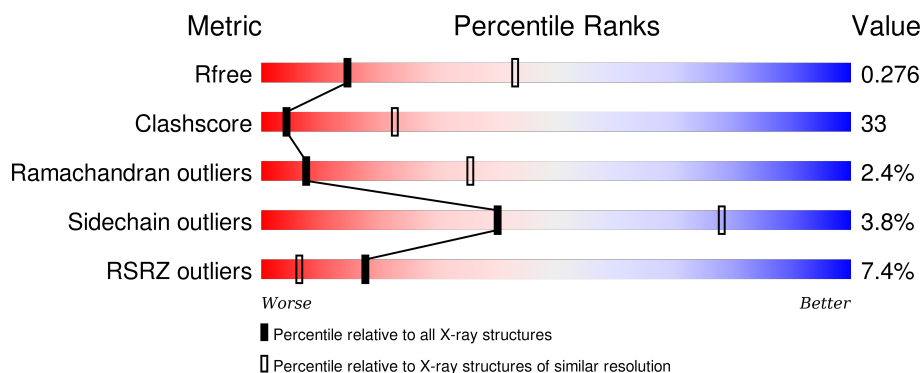
1 Overall quality at a glance

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}	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (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>

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Mol	Chain	Length	Quality of chain
2	D	15	<div><div></div><div>93%</div><div>7%</div></div>
2	F	15	<div><div>7%</div><div>87%</div><div>7%</div></div>
2	H	15	<div><div></div><div>93%</div><div>7%</div></div>
3	M	284	<div><div>12%</div><div>51%</div><div>48%</div><div></div></div>
3	N	284	<div><div>16%</div><div>51%</div><div>44%</div><div>5%</div></div>
3	P	284	<div><div>2%</div><div>56%</div><div>41%</div><div></div></div>
3	Q	284	<div><div>2%</div><div>50%</div><div>49%</div><div></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			

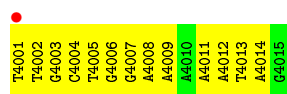
There are 4 discrepancies between the modelled and reference sequences:

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

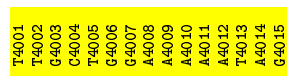
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

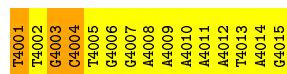
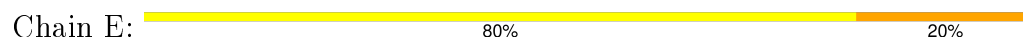
- Molecule 1: NFAT1 Monomeric Binding Site, Plus Strand



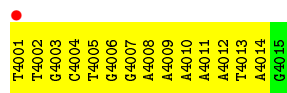
- Molecule 1: NFAT1 Monomeric Binding Site, Plus Strand



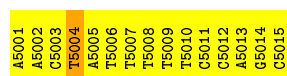
- Molecule 1: NFAT1 Monomeric Binding Site, Plus Strand



- 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

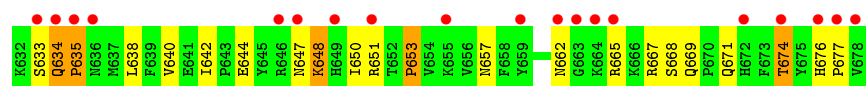
Chain M:  12% 51% 48%

V995
P996
L997
E998
W999
S403
Q404
S405
R411
I412
E413
V414
Q415
P416
K417
S418
H419
R420
H421
A422
H423
Y424
E425
T426
E427
G428
S429
R430
G431
A432
V433
K434
A435
P436
T437
G438
G439
H440
P441
A442
V443
D444
E450
N451
G455
L456
Q457
I458
P459
I460
T461
T462
A463
D464
E465
R466
I467
L468
K469
P470
H471
A472
F473
Q474
Y475
I479
V484
T485
T486
S488
P489
V493
L499
E500
Y501
P502
L503
E504
P505
M509
B510
D514
C515
I518
L519
K520
L521
R522
N523
A524
D525
V526
E527
L528
R529
E532
T533
D534
I535
G536
N539
R543
L544
V545
F546
R547
E552
S553
S554
G555
R556
I557
L560
Q561
N565
C569
S570
Q571
R572
S573
A574
E575
E576
L577
P578
V580
H579
V580
E581
R582
Q583
D584
S587
C588
Y591
Q594
Q595
M596
L597
L598
T599
G600
Q601
N602
F603
T604
S605
E606
S607
T612
E613
K614
T615
T616
D617
G618
Q619
Q620
T621
W622
T627
V628
K629
K630
D631
K632
S633
Q634
P635
N636
W637
L638
I642
P643
E644
V645
N646
K647
K648
H649
I650
R651
V656
V659
V660
I661
N662
G663
K664
R665
Q671
T674
V678

