



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 31, 2021 – 06:25 AM EDT

PDB ID : 2DY4
Title : Crystal structure of RB69 GP43 in complex with DNA containing Thymine Glycol
Authors : Aller, P.; Rould, M.A.; Hogg, M.; Wallace, S.S.; Doublie, S.
Deposited on : 2006-09-06
Resolution : 2.65 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.23.2
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.2

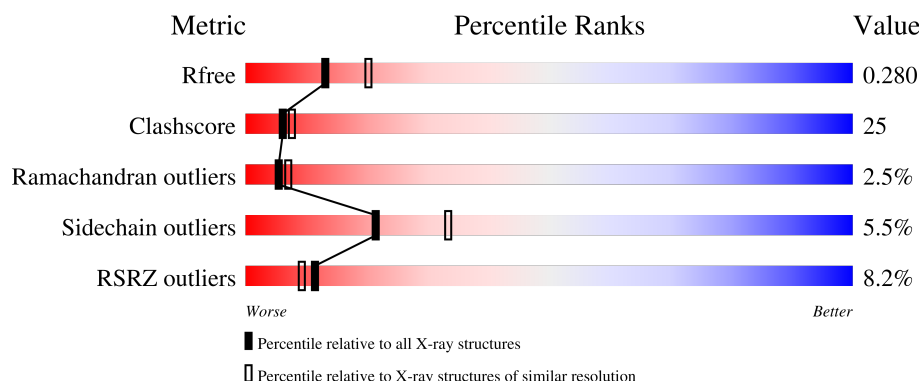
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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}	130704	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	E	18	 11% 6% 83% 6% 6%
1	G	18	 22% 67% 11%
1	I	18	 11% 72% 17%
1	K	18	 44% 94% 6%
2	F	15	 20% 7% 87% 7%

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Mol	Chain	Length	Quality of chain
2	H	15	<div><div></div><div>13%80%7%</div></div>
2	J	15	<div><div></div><div>93%7%</div></div>
2	L	15	<div><div></div><div>60%7%87%7%</div></div>
3	A	903	<div><div></div><div>6%59%37%. </div></div>
3	B	903	<div><div></div><div>5%63%32%. . </div></div>
3	C	903	<div><div></div><div>4%64%32%. </div></div>
3	D	903	<div><div></div><div>16%47%45%6%. </div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 31943 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 5'-D(*CP*GP*(CTG)P*GP*GP*AP*AP*TP*GP*A*CP*AP*GP*CP*CP*GP*CP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	17	Total	C	N	O	P	0	0	0
			348	165	69	99	15			
1	G	18	Total	C	N	O	P	0	0	0
			372	175	74	106	17			
1	I	18	Total	C	N	O	P	0	0	0
			372	175	74	106	17			
1	K	18	Total	C	N	O	P	0	0	0
			372	175	74	106	17			

- Molecule 2 is a DNA chain called 5'-D(*GP*CP*GP*GP*CP*TP*GP*T*CP*AP*TP*TP*CP*CP*A)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	14	Total	C	N	O	P	0	0	0
			276	133	51	80	12			
2	H	15	Total	C	N	O	P	0	0	0
			299	143	53	89	14			
2	J	15	Total	C	N	O	P	0	0	0
			299	143	53	89	14			
2	L	15	Total	C	N	O	P	0	0	0
			299	143	53	89	14			

- Molecule 3 is a protein called DNA polymerase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	A	902	Total	C	N	O	S	Se	0	0	0
			7302	4689	1213	1367	8	25			
3	B	888	Total	C	N	O	S	Se	0	0	0
			7175	4608	1193	1341	8	25			
3	C	900	Total	C	N	O	S	Se	0	0	0
			7300	4683	1214	1370	8	25			

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	D	890	Total	C	N	O	S	Se	0	0	0
			6923	4449	1130	1313	8	23			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	222	ALA	ASP	engineered mutation	UNP Q38087
A	327	ALA	ASP	engineered mutation	UNP Q38087
B	222	ALA	ASP	engineered mutation	UNP Q38087
B	327	ALA	ASP	engineered mutation	UNP Q38087
C	222	ALA	ASP	engineered mutation	UNP Q38087
C	327	ALA	ASP	engineered mutation	UNP Q38087
D	222	ALA	ASP	engineered mutation	UNP Q38087
D	327	ALA	ASP	engineered mutation	UNP Q38087

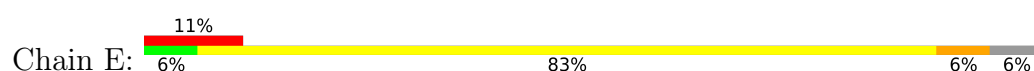
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	9	Total	O	0	0
			9	9		
4	F	5	Total	O	0	0
			5	5		
4	G	18	Total	O	0	0
			18	18		
4	H	9	Total	O	0	0
			9	9		
4	I	17	Total	O	0	0
			17	17		
4	J	4	Total	O	0	0
			4	4		
4	K	5	Total	O	0	0
			5	5		
4	L	2	Total	O	0	0
			2	2		
4	A	117	Total	O	0	0
			117	117		
4	B	205	Total	O	0	0
			205	205		
4	C	160	Total	O	0	0
			160	160		
4	D	55	Total	O	0	0
			55	55		

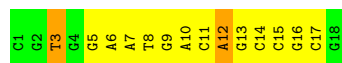
3 Residue-property plots [i](#)

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

- Molecule 1: 5'-D(*CP*GP*(CTG)P*GP*GP*AP*AP*TP*GP*A*CP*AP*GP*CP*CP*GP*CP*G)-3'



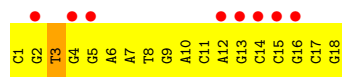
- Molecule 1: 5'-D(*CP*GP*(CTG)P*GP*GP*AP*AP*TP*GP*A*CP*AP*GP*CP*CP*GP*CP*G)-3'



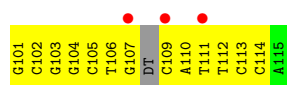
- Molecule 1: 5'-D(*CP*GP*(CTG)P*GP*GP*AP*AP*TP*GP*A*CP*AP*GP*CP*CP*GP*CP*G)-3'



- Molecule 1: 5'-D(*CP*GP*(CTG)P*GP*GP*AP*AP*TP*GP*A*CP*AP*GP*CP*CP*GP*CP*G)-3'



- Molecule 2: 5'-D(*GP*CP*GP*GP*CP*TP*GP*T*CP*AP*TP*TP*CP*CP*A)-3'

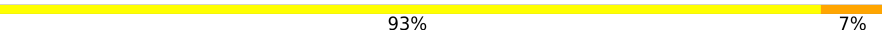


- Molecule 2: 5'-D(*GP*CP*GP*GP*CP*TP*GP*T*CP*AP*TP*TP*CP*CP*A)-3'

Chain H:  13% 80% 7%

G101
C102
G103
G104
C105
T106
G107
T108
C109
A110
T111
T112
C113
C114
A115

- Molecule 2: 5'-D(*GP*CP*GP*GP*CP*TP*GP*T*CP*AP*TP*TP*CP*CP*A)-3'

Chain J:  93% 7%

G101
C102
G103
G104
C105
T106
G107
T108
C109
A110
T111
T112
C113
C114
A115

- Molecule 2: 5'-D(*GP*CP*GP*GP*CP*TP*GP*T*CP*AP*TP*TP*CP*CP*A)-3'

Chain L:  7% 60% 87% 7%

G101
C102
G103
G104
C105
T106
G107
T108
C109
A110
T111
T112
C113
C114
A115

- Molecule 3: DNA polymerase

Chain A:  6% 59% 37% 0%

H1
K2
E3
L6
Q10
G12
D13
S14
I15
F16
E17
D21
R25
E26
R27
T28
R29
E32
S36
L37
C41
D51
P56
C57
T58
M64
M65
R66
D67
W71
I72
M75
E76
E81
A82
L83
S84
R85
D86
L90
E100
I101
K102
Y103

D104
H105
T106
N112
F113
E116
P120
D121
E125
P126
A129
H131
K130
P132
A135
S154
P155
Y156
G157
M158
V159
S163
L170
Q171
D176
E177
E181
M193
E194
K195
E196
L197
L198
M199
L202
N203
F204
W205
Q206
Q207
D208
V211
T212
D213
W216

N217
V218
F221
A222
I223
P224
Y225
R229
Q230
K231
F234
G235
E236
K240
R241
L242
H245
K251
E254
Y257
G258
S259
T262
S269
Y273
S287
D291
Y292
L293
S294
L298
N299
V300
G301
K302
L303
K304
P308
K311
H317
Q318
R319