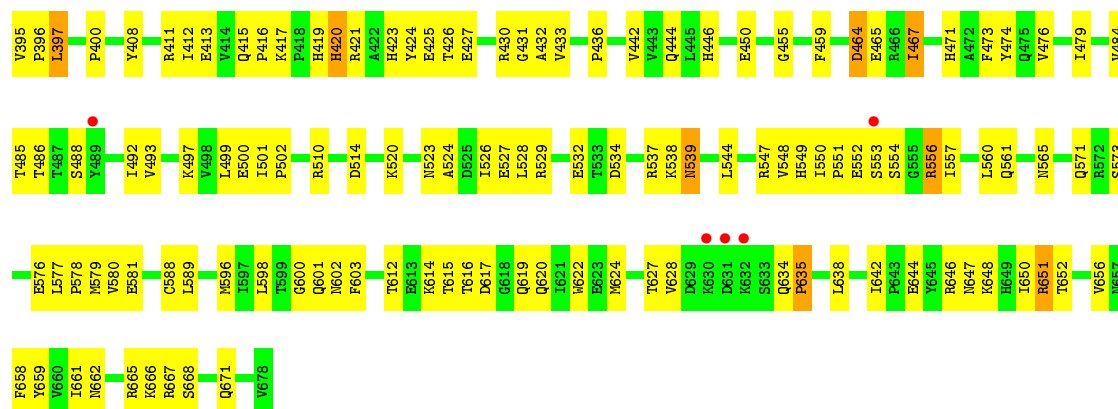
- Molecule 3: Nuclear factor of activated T-cells, cytoplasmic 2

Chain N:  16% 51% 44% 5%

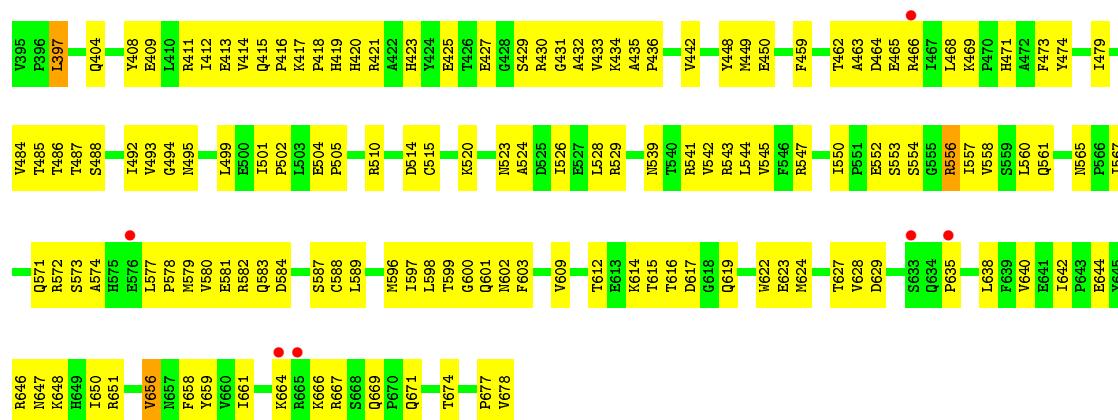
V995
P996
L997
P400
S403
Y408
R411
I412
E413
V414
Q415
P416
K417
P418
H419
H420
A422
H423
E424
Y424
T426
E427
R430
G431
A432
V433
K434
P436
H440
P441
V442
Y448
M449
E450
M451
L456
Q457
I458
F459
I460
A463
I467
L468
H471
A472
F473
S559
L560
Q561
N565
P566
S570
Q571
R572
S573
A574
H575
E576
L577
P578
M579
V580
E581
R582
Q583
D584
T585
I586
S587
C588
Y591
G592
G593
Q594
Q595
M596
L597
L598
T599
G600
Q601
N602
F603
T604
S605
V542
R543
L544
V545
F546
G547
V548
H549
P551
E552
S553
S554
S555
R556
I557
V558
K614
T615
T616
D617
Q618
Q619
Q620
W622
E623
T627
V628
K629
K630
D631



- 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
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 39717 reflections (0.003%)	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, 0.375 respectively for untwinned datasets, and 0.333, 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

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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

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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:P:485:THR:HG22	3:P:514:ASP:OD1	1.76	0.84
3:N:620:GLN:O	3:N:620:GLN:HG3	1.77	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
3:M:415:GLN:NE2	3:M:565:ASN:H	1.83	0.76
1:C:4012:DA:H2''	1:C:4013:DT:H5'	1.67	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:Q:415:GLN:HE22	3:Q:565:ASN:H	1.31	0.75
3:M:414:VAL:HG23	3:M:442:VAL:HB	1.67	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