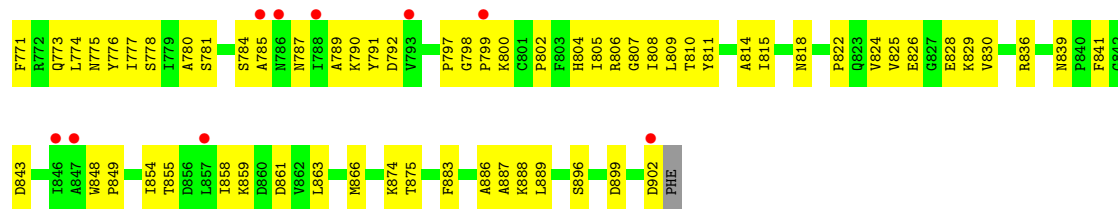
I326
R330
V331
L332
D335
R338
Q339
F340
D346
K347
G348
Y349
I353
S357
V358
F359
S360
P361
I362
D366
A367
L373
Q376
N377
K378
V379
I380
P381
Q382
H386
P387
H485
K486
M489
L490
A491
A492
Q493
K494
N495
G496
E497
I498
I499
L400
K500
P401
M402
R403
Y404
K405
Y406

V407
M408
S409
F410
V410
D411
L412
T413
S414
L415
I419
Q422
V423
L439
I443
S455
C456
S457
F458
P458
D466
R467
D468
V471
P472
T476
R477
F478
N480
Q481
R482
K483
E484
H485
K486
M489
L490
A491
A492
Q493
K494
N495
G496
E497
I498
I499
L400
K500
P401
M402
R403
Y404
K405
Y406

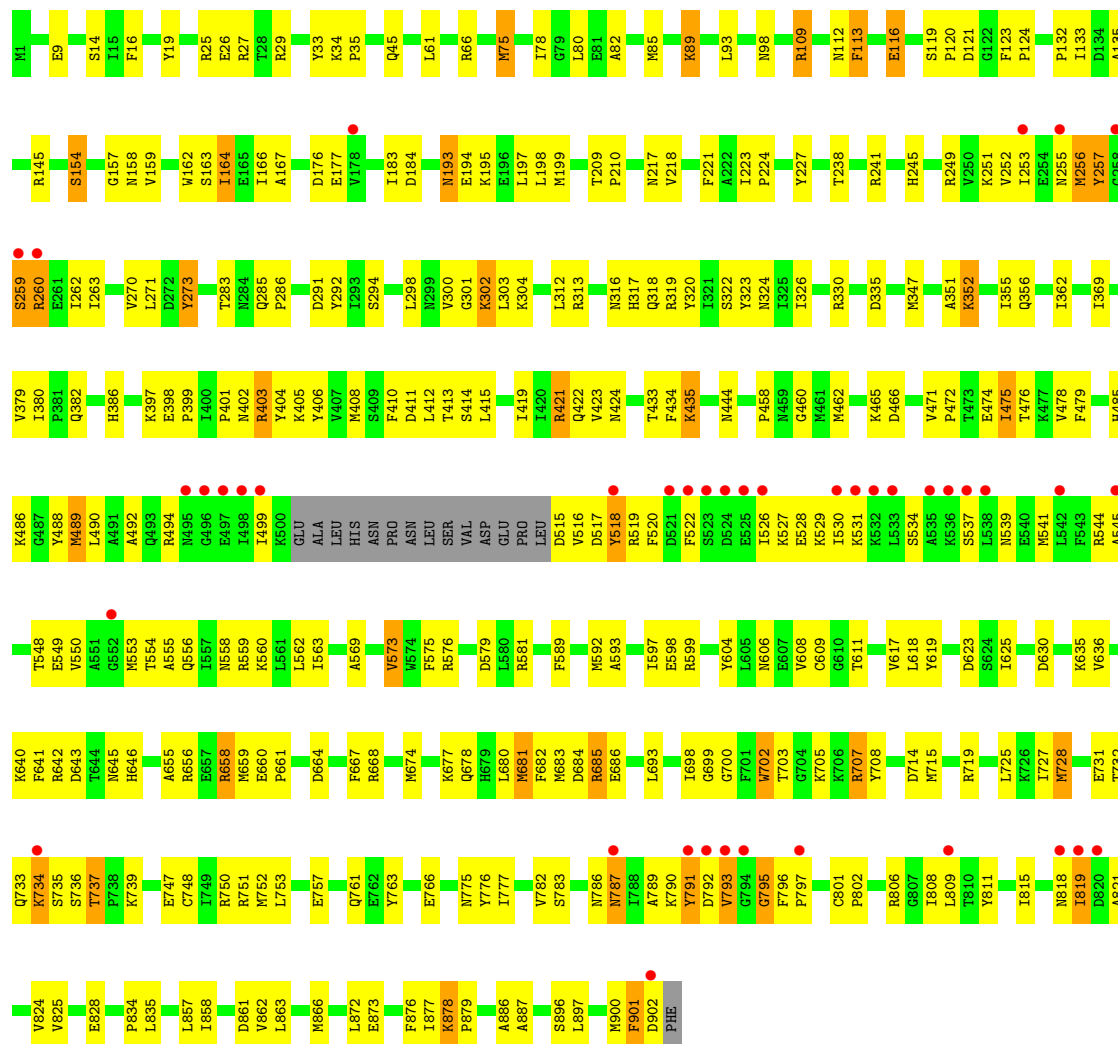
P506
N507
S509
V510
D511
L512
T513
S514
L515
D516
V517
R519
F520
D521
F522
S523
I526
K527
E528
K529
L530
K531
K532
L533
S534
K535
K536
S537
L538
M539
E540
M541
L542
T548
G552
M553
T554
A555
Q556
I557
N558
R559
K560
L561
L562
I563
L570
G571
N572
F573
Y578
H504
T587

M592
A593
L594
M595
Q596
I597
M602
M606
E607
T611
E612
G613
E614
A615
F616
V617
L618
Y619
G620
D621
T622
I625
A629
K631
L632
I633
V636
K640
F641
R642
H646
K653
F654
A655
R656
E657
R658
M659
E660
P661
A662
I663
M674
N675
M676
A677
K678
E770

L680
M681
F682
M683
D684
Q685
R685
I688
A689
G690
P691
G699
G700
F701
W702
K705
K706
R707
Y708
A709
L710
W711
V712
M715
E716
G717
K724
L725
K726
I727
M728
G729
L730
E731
T732
Q733
K734
S735
S736
T737
F738
K739
Q742
E747
L753
E757
E758
E762
K769
E770

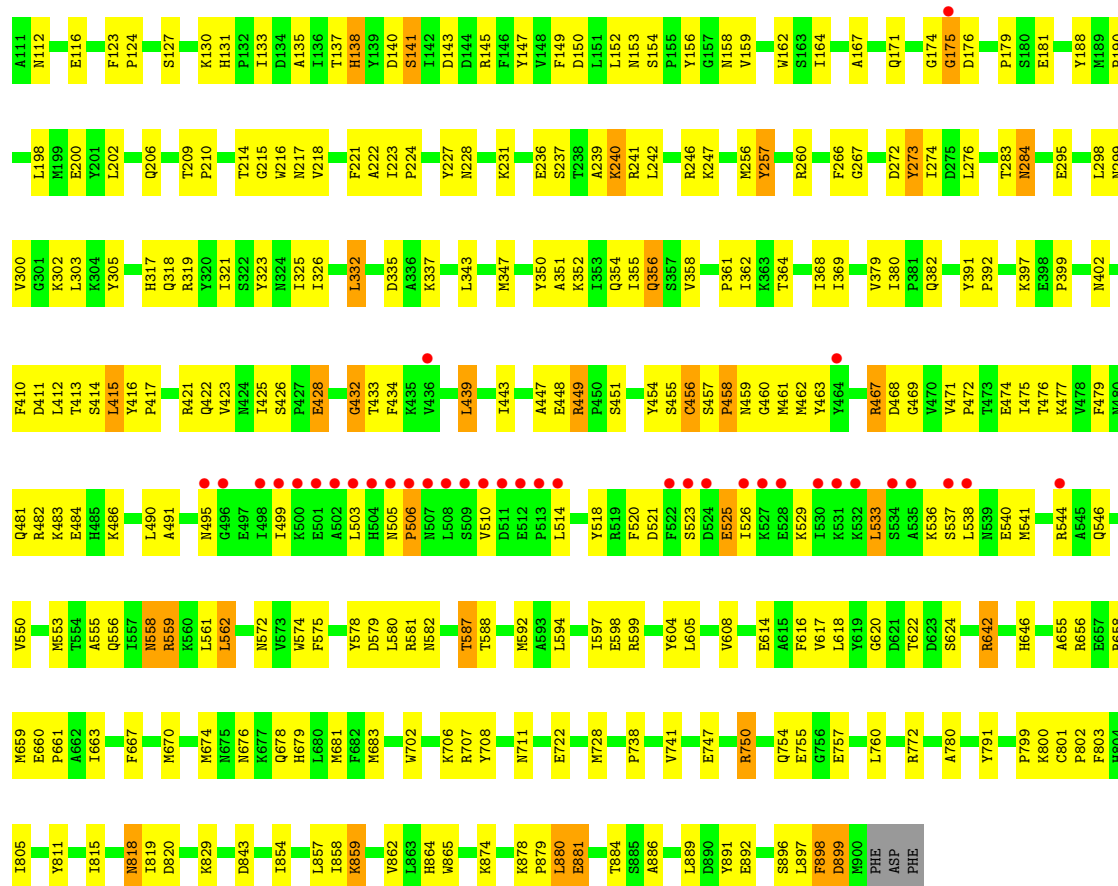


● Molecule 3: DNA polymerase

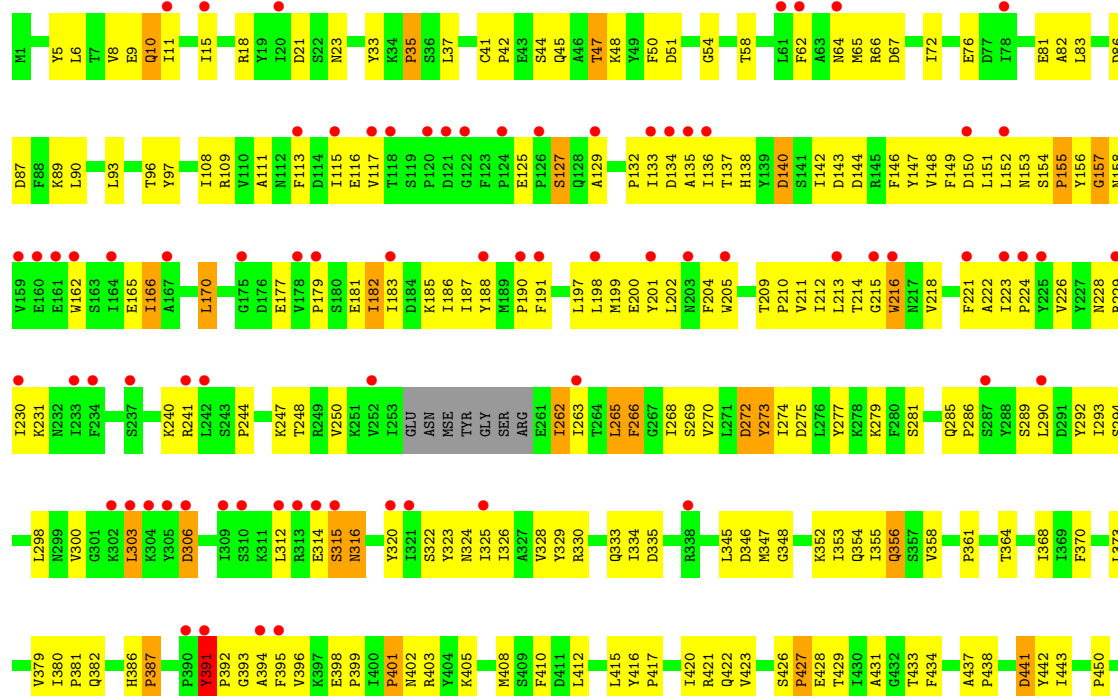


● Molecule 3: DNA polymerase





- Molecule 3: DNA polymerase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	132.61Å 122.63Å 168.69Å 90.00° 96.31° 90.00°	Depositor
Resolution (Å)	50.00 – 2.65 49.49 – 2.60	Depositor EDS
% Data completeness (in resolution range)	88.3 (50.00-2.65) 93.6 (49.49-2.60)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.54 (at 2.61Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.229 , 0.281 0.229 , 0.280	Depositor DCC
R_{free} test set	28873 reflections (9.49%)	wwPDB-VP
Wilson B-factor (Å ²)	47.3	Xtriage
Anisotropy	0.252	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 56.7	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	0.92	EDS
Total number of atoms	31943	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 3.13% 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

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

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	E	0.41	0/365	1.28	0/558
1	G	0.52	0/393	1.33	1/603 (0.2%)
1	I	0.60	0/393	1.31	2/603 (0.3%)
1	K	0.73	0/393	1.31	0/603
2	F	0.41	0/307	1.24	0/468
2	H	0.57	0/333	1.37	1/510 (0.2%)
2	J	0.54	0/333	1.30	1/510 (0.2%)
2	L	0.79	0/333	1.27	1/510 (0.2%)
3	A	0.39	0/7457	0.57	0/10050
3	B	0.42	0/7326	0.62	1/9873 (0.0%)
3	C	0.41	0/7454	0.59	1/10045 (0.0%)
3	D	0.30	0/7072	0.50	0/9590
All	All	0.41	0/32159	0.68	8/43923 (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	G	1	0
2	H	0	1
All	All	1	1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	255	ASN	N-CA-C	-5.75	95.47	111.00
1	G	12	DA	C4'-C3'-O3'	5.52	123.50	109.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	110	DA	C4'-C3'-C2'	5.47	108.03	103.10
2	J	113	DC	C4'-C3'-C2'	5.39	107.95	103.10
3	C	750	ARG	NE-CZ-NH2	-5.35	117.62	120.30
1	I	5	DG	O4'-C1'-C2'	5.18	110.05	105.90
1	I	9	DG	N9-C1'-C2'	5.18	122.44	112.60
2	H	108	DT	O4'-C1'-C2'	5.12	110.00	105.90

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	G	12	DA	C3'

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	115	DA	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	348	0	195	40	0
1	G	372	0	204	26	0
1	I	372	0	204	39	0
1	K	372	0	204	38	0
2	F	276	0	155	22	0
2	H	299	0	165	22	0
2	J	299	0	165	28	0
2	L	299	0	165	26	0
3	A	7302	0	7141	309	0
3	B	7175	0	6995	306	0
3	C	7300	0	7144	254	0
3	D	6923	0	6512	420	0
4	A	117	0	0	28	0
4	B	205	0	0	17	0
4	C	160	0	0	14	0
4	D	55	0	0	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	9	0	0	2	0
4	F	5	0	0	1	0
4	G	18	0	0	0	0
4	H	9	0	0	2	0
4	I	17	0	0	3	0
4	J	4	0	0	0	0
4	K	5	0	0	1	0
4	L	2	0	0	0	0
All	All	31943	0	29249	1491	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 25.