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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:P:524:ALA:O	3:P:528:LEU:HD13	1.89	0.72
3:N:457:GLN:NE2	3:N:500:GLU:OE2	2.20	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:4012:DA:H2''	1:G:4013:DT:C5'	2.21	0.71
1:G:4011:DA:H1'	1:G:4012:DA:H5''	1.73	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:471:HIS:CD2	3:P:474:TYR:HD2	2.11	0.68
3:P:415:GLN:HE21	3:P:416:PRO:HD2	1.56	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
3:Q:413:GLU:HG2	3:Q:510:ARG:HH22	1.56	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
2:F:5003:DC:H2''	2:F:5004:DT:OP2	1.93	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:4007:DG:H1'	1:G:4008:DA:H5''	1.75	0.67
3:P:520:LYS:NZ	3:P:523:ASN:HD21	1.93	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:M:468:LEU:HD23	3:M:561:GLN:NE2	2.08	0.67
3:Q:580:VAL:HB	3:Q:671:GLN:NE2	2.09	0.66
3:M:580:VAL:HB	3:M:671:GLN:NE2	2.10	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:N:421:ARG:NH2	3:N:430:ARG:NH2	2.44	0.66
3:M:578:PRO:HB3	3:M:602:ASN:O	1.96	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
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
2:B:5014:DG:H2''	2:B:5015:DC:O5'	1.98	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
3:M:489:TYR:CE2	3:M:500:GLU:HB3	2.32	0.64
2:F:5006:DT:H2''	2:F:5007:DT:H5'	1.78	0.64
3:P:580:VAL:HB	3:P:671:GLN:NE2	2.12	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:M:644:GLU:OE1	3:M:648:LYS:HD3	1.98	0.64
3:Q:584:ASP:HB2	3:Q:597:ILE:HB	1.79	0.64
1:A:4012:DA:H2''	1:A:4013:DT:H5'	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:N:577:LEU:HB2	3:N:578:PRO:CD	2.24	0.63
3:Q:614:LYS:HA	3:Q:619:GLN:O	1.97	0.63
3:M:520:LYS:HZ1	3:M:523:ASN:HD21	1.46	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:612:THR:O	3:Q:656:VAL:HG22	1.98	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
1:G:4007:DG:H2''	1:G:4008:DA:H5''	1.81	0.62
2:F:5015:DC:H5''	2:F:5015:DC:H6	1.64	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:Q:588:CYS:SG	3:Q:589:LEU:N	2.74	0.61
3:N:415:GLN:NE2	3:N:565:ASN:H	1.98	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

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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: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
3:N:578:PRO:HB2	3:N:668:SER:HB3	1.84	0.58
2:F:5002:DA:C4'	2:F:5003:DC:OP1	2.50	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:635:PRO:HB3	3:Q:552:GLU:OE1	2.04	0.58
3:N:487:THR:HG22	3:N:488:SER:N	2.19	0.58
2:F:5001:DA:H2''	2:F:5002:DA:H8	1.69	0.58
2:D:5006:DT:H2''	2:D:5007:DT:H5'	1.84	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:580:VAL:CG1	3:Q:671:GLN:HE21	2.17	0.57
3:Q:557:ILE:HD12	3:Q:557:ILE:N	2.20	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:Q:547:ARG:NH2	3:Q:561:GLN:OE1	2.34	0.56
3:M:417:LYS:HG3	3:M:434:LYS:O	2.05	0.56
3:Q:413:GLU:CG	3:Q:510:ARG:HH22	2.19	0.56
3:N:501:ILE:HG23	3:N:502:PRO:HD2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:578:PRO:HA	3:P:602:ASN:HB2	1.87	0.56
3:P:520:LYS:NZ	3:P:523:ASN:ND2	2.53	0.56
3:N:634:GLN:CB	3:N:635:PRO:HD2	2.36	0.56
2:B:5011:DC:H1'	2:B:5012:DC:H5'	1.87	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
3:N:580:VAL:HB	3:N:671:GLN:NE2	2.20	0.56
3:N:425:GLU:O	3:N:427:GLU:N	2.38	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:P:423:HIS:HB3	3:P:430:ARG:HB2	1.87	0.55
3:M:615:THR:OG1	3:M:619:GLN:HB2	2.06	0.55
3:Q:615:THR:HG22	3:Q:616:THR:H	1.71	0.55
3:P:578:PRO:HG2	3:P:668:SER:HB3	1.87	0.55
3:P:552:GLU:O	3:P:554:SER:N	2.39	0.55
1:G:4002:DT:C2'	1:G:4003:DG:C8	2.90	0.55
2:F:5014:DG:H2''	2:F:5015:DC:H5''	1.87	0.55
2:F:5006:DT:H2''	2:F:5007:DT:C5'	2.36	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:Q:419:HIS:HB3	3:Q:579:MET:SD	2.46	0.55
3:N:584:ASP:HB3	3:N:597:ILE:H	1.71	0.55
3:Q:419:HIS:HE1	3:Q:601:GLN:HG3	1.72	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:M:420:HIS:O	3:M:569:CYS:HA	2.06	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