All (1491) 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:I:14:DC:H2''	1:I:15:DC:H5''	1.21	1.17
2:J:111:DT:H2''	2:J:112:DT:H5'	1.16	1.13
3:B:164:ILE:HD12	3:B:164:ILE:H	1.13	1.09
2:L:104:DG:H2''	2:L:105:DC:H5''	1.32	1.07
1:G:11:DC:H2''	1:G:12:DA:H5''	1.34	1.05
3:B:347:MSE:HE1	3:B:562:LEU:HD11	1.43	1.00
3:B:556:GLN:HB3	4:B:990:HOH:O	1.61	0.99
3:D:212:ILE:HD11	3:D:345:LEU:HD21	1.45	0.98
1:I:15:DC:H2''	1:I:16:DG:H5'	1.45	0.97
3:D:619:TYR:HE1	3:D:621:ASP:HB2	1.30	0.96
3:B:82:ALA:H	3:B:382:GLN:HE21	1.06	0.96
2:J:111:DT:H2''	2:J:112:DT:C5'	1.95	0.95
3:C:112:ASN:HB3	3:C:214:THR:HG23	1.49	0.95
1:I:17:DC:H1'	4:I:435:HOH:O	1.67	0.94
3:C:897:LEU:HD23	3:C:897:LEU:H	1.31	0.94
3:D:218:VAL:HG12	3:D:223:ILE:HG13	1.48	0.93
3:D:356:GLN:H	3:D:356:GLN:HE21	0.94	0.93
3:A:863:LEU:HA	3:A:866:MSE:HE3	1.48	0.93
3:D:214:THR:HG22	3:D:215:GLY:H	1.30	0.93
3:D:356:GLN:H	3:D:356:GLN:NE2	1.66	0.92
3:B:736:SER:HA	4:B:910:HOH:O	1.68	0.92
3:B:793:VAL:HB	3:B:796:PHE:HB2	1.49	0.91
3:A:642:ARG:H	3:A:646:HIS:HD2	1.20	0.90
3:D:686:GLU:HB3	3:D:715:MSE:HE1	1.54	0.89
3:B:405:LYS:HA	3:B:699:GLY:HA3	1.55	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:10:DA:H2''	1:I:11:DC:H5'	1.55	0.89
3:B:530:ILE:HG13	3:B:531:LYS:H	1.38	0.89
3:B:732:THR:HG23	3:B:733:GLN:HE21	1.38	0.88
1:G:11:DC:C2'	1:G:12:DA:H5''	2.04	0.87
3:D:356:GLN:HE21	3:D:356:GLN:N	1.71	0.87
3:C:112:ASN:HD21	3:C:332:LEU:HD11	1.37	0.86
3:D:619:TYR:CE1	3:D:621:ASP:HB2	2.09	0.86
3:D:844:LYS:H	3:D:844:LYS:HD3	1.38	0.86
3:C:572:ASN:ND2	3:C:574:TRP:H	1.73	0.86
3:D:854:ILE:HD11	3:D:858:ILE:HD11	1.56	0.86
2:L:112:DT:H2''	2:L:113:DC:H5''	1.55	0.86
2:L:112:DT:C2'	2:L:113:DC:H5''	2.04	0.86
3:D:597:ILE:O	3:D:601:VAL:HG23	1.73	0.86
3:D:873:GLU:HA	3:D:877:ILE:HG12	1.57	0.85
3:A:495:ASN:HD21	3:A:521:ASP:HA	1.41	0.85
3:C:553:MSE:HA	4:C:1026:HOH:O	1.75	0.85
1:I:9:DG:H2''	1:I:10:DA:H5''	1.59	0.85
3:B:253:ILE:HD11	3:B:260:ARG:CZ	2.07	0.84
3:A:655:ALA:HA	3:A:659:MSE:HG3	1.60	0.84
1:E:6:DA:H2''	1:E:7:DA:C8	2.12	0.84
3:B:863:LEU:HA	3:B:866:MSE:HE3	1.60	0.84
3:D:489:MSE:HE3	3:D:490:LEU:HB2	1.57	0.84
1:G:7:DA:H2''	1:G:8:DT:H5'	1.58	0.84
3:D:6:LEU:HD22	3:D:211:VAL:HG11	1.60	0.83
3:A:90:LEU:HD22	3:A:353:ILE:HG22	1.59	0.83
2:J:104:DG:H2'	2:J:105:DC:C6	2.12	0.83
1:K:5:DG:H2''	1:K:6:DA:H5'	1.59	0.83
3:A:728:MSE:HG3	4:A:986:HOH:O	1.77	0.83
3:D:154:SER:HB3	3:D:155:PRO:HD2	1.60	0.83
3:D:137:THR:HB	3:D:328:VAL:HG21	1.58	0.83
1:I:14:DC:C2'	1:I:15:DC:H5''	2.07	0.83
2:L:105:DC:H2'	2:L:106:DT:H72	1.59	0.83
3:B:386:HIS:HB2	3:B:573:VAL:HG22	1.60	0.83
3:C:660:GLU:HB2	3:C:661:PRO:HD3	1.60	0.83
3:D:412:LEU:HD12	3:D:623:ASP:HA	1.61	0.82
3:A:486:LYS:HE3	3:A:556:GLN:HG2	1.62	0.82
2:L:104:DG:H2''	2:L:105:DC:C5'	2.08	0.82
3:B:75:MSE:HE3	3:B:75:MSE:HA	1.61	0.82
1:K:8:DT:H2''	1:K:9:DG:H5'	1.62	0.81
3:A:499:ILE:HD13	3:A:541:MSE:HG2	1.61	0.81
3:B:121:ASP:HA	3:B:819:ILE:HG21	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:303:LEU:HD23	3:D:303:LEU:H	1.44	0.81
1:I:12:DA:H2''	1:I:13:DG:C8	2.14	0.81
3:C:592:MSE:HE3	3:C:670:MSE:SE	2.30	0.81
3:A:660:GLU:HB2	3:A:661:PRO:HD3	1.63	0.81
3:A:738:PRO:HB3	3:A:780:ALA:O	1.80	0.80
2:F:106:DT:H2''	2:F:107:DG:H5''	1.63	0.80
3:C:412:LEU:HG	3:C:683:MSE:HE3	1.64	0.80
3:D:484:GLU:HG2	3:D:488:TYR:HE1	1.46	0.80
1:I:9:DG:H2''	1:I:10:DA:C5'	2.12	0.80
3:A:408:MSE:HE1	3:A:655:ALA:HB2	1.62	0.80
3:B:154:SER:HB3	3:B:313:ARG:HH12	1.46	0.80
3:C:503:LEU:HA	3:C:506:PRO:HG3	1.64	0.80
2:J:111:DT:C2'	2:J:112:DT:H5'	2.08	0.79
1:I:5:DG:H2''	1:I:6:DA:C5'	2.12	0.79
3:A:483:LYS:HE3	3:A:483:LYS:HA	1.64	0.79
3:C:392:PRO:O	3:C:587:THR:HG21	1.83	0.79
2:J:109:DC:H2''	2:J:110:DA:H5'	1.65	0.79
3:B:732:THR:HG23	3:B:733:GLN:NE2	1.98	0.78
3:C:240:LYS:HE3	3:C:246:ARG:HB3	1.64	0.78
1:I:5:DG:H2''	1:I:6:DA:H5'	1.65	0.77
3:A:347:MSE:HB2	3:A:558:ASN:HD21	1.50	0.77
3:D:137:THR:HG22	3:D:138:HIS:H	1.48	0.77
3:B:159:VAL:HG21	3:B:317:HIS:CD2	2.20	0.77
3:B:157:GLY:C	3:B:158:ASN:HD22	1.87	0.77
1:I:8:DT:H4'	4:I:192:HOH:O	1.86	0.76
3:B:224:PRO:HA	3:B:263:ILE:HD12	1.66	0.76
1:G:9:DG:H2''	1:G:10:DA:H5'	1.68	0.76
3:A:739:LYS:HD3	3:A:778:SER:HA	1.65	0.76
1:E:13:DG:O5'	3:A:800:LYS:HG2	1.85	0.76
1:K:13:DG:H2''	1:K:14:DC:H5'	1.65	0.76
3:D:833:LEU:HD22	3:D:866:MSE:HE3	1.68	0.76
3:A:176:ASP:HA	3:A:319:ARG:HH21	1.51	0.75
3:C:523:SER:HB2	3:C:525:GLU:HG2	1.68	0.75
3:A:700:GLY:HA2	3:A:753:LEU:HD22	1.69	0.75
3:C:454:TYR:HD2	3:C:462:MSE:HE2	1.51	0.75
3:D:136:ILE:HG23	3:D:149:PHE:HB2	1.66	0.75
1:K:8:DT:H2'	1:K:9:DG:C8	2.22	0.75
3:A:775:ASN:HD21	3:A:777:ILE:HB	1.51	0.75
3:D:784:SER:HA	3:D:829:LYS:HA	1.67	0.75
3:A:514:LEU:HD21	3:A:529:LYS:HE2	1.67	0.75
3:C:221:PHE:O	3:C:224:PRO:HD2	1.86	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:824:VAL:HA	3:D:849:PRO:HB3	1.69	0.75
3:D:399:PRO:HB3	3:D:619:TYR:HD2	1.52	0.74
1:I:10:DA:H2''	1:I:11:DC:C5'	2.16	0.74
2:J:114:DC:H2''	2:J:115:DA:H5''	1.68	0.74
3:A:100:GLU:HG2	3:A:102:LYS:HE2	1.67	0.74
1:K:8:DT:H2'	1:K:9:DG:H8	1.52	0.74
3:A:848:TRP:HB2	3:A:849:PRO:HD2	1.69	0.74
3:B:116:GLU:HB2	3:B:135:ALA:HB3	1.69	0.74
3:B:735:SER:HB3	3:B:737:THR:HG23	1.67	0.74
3:A:739:LYS:CD	3:A:739:LYS:H	1.99	0.74
3:B:818:ASN:ND2	3:B:821:ALA:HB2	2.02	0.74
3:D:700:GLY:HA2	3:D:753:LEU:HD22	1.69	0.74
3:A:213:LEU:HD13	3:A:223:ILE:HD11	1.68	0.74
3:B:298:LEU:O	3:B:300:VAL:HG23	1.88	0.74
1:I:6:DA:H2''	1:I:7:DA:C8	2.23	0.73
3:D:730:LEU:HD23	3:D:730:LEU:H	1.52	0.73
3:A:392:PRO:O	3:A:587:THR:HG21	1.88	0.73
3:D:300:VAL:HG21	3:D:330:ARG:HH12	1.52	0.73
3:D:514:LEU:HB3	3:D:516:VAL:HG13	1.69	0.73
3:A:631:LYS:HB2	3:A:631:LYS:NZ	2.04	0.73
1:I:13:DG:H2''	1:I:14:DC:H5'	1.71	0.73
3:D:218:VAL:HG13	3:D:222:ALA:HB3	1.69	0.73
3:A:112:ASN:HB2	4:A:987:HOH:O	1.89	0.73
3:B:700:GLY:HA2	3:B:753:LEU:HD22	1.70	0.72
3:D:250:VAL:HG13	3:D:263:ILE:HG12	1.71	0.72
2:H:104:DG:H2''	2:H:105:DC:O5'	1.88	0.72
3:A:776:TYR:HB2	3:A:866:MSE:HE1	1.71	0.72
3:B:732:THR:CG2	3:B:733:GLN:HE21	2.03	0.72
2:L:106:DT:H2''	2:L:107:DG:H5''	1.72	0.72
3:A:443:ILE:HD13	3:A:595:GLN:HB2	1.71	0.72
3:B:163:SER:H	3:B:318:GLN:HE22	1.37	0.72
3:D:492:ALA:HA	3:D:495:ASN:HB3	1.72	0.72
3:D:790:LYS:O	3:D:790:LYS:HD3	1.89	0.72
2:F:106:DT:H2''	2:F:107:DG:C5'	2.20	0.72
3:B:223:ILE:HB	3:B:224:PRO:HD3	1.70	0.72
3:C:153:ASN:HD22	3:C:158:ASN:CG	1.93	0.71
3:D:523:SER:HB2	3:D:527:LYS:CB	2.20	0.71
3:A:592:MSE:HE1	3:A:674:MSE:HG3	1.71	0.71
3:B:589:PHE:HE1	3:B:681:MSE:HE2	1.55	0.71
3:D:405:LYS:O	3:D:690:GLY:HA2	1.91	0.71
3:D:604:TYR:OH	3:D:658:ARG:HG3	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:347:MSE:HG2	3:D:358:VAL:HG13	1.72	0.71
3:A:422:GLN:HE22	3:A:681:MSE:HG2	1.56	0.71
3:A:507:ASN:C	3:A:508:LEU:HD22	2.10	0.71
3:A:468:ASP:HA	4:A:997:HOH:O	1.90	0.71
3:B:253:ILE:O	3:B:259:SER:HA	1.90	0.71
3:C:295:GLU:O	3:C:299:ASN:HA	1.91	0.71
3:D:202:LEU:HB3	3:D:241:ARG:HD3	1.72	0.71
3:B:435:LYS:H	3:B:435:LYS:HD3	1.54	0.70
3:D:486:LYS:HA	4:D:916:HOH:O	1.91	0.70
3:D:702:TRP:CE2	3:D:708:TYR:HB3	2.27	0.70
3:B:303:LEU:HD13	3:B:319:ARG:HD2	1.72	0.70
3:B:408:MSE:HE1	3:B:655:ALA:HB2	1.73	0.70
3:C:572:ASN:HD22	3:C:574:TRP:H	1.38	0.70
3:C:21:ASP:OD2	3:C:25:ARG:HG3	1.92	0.70
3:C:104:ASP:OD1	3:C:106:THR:HB	1.91	0.70
2:L:110:DA:H2''	2:L:111:DT:O4'	1.92	0.70
3:B:164:ILE:H	3:B:164:ILE:CD1	1.90	0.70
3:B:735:SER:CB	3:B:737:THR:HG23	2.22	0.70
3:D:370:PHE:HA	3:D:380:ILE:HD11	1.73	0.69
3:D:730:LEU:HG	3:D:731:GLU:H	1.57	0.69
3:A:218:VAL:HG23	3:A:222:ALA:HB3	1.74	0.69
3:D:803:PHE:CZ	3:D:845:CYS:HB3	2.27	0.69
3:D:326:ILE:O	3:D:330:ARG:HG2	1.92	0.69
3:D:802:PRO:HB2	3:D:804:HIS:CE1	2.27	0.69
2:H:107:DG:H5'	4:H:306:HOH:O	1.92	0.69
3:A:347:MSE:HE1	3:A:562:LEU:HD11	1.75	0.69
3:B:435:LYS:HD3	3:B:435:LYS:N	2.08	0.69
3:B:797:PRO:HG3	3:B:806:ARG:NH1	2.08	0.69
3:D:213:LEU:HB3	3:D:270:VAL:HG12	1.73	0.69
3:D:731:GLU:OE2	3:D:879:PRO:HB3	1.92	0.69
1:K:5:DG:H2''	1:K:6:DA:C5'	2.21	0.69
3:B:733:GLN:O	3:B:734:LYS:C	2.30	0.69
3:C:343:LEU:HG	4:C:1053:HOH:O	1.92	0.69
3:C:604:TYR:OH	3:C:658:ARG:HB3	1.93	0.69
3:D:8:VAL:HG11	3:D:93:LEU:HD13	1.75	0.69
3:D:779:ILE:HD11	3:D:866:MSE:HE1	1.73	0.69
3:D:117:VAL:HG12	3:D:133:ILE:HA	1.73	0.69
2:H:110:DA:H2''	2:H:111:DT:H5'	1.74	0.68
3:B:303:LEU:HD12	3:B:323:TYR:HA	1.74	0.68
3:C:412:LEU:HD13	3:C:415:LEU:HD13	1.75	0.68
3:D:109:ARG:HB2	3:D:211:VAL:HG23	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:106:DT:C2'	2:F:107:DG:H5''	2.22	0.68
3:D:90:LEU:HG	3:D:353:ILE:HG22	1.75	0.68
2:F:111:DT:H1'	4:F:577:HOH:O	1.93	0.68
3:C:81:GLU:HG2	3:C:83:LEU:HD22	1.73	0.68
3:C:482:ARG:C	3:C:484:GLU:H	1.96	0.68
3:A:642:ARG:H	3:A:646:HIS:CD2	2.08	0.68
3:D:458:PRO:HG3	3:D:592:MSE:SE	2.43	0.68
3:A:739:LYS:HD2	3:A:778:SER:O	1.94	0.68
1:I:13:DG:H2''	1:I:14:DC:C5'	2.24	0.68
3:C:881:GLU:HG3	3:C:891:TYR:HE1	1.59	0.68
3:D:737:THR:HG22	3:D:875:THR:HB	1.76	0.68
4:E:449:HOH:O	2:F:110:DA:H1'	1.93	0.67
3:B:75:MSE:HA	3:B:75:MSE:CE	2.23	0.67
3:D:427:PRO:HG2	4:D:953:HOH:O	1.94	0.67
3:B:326:ILE:CG2	3:B:330:ARG:HE	2.06	0.67
3:C:52:ILE:HD12	3:C:428:GLU:HG3	1.77	0.67
3:D:830:VAL:HA	3:D:850:SER:H	1.58	0.67
1:I:9:DG:C2'	1:I:10:DA:H5''	2.23	0.67
3:A:485:HIS:HB3	3:A:556:GLN:HE21	1.58	0.67
3:C:171:GLN:HA	3:C:175:GLY:HA2	1.77	0.67
3:C:495:ASN:O	3:C:499:ILE:HG12	1.94	0.67
3:A:602:ASN:HD21	3:A:617:VAL:H	1.42	0.67
3:C:152:LEU:HD11	3:C:190:PRO:HB2	1.76	0.67
3:D:132:PRO:HB3	3:D:229:ARG:NH2	2.10	0.67
3:A:403:ARG:HD2	3:A:887:ALA:O	1.95	0.67
2:J:105:DC:H2''	2:J:106:DT:H5'	1.77	0.66
3:C:175:GLY:HA3	3:C:319:ARG:HH21	1.59	0.66
3:D:821:ALA:HB1	3:D:855:THR:HG21	1.78	0.66
3:A:559:ARG:O	3:A:563:ILE:HG13	1.94	0.66
3:C:130:LYS:HE3	3:C:131:HIS:CE1	2.29	0.66
2:L:105:DC:H2'	2:L:106:DT:C7	2.24	0.66
3:B:82:ALA:H	3:B:382:GLN:NE2	1.88	0.66
3:D:471:VAL:HB	3:D:472:PRO:HD3	1.77	0.66
1:E:18:DG:OP1	1:E:18:DG:H3'	1.96	0.66
2:H:107:DG:H2''	2:H:108:DT:O5'	1.94	0.66
2:H:110:DA:H2''	2:H:111:DT:C5'	2.26	0.66
3:B:164:ILE:HD12	3:B:164:ILE:N	1.98	0.66
3:C:298:LEU:HB2	3:C:300:VAL:HG12	1.78	0.66
3:A:338:ARG:HB3	3:A:340:PHE:CE1	2.30	0.66
3:C:78:ILE:HG13	3:C:80:LEU:HD23	1.77	0.66
1:E:2:DG:OP1	3:A:361:PRO:HD2	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:16:DG:H2''	1:I:17:DC:O5'	1.94	0.66