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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:O	3:P:628:VAL:HG23	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:P:425:GLU:C	3:P:427:GLU:H	2.12	0.53
3:M:520:LYS:NZ	3:M:523:ASN:HD21	2.06	0.53
2:H:5001:DA:HO5'	2:H:5001:DA:H8	1.54	0.53
1:A:4011:DA:H1'	1:A:4012:DA:H5''	1.91	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:Q:552:GLU:C	3:Q:554:SER:H	2.12	0.52
3:Q:423:HIS:CA	3:Q:430:ARG:HD2	2.39	0.52
3:N:412:ILE:O	3:N:412:ILE:HG22	2.09	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:N:440:HIS:CD2	3:N:514:ASP:HB3	2.44	0.52
3:M:425:GLU:C	3:M:427:GLU:H	2.12	0.52
3:P:471:HIS:CD2	3:P:473:PHE:H	2.27	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: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: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
3:M:467:ILE:CG2	3:M:469:LYS:HE3	2.39	0.52
1:C:4002:DT:C2'	1:C:4003:DG:C8	2.93	0.52
3:Q:552:GLU:O	3:Q:554:SER:N	2.43	0.52
3:N:397:LEU:HD11	3:N:493:VAL:HB	1.90	0.52
3:P:580:VAL:HG13	3:P:598:LEU:HG	1.91	0.52
3:N:448:TYR:CE1	3:N:450:GLU:HB3	2.44	0.52
1:C:4007:DG:OP1	3:N:665:ARG:NH2	2.42	0.52

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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: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:N:417:LYS:HG3	3:N:434:LYS:O	2.10	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:Q:488:SER:HB3	3:Q:501:ILE:HD11	1.93	0.51
3:M:607:SER:OG	3:M:662:ASN:ND2	2.44	0.51
3:P:421:ARG:NH1	3:P:571:GLN:HG3	2.26	0.51
3:N:411:ARG:HG3	3:N:412:ILE:N	2.25	0.51
3:M:661:ILE:HG23	3:M:663:GLY:O	2.11	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
3:M:479:ILE:HG22	3:M:484:VAL:CG2	2.40	0.50
3:N:565:ASN:HB3	3:N:566:PRO:HD2	1.93	0.50
3:N:523:ASN:O	3:N:527:GLU:HG3	2.11	0.50
1:E:4002:DT:H2''	1:E:4003:DG:O5'	2.10	0.50
3:P:671:GLN:HA	3:P:671:GLN:OE1	2.12	0.50
3:P:479:ILE:HG22	3:P:484:VAL:HG21	1.94	0.50
3:M:423:HIS:HB3	3:M:430:ARG:CG	2.41	0.50
3:P:552:GLU:C	3:P:554:SER:N	2.65	0.50
3:N:548:VAL:HG22	3:N:549:HIS:N	2.26	0.50
3:P:421:ARG:HH11	3:P:571:GLN:HG3	1.77	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
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

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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:Q:659:TYR:HE1	3:Q:661:ILE:HD11	1.77	0.50
3:N:463:ALA:HB2	3:N:543:ARG:HG3	1.93	0.50
3:P:421:ARG:NH2	3:P:430:ARG:NH2	2.59	0.49
3:N:467:ILE:CG1	3:Q:583:GLN:O	2.56	0.49
3:P:486:THR:HG22	3:P:501:ILE:HG13	1.94	0.49
3:N:481:GLY:C	3:N:483:THR:H	2.15	0.49
3:M:412:ILE:HG22	3:M:412:ILE:O	2.12	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
3:M:488:SER:HB2	3:M:499:LEU:HD11	1.93	0.49
1:E:4012:DA:H1'	1:E:4013:DT:H5''	1.93	0.49
3:M:520:LYS:NZ	3:M:521:LEU:O	2.44	0.49
3:P:634:GLN:CB	3:P:635:PRO:HD2	2.42	0.49
3:N:603:PHE:HD1	3:N:638:LEU:HG	1.77	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:Q:541:ARG:HH12	3:Q:669:GLN:CD	2.16	0.49
3:N:584:ASP:HB2	3:N:597:ILE:HB	1.95	0.49
3:M:459:PHE:CZ	3:M:545:VAL:HG11	2.47	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
3:N:459:PHE:CZ	3:N:545:VAL:HG11	2.47	0.49
2:H:5010:DT:H1'	2:H:5011:DC:H5''	1.95	0.49
3:N:653:PRO:CG	3:N:677:PRO:HD2	2.40	0.49
3:N:628:VAL:HG12	3:N:640:VAL:HG22	1.94	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
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:HH11	3:M:411:ARG:HG2	1.78	0.49
2:H:5011:DC:H1'	2:H:5012:DC:H5'	1.94	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