3:B:527:LYS:HA	3:B:530:ILE:HD11	1.76	0.66
3:C:391:TYR:HB2	3:C:392:PRO:HD2	1.76	0.66
1:K:8:DT:H4'	1:K:8:DT:OP1	1.96	0.66
3:B:458:PRO:HG3	3:B:592:MSE:SE	2.46	0.66
3:C:556:GLN:HB3	4:C:1026:HOH:O	1.96	0.66
3:B:326:ILE:O	3:B:330:ARG:HG2	1.95	0.65
3:B:593:ALA:CB	3:B:681:MSE:HE3	2.25	0.65
3:D:191:PHE:HE2	3:D:200:GLU:HG3	1.61	0.65
3:C:540:GLU:O	3:C:544:ARG:HG2	1.96	0.65
3:A:170:LEU:HA	3:A:177:GLU:HG2	1.79	0.65
3:A:874:LYS:HB3	4:A:964:HOH:O	1.96	0.65
1:G:9:DG:H2''	1:G:10:DA:C5'	2.26	0.65
3:A:810:THR:OG1	3:A:843:ASP:HB2	1.96	0.65
3:D:768:GLU:HG2	3:D:872:LEU:HD21	1.79	0.65
2:L:112:DT:H2''	2:L:113:DC:O4'	1.97	0.65
3:D:244:PRO:HD3	3:D:268:ILE:HD11	1.79	0.64
3:A:193:ASN:HD21	3:A:196:GLU:HG3	1.61	0.64
3:A:555:ALA:N	4:A:960:HOH:O	2.30	0.64
3:B:422:GLN:HG3	3:B:678:GLN:O	1.96	0.64
3:B:516:VAL:H	3:B:544:ARG:NH1	1.94	0.64
3:C:439:LEU:HD21	3:C:588:THR:HG23	1.78	0.64
1:E:5:DG:C2'	1:E:6:DA:H5''	2.27	0.64
3:C:458:PRO:HB2	3:C:588:THR:HG22	1.79	0.64
1:K:3:CTG:H2''	1:K:4:DG:C8	2.32	0.64
3:C:231:LYS:HE3	3:C:236:GLU:HG3	1.79	0.64
3:C:455:SER:OG	3:C:676:ASN:HA	1.98	0.64
3:D:592:MSE:HE3	3:D:670:MSE:SE	2.48	0.64
3:D:649:ASP:CG	3:D:719:ARG:HH22	2.01	0.64
3:B:541:MSE:HE3	3:B:544:ARG:NH2	2.12	0.64
3:C:218:VAL:HG22	3:C:223:ILE:HG13	1.80	0.64
3:D:492:ALA:HA	3:D:495:ASN:CB	2.27	0.64
2:L:112:DT:H2''	2:L:113:DC:C5'	2.27	0.64
3:D:355:ILE:O	3:D:358:VAL:HG23	1.97	0.64
3:D:484:GLU:HG2	3:D:488:TYR:CE1	2.29	0.64
3:D:504:HIS:C	3:D:506:PRO:HD3	2.17	0.64
3:A:738:PRO:HB3	3:A:780:ALA:C	2.18	0.64
3:A:811:TYR:OH	3:A:822:PRO:HG2	1.98	0.64
3:B:668:ARG:HG3	3:B:668:ARG:HH11	1.62	0.64
3:D:416:TYR:O	3:D:420:ILE:HG13	1.98	0.64
3:D:668:ARG:NH1	3:D:668:ARG:HB2	2.12	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:106:DT:H1'	2:F:107:DG:H5''	1.80	0.64
3:A:83:LEU:HD12	3:A:83:LEU:H	1.62	0.64
3:B:757:GLU:O	3:B:761:GLN:HG3	1.97	0.64
2:H:113:DC:O5'	3:B:734:LYS:HB2	1.98	0.63
1:K:8:DT:H2''	1:K:9:DG:C5'	2.28	0.63
3:A:822:PRO:HD2	3:A:855:THR:HB	1.80	0.63
3:D:856:ASP:HA	3:D:859:LYS:HB3	1.80	0.63
3:A:13:ASP:OD1	3:A:66:ARG:HB2	1.98	0.63
3:A:231:LYS:HG3	3:A:236:GLU:HA	1.79	0.63
3:B:397:LYS:HD3	3:B:619:TYR:HA	1.81	0.63
3:B:598:GLU:HG3	3:B:617:VAL:HG11	1.80	0.63
1:E:11:DC:H2''	1:E:12:DA:H5'	1.79	0.63
1:E:9:DG:H2'	1:E:11:DC:C6	2.34	0.63
3:A:251:LYS:HD2	3:A:262:ILE:HD11	1.80	0.63
3:B:403:ARG:HH11	3:B:403:ARG:CB	2.12	0.63
3:B:658:ARG:NE	3:D:897:LEU:HD11	2.13	0.63
1:K:9:DG:H2''	1:K:10:DA:O5'	1.99	0.63
3:A:387:PRO:HB2	4:A:998:HOH:O	1.98	0.63
3:B:304:LYS:HD2	3:B:304:LYS:N	2.12	0.63
3:A:620:GLY:O	3:A:621:ASP:HB2	1.99	0.63
3:D:273:TYR:OH	3:D:335:ASP:HA	1.99	0.63
3:D:41:CYS:HB2	3:D:42:PRO:HD2	1.81	0.62
3:D:398:GLU:OE1	3:D:705:LYS:HE3	1.98	0.62
3:D:642:ARG:HG2	3:D:646:HIS:HD2	1.63	0.62
1:G:14:DC:H2''	1:G:15:DC:H5'	1.81	0.62
2:H:101:DG:H8	2:H:101:DG:HO5'	1.47	0.62
3:A:304:LYS:O	3:A:319:ARG:HD3	1.99	0.62
3:C:467:ARG:H	3:C:467:ARG:HD3	1.64	0.62
1:I:2:DG:OP2	3:C:361:PRO:HD2	2.00	0.62
3:D:166:ILE:HB	4:D:934:HOH:O	1.99	0.62
3:B:403:ARG:HH11	3:B:403:ARG:HB3	1.64	0.62
3:A:655:ALA:HA	3:A:659:MSE:CG	2.27	0.62
3:A:685:ARG:NH1	3:A:688:ILE:HG13	2.15	0.62
3:B:589:PHE:CE1	3:B:681:MSE:HE2	2.33	0.62
3:D:272:ASP:OD2	3:D:274:ILE:HG22	1.99	0.62
3:D:725:LEU:HD11	3:D:750:ARG:HG3	1.82	0.62
1:E:14:DC:H2''	1:E:15:DC:H5'	1.81	0.62
3:A:839:ASN:HD22	3:A:841:PHE:HB2	1.63	0.62
3:C:818:ASN:OD1	3:C:857:LEU:HD11	2.00	0.62
2:J:103:DG:H2''	2:J:104:DG:O5'	1.99	0.62
1:K:16:DG:H2''	1:K:17:DC:H5''	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:790:LYS:HE2	3:B:802:PRO:HD3	1.81	0.62
3:D:841:PHE:HZ	3:D:861:ASP:HB3	1.64	0.62
3:A:130:LYS:HE2	4:A:956:HOH:O	2.00	0.62
3:C:520:PHE:HA	4:C:937:HOH:O	2.00	0.61
3:D:520:PHE:HA	4:D:931:HOH:O	2.00	0.61
1:E:12:DA:H2''	1:E:13:DG:O5'	2.00	0.61
1:G:7:DA:H2''	1:G:8:DT:C5'	2.29	0.61
2:J:108:DT:H2''	2:J:109:DC:H5'	1.82	0.61
3:B:162:TRP:CZ3	3:B:164:ILE:HG13	2.35	0.61
3:A:82:ALA:O	3:A:382:GLN:HG3	2.00	0.61
3:C:164:ILE:N	4:C:983:HOH:O	2.27	0.61
3:B:303:LEU:HB2	3:B:323:TYR:CD1	2.36	0.61
3:B:541:MSE:HE3	3:B:544:ARG:HH22	1.65	0.61
1:E:11:DC:H2''	1:E:12:DA:C5'	2.31	0.61
3:C:421:ARG:HD3	3:C:476:THR:OG1	1.99	0.61
3:D:686:GLU:CB	3:D:715:MSE:HE1	2.28	0.61
3:B:257:TYR:CE1	3:B:786:ASN:HB3	2.35	0.61
3:D:496:GLY:O	3:D:499:ILE:HB	2.01	0.61
3:A:443:ILE:HD13	3:A:595:GLN:CB	2.30	0.61
3:D:277:TYR:O	3:D:281:SER:HB2	2.01	0.61
3:D:553:MSE:O	3:D:556:GLN:HG3	2.00	0.61
3:D:825:VAL:HB	3:D:828:GLU:HB2	1.81	0.61
3:A:85:MSE:HE1	3:A:366:ASP:OD2	2.01	0.61
3:A:606:ASN:OD1	3:A:616:PHE:HE1	1.84	0.61
2:L:114:DC:H2''	2:L:115:DA:O4'	2.01	0.60
3:A:707:ARG:HD3	3:A:729:GLY:HA3	1.83	0.60
3:D:402:ASN:CG	3:D:403:ARG:H	2.04	0.60
3:D:465:LYS:HD2	3:D:677:LYS:HA	1.83	0.60
1:K:13:DG:H2''	1:K:14:DC:C5'	2.32	0.60
3:B:132:PRO:HA	3:B:194:GLU:OE2	2.01	0.60
3:B:421:ARG:HD3	3:B:475:ILE:HD12	1.82	0.60
3:C:343:LEU:HD11	3:C:558:ASN:ND2	2.15	0.60
1:K:2:DG:O6	3:D:279:LYS:HD2	2.01	0.60
3:A:347:MSE:HB2	3:A:558:ASN:ND2	2.16	0.60
3:B:159:VAL:HG11	3:B:317:HIS:HB2	1.83	0.60
3:D:9:GLU:O	3:D:15:ILE:HG13	2.01	0.60
3:D:214:THR:HG22	3:D:215:GLY:N	2.10	0.60
3:D:714:ASP:HB2	3:D:719:ARG:HD3	1.83	0.60
1:E:6:DA:H2''	1:E:7:DA:N7	2.15	0.60
3:D:262:ILE:HD12	3:D:262:ILE:N	2.16	0.60
3:A:606:ASN:HD21	3:A:614:GLU:H	1.47	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:494:ARG:CB	3:B:494:ARG:HH11	2.15	0.60
3:C:112:ASN:HD21	3:C:332:LEU:CD1	2.14	0.60
3:C:791:TYR:CD2	3:C:801:CYS:HA	2.36	0.60
3:D:142:ILE:HD12	3:D:143:ASP:N	2.17	0.60
2:H:106:DT:H2''	2:H:107:DG:H5'	1.83	0.60
1:I:7:DA:H2''	1:I:8:DT:O5'	2.02	0.60
3:A:405:LYS:HA	3:A:699:GLY:HA3	1.84	0.60
3:D:434:PHE:CZ	3:D:460:GLY:HA2	2.36	0.60
2:F:111:DT:H2''	2:F:112:DT:C5'	2.31	0.60
1:G:12:DA:H2''	1:G:13:DG:C8	2.36	0.60
3:B:294:SER:HB2	3:B:301:GLY:HA2	1.82	0.60
3:A:502:ALA:HA	3:A:538:LEU:HD23	1.82	0.60
3:A:554:THR:C	4:A:960:HOH:O	2.41	0.60
3:A:784:SER:HB3	3:A:829:LYS:HG2	1.81	0.60
3:C:711:ASN:ND2	3:C:754:GLN:HE21	2.00	0.60
3:D:890:ASP:HB3	4:D:949:HOH:O	2.02	0.60
3:A:386:HIS:HB2	3:A:573:VAL:HB	1.84	0.59
3:A:625:ILE:HG12	3:A:683:MSE:HE1	1.83	0.59
3:C:655:ALA:O	3:C:660:GLU:HG2	2.02	0.59
3:B:285:GLN:HG3	3:B:286:PRO:HD2	1.84	0.59
3:B:636:VAL:O	3:B:640:LYS:HG3	2.02	0.59
3:D:730:LEU:HD12	3:D:883:PHE:CZ	2.37	0.59
3:A:81:GLU:OE2	3:A:83:LEU:HG	2.03	0.59
3:C:112:ASN:HB3	3:C:214:THR:CG2	2.30	0.59
2:F:102:DC:H2''	2:F:103:DG:OP2	2.02	0.59
2:J:101:DG:HO5'	2:J:101:DG:H8	1.50	0.59
3:B:303:LEU:C	3:B:304:LYS:HD2	2.23	0.59
1:I:6:DA:H2''	1:I:7:DA:H8	1.66	0.59
1:K:3:CTG:H2''	1:K:4:DG:H8	1.66	0.59
3:A:791:TYR:O	3:A:798:GLY:N	2.36	0.59
3:D:510:VAL:O	3:D:533:LEU:HD13	2.02	0.59
2:J:105:DC:H2''	2:J:106:DT:C5'	2.32	0.59
1:K:13:DG:H2'	1:K:14:DC:C6	2.38	0.59
3:A:194:GLU:OE1	3:A:229:ARG:HD2	2.02	0.59
3:C:273:TYR:OH	3:C:335:ASP:HA	2.02	0.59
3:D:731:GLU:N	4:D:925:HOH:O	2.35	0.59
1:K:1:DC:H4'	3:D:572:ASN:HD21	1.68	0.59
3:B:82:ALA:N	3:B:382:GLN:HE21	1.90	0.59
3:C:1:MSE:HE1	3:C:107:LYS:HE3	1.84	0.59
2:L:105:DC:H4'	2:L:105:DC:OP1	2.03	0.58
3:B:731:GLU:HB3	3:B:737:THR:HG21	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:708:TYR:O	3:D:730:LEU:HD22	2.03	0.58
3:C:757:GLU:HB2	3:C:889:LEU:HD22	1.84	0.58
3:A:90:LEU:CD2	3:A:353:ILE:HG22	2.31	0.58
3:A:513:PRO:HG3	3:A:537:SER:HB3	1.84	0.58
3:D:202:LEU:HD13	3:D:241:ARG:HD2	1.86	0.58
3:D:306:ASP:HB2	3:D:315:SER:OG	2.03	0.58
3:D:330:ARG:O	3:D:334:ILE:HG13	2.02	0.58
3:D:844:LYS:HD3	3:D:844:LYS:N	2.15	0.58
1:I:2:DG:H2''	1:I:3:CTG:OP2	2.04	0.58
1:I:8:DT:H2'	1:I:9:DG:C8	2.37	0.58
3:A:791:TYR:HA	3:A:799:PRO:HD2	1.84	0.58
3:A:807:GLY:HA3	4:A:972:HOH:O	2.03	0.58
3:D:642:ARG:HG3	3:D:643:ASP:OD2	2.03	0.58
3:D:832:VAL:HB	4:D:957:HOH:O	2.02	0.58
3:A:896:SER:HB3	3:A:899:ASP:OD1	2.03	0.58
3:D:392:PRO:HD2	3:D:584:THR:HG22	1.86	0.58
3:D:496:GLY:HA2	3:D:499:ILE:HD12	1.84	0.58
3:A:129:ALA:HA	3:A:225:TYR:CE1	2.39	0.58
3:A:784:SER:HA	3:A:829:LYS:HA	1.85	0.58
3:A:734:LYS:HE2	3:A:737:THR:OG1	2.04	0.58
3:A:485:HIS:HB3	3:A:556:GLN:NE2	2.18	0.58
3:D:422:GLN:HG3	3:D:678:GLN:O	2.04	0.58
3:B:386:HIS:CD2	4:B:1064:HOH:O	2.56	0.58
3:D:10:GLN:HG3	3:D:65:MSE:SE	2.53	0.58
3:D:830:VAL:HG22	3:D:831:TYR:H	1.69	0.58
3:A:64:ASN:ND2	3:A:67:ASP:H	2.02	0.58
3:A:489:MSE:HE2	3:A:490:LEU:HG	1.86	0.58
3:B:435:LYS:O	3:B:435:LYS:HG2	2.04	0.58
3:C:897:LEU:H	3:C:897:LEU:CD2	2.11	0.58
3:A:775:ASN:ND2	3:A:777:ILE:HB	2.16	0.57
3:A:776:TYR:CB	3:A:866:MSE:HE1	2.34	0.57
3:B:271:LEU:HD11	3:B:356:GLN:HA	1.85	0.57
1:E:4:DG:H2''	1:E:5:DG:O5'	2.05	0.57
1:G:7:DA:H2'	1:G:8:DT:H72	1.86	0.57
1:G:14:DC:H2''	1:G:15:DC:C5'	2.34	0.57
2:L:103:DG:H2''	2:L:104:DG:C8	2.39	0.57
3:D:51:ASP:HA	3:D:379:VAL:HG22	1.85	0.57
3:D:495:ASN:HD22	3:D:521:ASP:HA	1.68	0.57
2:H:114:DC:OP1	3:B:728:MSE:HE3	2.04	0.57
1:I:5:DG:H2''	1:I:6:DA:H5''	1.86	0.57
3:A:739:LYS:CD	3:A:739:LYS:N	2.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:158:ASN:HD22	3:B:158:ASN:N	2.02	0.57
3:C:52:ILE:HB	3:C:428:GLU:HG2	1.85	0.57
3:B:421:ARG:HD2	3:B:476:THR:OG1	2.03	0.57
3:B:534:SER:OG	3:B:537:SER:HB2	2.05	0.57
3:B:685:ARG:NH2	3:B:714:ASP:OD1	2.37	0.57
3:C:555:ALA:O	3:C:559:ARG:HG2	2.04	0.57
3:D:509:SER:HB2	3:D:533:LEU:HA	1.87	0.57
3:B:183:ILE:HG23	3:B:184:ASP:N	2.19	0.57
3:B:227:TYR:CD2	3:B:263:ILE:HD13	2.40	0.57
3:B:312:LEU:HD12	3:B:320:TYR:HB2	1.86	0.57
3:B:703:THR:OG1	3:B:707:ARG:HD3	2.05	0.57
3:C:711:ASN:HD21	3:C:754:GLN:HE21	1.51	0.57
3:D:514:LEU:HD23	3:D:541:MSE:HE1	1.87	0.57
3:A:471:VAL:HB	3:A:472:PRO:CD	2.34	0.57
3:A:800:LYS:HB2	3:A:800:LYS:NZ	2.20	0.57
3:B:245:HIS:HE1	4:B:961:HOH:O	1.85	0.57
3:C:477:LYS:O	3:C:481:GLN:HG3	2.04	0.57
3:D:730:LEU:HD23	3:D:730:LEU:N	2.19	0.57
3:A:806:ARG:HA	3:A:809:LEU:HD12	1.86	0.57
3:D:396:VAL:HG21	3:D:706:LYS:HE2	1.86	0.57
3:D:833:LEU:CD2	3:D:866:MSE:HE3	2.35	0.57
1:E:9:DG:H2''	1:E:11:DC:O4'	2.05	0.57
3:B:593:ALA:HB1	3:B:681:MSE:HE3	1.87	0.57
3:A:807:GLY:CA	4:A:972:HOH:O	2.52	0.57
3:C:42:PRO:HG2	3:C:45:GLN:HG3	1.86	0.57
3:D:300:VAL:HG21	3:D:330:ARG:NH1	2.20	0.57
3:A:6:LEU:CD1	3:A:26:GLU:HG3	2.35	0.56
3:A:597:ILE:HD11	3:A:663:ILE:HG23	1.86	0.56
3:A:771:PHE:HA	3:A:774:LEU:HD12	1.86	0.56
3:B:478:VAL:HG13	3:B:559:ARG:HG3	1.87	0.56