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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: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:418:PRO:O	3:Q:567:ILE:HA	2.14	0.48
3:Q:584:ASP:CB	3:Q:597:ILE:HB	2.44	0.48
3:Q:550:ILE:HB	3:Q:558:VAL:HB	1.95	0.48
3:Q:411:ARG:HG2	3:Q:411:ARG:HH11	1.79	0.48
3:N:602:ASN:HD22	3:Q:449:MET:HG3	1.78	0.48
3:M:576:GLU:HG3	3:M:576:GLU:O	2.14	0.48
3:P:580:VAL:CG1	3:P:598:LEU:HG	2.44	0.48
3:P:411:ARG:HG3	3:P:412:ILE:N	2.28	0.48
2:B:5007:DT:H1'	2:B:5008:DT:H5'	1.95	0.48
3:N:547:ARG:HB2	3:N:560:LEU:O	2.13	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
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:P:471:HIS:HE1	3:P:539:ASN:ND2	2.12	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
1:G:4013:DT:H2''	1:G:4014:DA:C8	2.49	0.47
3:N:400:PRO:HG3	3:Q:599:THR:HG21	1.96	0.47
3:M:532:GLU:OE1	3:M:534:ASP:HB2	2.14	0.47
1:C:4002:DT:H2'	1:C:4003:DG:C8	2.49	0.47
3:P:474:TYR:CZ	3:P:520:LYS:HD3	2.49	0.47
3:N:468:LEU:HD21	3:N:545:VAL:HG13	1.96	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
3:N:577:LEU:CB	3:N:578:PRO:HD3	2.31	0.47
3:P:423:HIS:CB	3:P:430:ARG:HD2	2.44	0.47
3:N:580:VAL:HB	3:N:671:GLN:HE21	1.78	0.47
1:C:4014:DA:H1'	1:C:4015:DG:H5'	1.95	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:P:615:THR:OG1	3:P:619:GLN:HB2	2.15	0.47
3:N:584:ASP:O	3:N:584:ASP:OD2	2.32	0.47
3:Q:474:TYR:CE1	3:Q:520:LYS:HD3	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:420:HIS:CD2	3:Q:433:VAL:HA	2.50	0.47
3:P:556:ARG:HH11	3:P:556:ARG:HG2	1.80	0.47
3:Q:552:GLU:C	3:Q:554:SER:N	2.68	0.47
3:M:617:ASP:O	3:M:619:GLN:NE2	2.44	0.47
2:H:5007:DT:C6	2:H:5008:DT:H72	2.50	0.47
3:Q:579:MET:O	3:Q:600:GLY:HA3	2.14	0.47
3:N:489:TYR:CZ	3:N:500:GLU:CB	2.98	0.47
3:N:440:HIS:CD2	3:N:514:ASP:CB	2.97	0.47
3:P:444:GLN:OE1	3:P:510:ARG:NH1	2.48	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:556:ARG:HG2	3:N:556:ARG:HH11	1.80	0.47
3:N:413:GLU:HG2	3:N:510:ARG:HH22	1.80	0.47
1:G:4003:DG:C2'	1:G:4004:DC:C5'	2.79	0.46
3:Q:615:THR:HB	3:Q:617:ASP:OD2	2.15	0.46
3:M:552:GLU:C	3:M:554:SER:H	2.18	0.46
3:M:397:LEU:HD11	3:M:493:VAL:HB	1.97	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: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: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: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:489:TYR:CZ	3:N:500:GLU:HB2	2.50	0.46
3:N:411:ARG:HG2	3:N:411:ARG:HH11	1.79	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:Q:465:GLU:CD	3:Q:469:LYS:HE2	2.35	0.46
3:N:596:MET:HB2	3:N:642:ILE:HD11	1.97	0.46
3:M:462:THR:HG22	3:M:463:ALA:N	2.30	0.46
3:Q:520:LYS:NZ	3:Q:523:ASN:HD21	2.13	0.46
3:Q:411:ARG:HG3	3:Q:412:ILE:N	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:622:TRP:CG	3:P:646:ARG:HD3	2.50	0.46
1:A:4001:DT:H2'	1:A:4002:DT:H72	1.98	0.46
3:P:431:GLY:C	3:P:479:ILE:HD11	2.36	0.46
3:P:408:TYR:HB3	3:P:560:LEU:HD11	1.96	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:547:ARG:NE	3:M:561:GLN:OE1	2.50	0.45
3:P:501:ILE:HG23	3:P:502:PRO:HD2	1.97	0.45
3:M:604:THR:CG2	3:M:605:SER:N	2.73	0.45
3:Q:462:THR:CB	3:Q:465:GLU:HB2	2.45	0.45
3:M:403:SER:O	3:M:560:LEU:HD13	2.17	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:552:GLU:O	3:N:554:SER:N	2.49	0.45
3:N:550:ILE:HB	3:N:558:VAL:HB	1.97	0.45
3:N:480:THR:HG22	3:N:480:THR:O	2.16	0.45
2:F:5002:DA:H1'	2:F:5003:DC:C6	2.51	0.45
2:B:5013:DA:H2''	2:B:5014:DG:OP2	2.16	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:661:ILE:HA	3:Q:666:LYS:O	2.16	0.45
3:Q:412:ILE:O	3:Q:412:ILE:HG22	2.17	0.45
3:N:442:VAL:HG13	3:N:511:ALA:O	2.16	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
2:D:5008:DT:H1'	2:D:5009:DT:H5''	1.99	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:587:SER:HA	3:Q:674:THR:O	2.17	0.45
3:Q:504:GLU:HA	3:Q:505:PRO:HD3	1.86	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:Q:459:PHE:CZ	3:Q:545:VAL:HG11	2.53	0.44
3:P:548:VAL:HG22	3:P:549:HIS:N	2.32	0.44

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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:Q:419:HIS:CE1	3:Q:601:GLN:HG3	2.51	0.44
3:M:552:GLU:C	3:M:554:SER:N	2.71	0.44
3:Q:609:VAL:HG21	3:Q:640:VAL:CG2	2.48	0.44
3:P:547:ARG:NH2	3:P:561:GLN:OE1	2.39	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:N:417:LYS:HG2	3:N:436:PRO:HA	1.99	0.44
3:M:584:ASP:HB3	3:M:597:ILE:H	1.82	0.44
2:B:5001:DA:H2''	2:B:5002:DA:C8	2.53	0.44
3:P:424:TYR:CE2	3:P:520:LYS:HG3	2.53	0.44
3:M:440:HIS:CD2	3:M:514:ASP:HB3	2.52	0.44
3:N:581:GLU:HG2	3:N:599:THR:O	2.18	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: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: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
3:N:613:GLU:HB2	3:N:622:TRP:HB3	1.99	0.44
1:G:4002:DT:C2'	1:G:4003:DG:H8	2.28	0.44
2:F:5004:DT:H2''	2:F:5005:DA:OP2	2.17	0.44
3:Q:584:ASP:CB	3:Q:597:ILE:H	2.31	0.44
3:P:662:ASN:HB2	3:P:666:LYS:CB	2.48	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
3:M:489:TYR:CZ	3:M:500:GLU:CB	3.01	0.44
3:N:570:SER:OG	3:N:572:ARG:HB2	2.18	0.44
1:A:4012:DA:H1'	1:A:4013:DT:H5''	1.99	0.44
3:M:520:LYS:NZ	3:M:523:ASN:ND2	2.66	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:Q:471:HIS:CE1	3:Q:474:TYR:HD2	2.36	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
1:E:4007:DG:H2''	1:E:4008:DA:H5'	1.96	0.43

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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:HG2	3:P:556:ARG:NH1	2.33	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:M:484:VAL:CG1	3:M:515:CYS:HB3	2.49	0.43
3:Q:601:GLN:OE1	3:Q:601:GLN:HA	2.19	0.43
3:Q:465:GLU:HG3	3:Q:466:ARG:N	2.34	0.43
3:Q:659:TYR:HE1	3:Q:661:ILE:CD1	2.31	0.43
3:Q:650:ILE:HG13	3:Q:677:PRO:HB3	2.01	0.43
1:G:4003:DG:C4'	1:G:4003:DG:OP1	2.56	0.43
1:C:4012:DA:H2''	1:C:4013:DT:C5'	2.44	0.43
3:Q:471:HIS:CE1	3:Q:473:PHE:HB2	2.53	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: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
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
1:E:4001:DT:H6	1:E:4001:DT:HO5'	1.65	0.43
3:P:430:ARG:HG2	3:P:430:ARG:NH1	2.33	0.42
3:Q:547:ARG:HB2	3:Q:560:LEU:O	2.18	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
2:B:5005:DA:C1'	2:B:5006:DT:H5''	2.45	0.42
3:M:557:ILE:HD12	3:M:557:ILE:H	1.84	0.42
3:M:423:HIS:CA	3:M:430:ARG:HD2	2.49	0.42
3:N:520:LYS:NZ	3:N:523:ASN:HD21	2.17	0.42
3:Q:474:TYR:CZ	3:Q:520:LYS:HD3	2.54	0.42
3:N:651:ARG:HA	3:N:651:ARG:NE	2.34	0.42
3:M:584:ASP:CB	3:M:597:ILE:H	2.32	0.42
3:M:526:ILE:O	3:M:529:ARG:HB3	2.20	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
3:M:603:PHE:CD1	3:M:638:LEU:HG	2.55	0.42

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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:P:415:GLN:NE2	3:P:565:ASN:H	2.18	0.42
3:P:651:ARG:HA	3:P:651:ARG:NE	2.33	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:450:GLU:HA	3:P:450:GLU:OE2	2.19	0.42
3:M:484:VAL:HG13	3:M:515:CYS:HB3	2.01	0.42
3:P:615:THR:HG22	3:P:616:THR:N	2.35	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:M:526:ILE:HD13	3:M:526:ILE:HA	1.85	0.42
3:M:504:GLU:HA	3:M:505:PRO:HD3	1.78	0.42
2:D:5009:DT:H2"	2:D:5010:DT:H71	2.02	0.42
1:E:4010:DA:H1'	1:E:4011:DA:H5'	2.02	0.42
1:C:4012:DA:H1'	1:C:4013:DT:H5"	2.02	0.42
3:Q:526:ILE:O	3:Q:529:ARG:HB3	2.20	0.42
3:N:489:TYR:CE2	3:N:500:GLU:CB	2.99	0.42
3:Q:615:THR:OG1	3:Q:619:GLN:HB2	2.20	0.42
3:P:415:GLN:HE22	3:P:565:ASN:H	1.68	0.42
3:N:657:ASN:HA	3:N:671:GLN:O	2.19	0.42
3:M:425:GLU:O	3:M:427:GLU:N	2.50	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:488:SER:HB3	3:P:501:ILE:CD1	2.48	0.41
3:P:400:PRO:HB3	3:P:467:ILE:HD11	2.01	0.41
2:D:5009:DT:H1'	2:D:5010:DT:H5'	2.03	0.41
3:P:551:PRO:O	3:P:551:PRO:HG2	2.20	0.41
3:N:571:GLN:O	3:N:572:ARG:C	2.58	0.41
3:Q:488:SER:HB3	3:Q:501:ILE:CD1	2.51	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: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:615:THR:C	3:N:617:ASP:N	2.72	0.41
3:Q:486:THR:HG22	3:Q:501:ILE:HG13	2.03	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:Q:423:HIS:HB3	3:Q:430:ARG:HD2	2.01	0.41
1:G:4007:DG:H2"	1:G:4008:DA:H5'	2.02	0.41
2:B:5001:DA:H2"	2:B:5002:DA:H8	1.85	0.41

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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:Q:479:ILE:HG22	3:Q:484:VAL:HG21	2.02	0.41
3:P:395:VAL:HA	3:P:396:PRO:HD3	1.79	0.41
3:Q:418:PRO:CD	3:Q:581:GLU:HB3	2.50	0.41
3:Q:550:ILE:C	3:Q:557:ILE:HG23	2.41	0.41
2:D:5009:DT:C2'	2:D:5010:DT:H71	2.51	0.41
3:Q:520:LYS:NZ	3:Q:523:ASN:ND2	2.68	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:M:433:VAL:HG11	3:M:544:LEU:HD11	2.01	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:M:581:GLU:HG2	3:M:599:THR:O	2.20	0.41
3:M:423:HIS:HB3	3:M:430:ARG:CD	2.50	0.41
3:M:612:THR:HA	3:M:622:TRP:O	2.21	0.41
3:Q:650:ILE:O	3:Q:677:PRO:HB3	2.21	0.41
3:M:628:VAL:O	3:M:630:LYS:N	2.54	0.41
3:Q:623:GLU:O	3:Q:624:MET:HB2	2.21	0.41
3:M:444:GLN:HA	3:M:509:MET:O	2.21	0.41
1:E:4012:DA:C2'	1:E:4013:DT:C5'	2.95	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	2.51	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
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
1:G:4004:DC:H2'	3:Q:429:SER:O	2.20	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
3:Q:577:LEU:O	3:Q:602:ASN:ND2	2.48	0.41
3:Q:501:ILE:HG23	3:Q:502:PRO:HD2	2.02	0.41
3:Q:580:VAL:HG11	3:Q:671:GLN:HE21	1.85	0.41
3:Q:408:TYR:HE1	3:Q:558:VAL:HG21	1.86	0.41
2:D:5010:DT:H1'	2:D:5011:DC:H5'	2.03	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:N:579:MET:O	3:N:579:MET:HG3	2.20	0.41
3:Q:417:LYS:HG3	3:Q:434:LYS:O	2.21	0.41
3:Q:486:THR:HG22	3:Q:487:THR:O	2.21	0.41
3:N:500:GLU:C	3:N:501:ILE:HD12	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:4002:DT:C2'	1:E:4003:DG:O5'	2.66	0.41
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:573:SER:O	3:Q:577:LEU:HB2	2.21	0.40
3:N:647:ASN:HD22	3:N:650:ILE:HG22	1.87	0.40
2:B:5006:DT:H2''	2:B:5007:DT:C5'	2.49	0.40
3:N:501:ILE:HG23	3:N:502:PRO:CD	2.49	0.40
3:Q:541:ARG:NH1	3:Q:669:GLN:OE1	2.54	0.40
3:N:548:VAL:CG2	3:N:549:HIS:N	2.84	0.40
3:N:419:HIS:O	3:N:420:HIS: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
3:M:455:GLY:HA3	3:M:500:GLU:OE2	2.22	0.40
3:N:650:ILE:HG13	3:N:677:PRO:HB3	2.02	0.40
2:H:5001:DA:C2'	2:H:5002:DA:C8	3.00	0.40
3:N:408:TYR:HD1	3:N:558:VAL:HG11	1.86	0.40
3:M:556:ARG:NH1	3:M:556:ARG:HG2	2.36	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:NH1	3:M:411:ARG:HG2	2.36	0.40
3:N:628:VAL:O	3:N:630:LYS:N	2.54	0.40
3:Q:463:ALA:HA	3:Q:543:ARG:CD	2.48	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:N:456:LEU:HA	3:N:456:LEU:HD12	1.84	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%)	9	40
3	N	282/284 (99%)	251 (89%)	21 (7%)	10 (4%)	4	24
3	P	282/284 (99%)	254 (90%)	21 (7%)	7 (2%)	7	34
3	Q	282/284 (99%)	251 (89%)	27 (10%)	4 (1%)	14	51
All	All	1128/1136 (99%)	1008 (89%)	93 (8%)	27 (2%)	7	35

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%)	51	84
3	N	247/254 (97%)	230 (93%)	17 (7%)	19	56
3	P	247/254 (97%)	240 (97%)	7 (3%)	51	84
3	Q	247/254 (97%)	240 (97%)	7 (3%)	51	84
All	All	988/1016 (97%)	950 (96%)	38 (4%)	40	78

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

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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

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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%)	-0.29	1 (6%) 21 7	34, 44, 84, 95	0
1	C	15/15 (100%)	-0.45	0 100 100	33, 42, 77, 87	0
1	E	15/15 (100%)	-0.09	0 100 100	47, 57, 103, 112	0
1	G	15/15 (100%)	0.12	1 (6%) 21 7	44, 55, 96, 103	0
2	B	15/15 (100%)	-0.19	0 100 100	18, 48, 79, 80	0
2	D	15/15 (100%)	-0.37	0 100 100	27, 45, 62, 63	0
2	F	15/15 (100%)	-0.16	0 100 100	35, 67, 101, 117	0
2	H	15/15 (100%)	-0.14	0 100 100	38, 62, 83, 96	0
3	M	284/284 (100%)	0.38	34 (11%) 6 2	16, 65, 120, 142	0
3	N	284/284 (100%)	0.56	46 (16%) 3 1	17, 76, 124, 141	0
3	P	284/284 (100%)	-0.17	5 (1%) 71 43	22, 54, 94, 130	0
3	Q	284/284 (100%)	-0.09	6 (2%) 67 36	25, 62, 101, 126	0
All	All	1256/1256 (100%)	0.13	93 (7%) 17 6	16, 62, 114, 142	0

All (93) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	N	576	GLU	6.2
3	M	633	SER	6.2
3	M	664	LYS	6.1
3	M	637	MET	5.5
3	M	665	ARG	5.5
3	M	635	PRO	5.3
3	P	631	ASP	5.0
3	N	586	ASP	5.0
3	M	618	GLY	5.0
3	M	627	THR	4.9
3	M	631	ASP	4.8

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Mol	Chain	Res	Type	RSRZ
3	N	619	GLN	4.7
3	N	575	HIS	4.5
3	M	605	SER	4.5
3	N	636	ASN	4.4
3	N	672	HIS	4.3
3	M	591	TYR	4.1
3	N	635	PRO	4.1
3	N	555	GLY	4.1
3	P	630	LYS	4.1
3	N	677	PRO	4.1
3	N	631	ASP	4.0
3	N	616	THR	4.0
3	M	634	GLN	4.0
3	N	651	ARG	3.9
3	M	606	GLU	3.9
3	N	592	GLY	3.8
3	N	663	GLY	3.8
3	N	574	ALA	3.8
3	N	591	TYR	3.7
3	N	585	THR	3.6
3	M	576	GLU	3.6
3	M	604	THR	3.5
3	N	617	ASP	3.4
3	N	602	ASN	3.4
3	M	651	ARG	3.3
3	N	665	ARG	3.3
3	N	634	GLN	3.2
3	M	399	TRP	3.2
3	M	649	HIS	3.2
3	M	588	CYS	3.2
3	M	595	GLN	3.2
3	N	633	SER	3.0
3	P	632	LYS	3.0
3	Q	665	ARG	3.0
3	N	595	GLN	3.0
3	N	678	VAL	3.0
3	N	659	TYR	2.9
3	M	587	SER	2.9
3	N	655	LYS	2.9
3	P	489	TYR	2.9
3	N	664	LYS	2.9
3	M	628	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
3	M	620	GLN	2.8
3	N	649	HIS	2.8
3	N	594	GLN	2.8
3	Q	664	LYS	2.7
3	N	674	THR	2.7
3	M	617	ASP	2.7
3	N	676	HIS	2.7
3	N	662	ASN	2.7
3	N	647	ASN	2.7
3	M	573	SER	2.6
3	P	553	SER	2.6
3	M	594	GLN	2.6
3	M	584	ASP	2.5
3	Q	576	GLU	2.5
3	N	593	GLY	2.5
3	M	659	TYR	2.5
3	M	619	GLN	2.4
3	N	599	THR	2.4
3	N	621	ILE	2.4
1	A	4001	DT	2.3
3	M	582	ARG	2.3
3	M	577	LEU	2.3
3	N	646	ARG	2.3
3	M	615	THR	2.2
3	N	627	THR	2.2
3	N	614	LYS	2.2
3	N	597	ILE	2.2
3	N	615	THR	2.2
3	N	623	GLU	2.2
1	G	4001	DT	2.2
3	N	601	GLN	2.1
3	M	556	ARG	2.1
3	N	622	TRP	2.1
3	Q	633	SER	2.1
3	Q	635	PRO	2.1
3	N	553	SER	2.0
3	Q	466	ARG	2.0
3	N	451	ASN	2.0
3	M	575	HIS	2.0
3	M	629	ASP	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.