2:L:106:DT:H5''	2:L:106:DT:H6	1.70	0.56
3:C:750:ARG:NH2	3:C:755:GLU:OE1	2.38	0.56
3:D:147:TYR:HA	3:D:187:ILE:HG23	1.87	0.56
3:D:831:TYR:HB2	3:D:848:TRP:CB	2.35	0.56
1:E:14:DC:H2'	1:E:15:DC:C6	2.40	0.56
3:A:157:GLY:C	3:A:158:ASN:HD22	2.09	0.56
3:A:163:SER:N	3:A:318:GLN:OE1	2.35	0.56
3:A:685:ARG:HH11	3:A:688:ILE:HG13	1.69	0.56
3:B:410:PHE:HB3	3:B:683:MSE:HG2	1.87	0.56
3:C:218:VAL:HA	3:C:222:ALA:HB3	1.86	0.56
3:D:35:PRO:HD2	3:D:64:ASN:O	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:116:GLU:HB3	3:D:135:ALA:HB3	1.87	0.56
3:D:212:ILE:CD1	3:D:345:LEU:HD21	2.29	0.56
3:D:873:GLU:HG2	3:D:877:ILE:CD1	2.35	0.56
1:K:11:DC:H2''	1:K:12:DA:H5'	1.87	0.56
3:A:101:ILE:HG21	3:A:349:TYR:HB3	1.88	0.56
3:B:660:GLU:HB3	3:B:661:PRO:HD3	1.87	0.56
3:C:181:GLU:CD	3:C:181:GLU:H	2.08	0.56
3:C:523:SER:CB	3:C:525:GLU:HG2	2.35	0.56
3:C:599:ARG:HA	4:C:920:HOH:O	2.06	0.56
3:B:351:ALA:O	3:B:352:LYS:HB2	2.05	0.56
3:B:530:ILE:HG13	3:B:531:LYS:N	2.15	0.56
3:C:216:TRP:O	3:C:217:ASN:HB2	2.06	0.56
1:E:2:DG:OP2	3:A:362:ILE:HD12	2.05	0.56
3:C:503:LEU:HD21	3:C:538:LEU:HB3	1.86	0.56
3:D:530:ILE:HD13	3:D:530:ILE:N	2.19	0.56
3:D:803:PHE:CE1	3:D:845:CYS:HB3	2.41	0.56
2:L:106:DT:H2''	2:L:107:DG:C5'	2.35	0.56
3:A:712:VAL:HG22	3:A:724:LYS:O	2.06	0.56
3:B:221:PHE:O	3:B:224:PRO:HD2	2.05	0.56
3:D:546:GLN:HA	3:D:546:GLN:OE1	2.05	0.56
2:F:111:DT:H2''	2:F:112:DT:H5'	1.87	0.56
1:K:5:DG:H2'	1:K:6:DA:C8	2.40	0.56
3:A:231:LYS:O	3:A:234:PHE:O	2.23	0.56
3:A:410:PHE:HZ	3:A:659:MSE:HE3	1.69	0.56
3:C:175:GLY:CA	3:C:319:ARG:HH21	2.19	0.56
3:C:434:PHE:CE1	3:C:460:GLY:HA2	2.40	0.56
3:D:223:ILE:HB	3:D:224:PRO:HD3	1.86	0.56
3:D:416:TYR:N	4:D:958:HOH:O	2.32	0.56
3:B:494:ARG:HH11	3:B:494:ARG:HB3	1.70	0.56
3:D:752:MSE:HE3	3:D:889:LEU:HD12	1.87	0.56
3:B:245:HIS:HD2	4:B:957:HOH:O	1.88	0.56
3:C:150:ASP:OD2	3:C:321:ILE:HG13	2.06	0.56
3:C:171:GLN:NE2	3:C:303:LEU:HD22	2.21	0.56
3:D:216:TRP:CZ2	3:D:293:ILE:HD13	2.41	0.56
3:D:222:ALA:O	3:D:226:VAL:HG23	2.06	0.56
3:D:329:TYR:O	3:D:333:GLN:HG3	2.05	0.56
3:D:421:ARG:NE	3:D:476:THR:OG1	2.39	0.56
3:A:362:ILE:HD11	3:A:572:ASN:CG	2.26	0.55
3:B:197:LEU:C	3:B:197:LEU:HD23	2.26	0.55
3:D:588:THR:O	3:D:591:GLN:HB2	2.05	0.55
1:E:13:DG:H2''	1:E:14:DC:O5'	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:18:DG:N3	1:E:18:DG:H2'	2.22	0.55
3:A:116:GLU:HB2	3:A:135:ALA:HB3	1.87	0.55
3:A:739:LYS:HD2	3:A:739:LYS:N	2.21	0.55
3:D:146:PHE:HB2	3:D:186:ILE:HG22	1.88	0.55
3:D:348:GLY:HA2	3:D:353:ILE:CD1	2.37	0.55
3:A:113:PHE:CE1	3:A:218:VAL:HG21	2.41	0.55
3:C:482:ARG:HG3	3:C:559:ARG:HB2	1.86	0.55
3:D:566:LEU:O	3:D:570:LEU:HD23	2.06	0.55
3:D:801:CYS:SG	3:D:802:PRO:HD2	2.47	0.55
3:D:873:GLU:HG2	3:D:877:ILE:HD13	1.87	0.55
3:B:322:SER:O	3:B:326:ILE:HG12	2.07	0.55
3:C:25:ARG:HD2	4:C:958:HOH:O	2.06	0.55
3:D:493:GLN:HG2	3:D:546:GLN:HE22	1.72	0.55
3:A:394:ALA:N	4:A:1011:HOH:O	2.37	0.55
3:D:402:ASN:CG	3:D:403:ARG:N	2.60	0.55
3:B:253:ILE:HD11	3:B:260:ARG:NH1	2.21	0.55
3:C:143:ASP:O	3:C:145:ARG:HG2	2.07	0.55
3:D:511:ASP:O	3:D:533:LEU:HD11	2.07	0.55
1:I:4:DG:H2''	1:I:5:DG:O5'	2.07	0.55
3:A:287:SER:HB3	3:A:292:TYR:CD1	2.41	0.55
3:C:457:SER:O	3:C:459:ASN:N	2.39	0.55
3:C:818:ASN:C	3:C:818:ASN:HD22	2.10	0.55
3:D:470:VAL:HG13	3:D:471:VAL:N	2.20	0.55
3:D:887:ALA:O	3:D:888:LYS:HB3	2.05	0.55
3:A:485:HIS:CB	3:A:556:GLN:HE21	2.19	0.55
3:A:726:LYS:HE3	3:A:728:MSE:CG	2.37	0.55
3:C:422:GLN:HG3	3:C:678:GLN:O	2.07	0.55
3:D:426:SER:O	3:D:428:GLU:N	2.40	0.55
3:D:443:ILE:HD13	3:D:595:GLN:HB2	1.89	0.55
3:A:221:PHE:O	3:A:224:PRO:HD2	2.07	0.55
3:B:121:ASP:HA	3:B:819:ILE:CG2	2.34	0.55
3:B:776:TYR:HB2	3:B:866:MSE:HE1	1.89	0.55
3:D:188:TYR:CD2	3:D:190:PRO:HD3	2.42	0.55
3:C:52:ILE:HG12	4:C:926:HOH:O	2.07	0.55
3:D:617:VAL:HG23	3:D:617:VAL:O	2.07	0.55
3:C:223:ILE:HB	3:C:224:PRO:HD3	1.89	0.54
3:C:237:SER:O	3:C:240:LYS:HG2	2.07	0.54
3:A:592:MSE:HE1	3:A:674:MSE:CG	2.37	0.54
3:D:64:ASN:HD21	3:D:67:ASP:H	1.55	0.54
3:D:137:THR:HG22	3:D:138:HIS:N	2.19	0.54
3:D:455:SER:OG	3:D:676:ASN:HA	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:37:LEU:HD21	3:A:72:ILE:HD11	1.88	0.54
3:A:631:LYS:HB2	3:A:631:LYS:HZ3	1.72	0.54
3:D:151:LEU:HD22	3:D:152:LEU:H	1.71	0.54
3:D:497:GLU:C	3:D:499:ILE:H	2.11	0.54
2:J:101:DG:H2''	2:J:102:DC:H6	1.72	0.54
1:K:4:DG:H4'	3:D:391:TYR:O	2.07	0.54
3:B:405:LYS:HA	3:B:699:GLY:CA	2.34	0.54
3:B:700:GLY:HA2	3:B:753:LEU:CD2	2.36	0.54
3:D:403:ARG:HA	4:D:917:HOH:O	2.08	0.54
3:D:485:HIS:HB3	3:D:556:GLN:HB3	1.90	0.54
3:A:376:GLN:HG3	3:A:378:LYS:HG3	1.90	0.54
3:C:443:ILE:O	3:C:599:ARG:NH2	2.33	0.54
3:A:482:ARG:HE	3:A:560:LYS:HB2	1.72	0.54
3:B:291:ASP:HB2	3:B:302:LYS:HG3	1.89	0.54
3:C:656:ARG:HA	3:C:660:GLU:HG3	1.90	0.54
2:L:106:DT:H2''	2:L:107:DG:O4'	2.07	0.54
3:C:482:ARG:HG2	3:C:556:GLN:HG2	1.90	0.54
3:D:81:GLU:CD	3:D:83:LEU:HD21	2.28	0.54
3:D:348:GLY:HA2	3:D:353:ILE:HD11	1.90	0.54
3:B:256:MSE:HG2	3:B:257:TYR:CD2	2.42	0.54
3:B:818:ASN:HD22	3:B:857:LEU:CD1	2.20	0.54
3:C:167:ALA:HA	3:C:176:ASP:CB	2.38	0.54
3:C:587:THR:HG22	3:C:588:THR:N	2.21	0.54
3:D:599:ARG:HB3	3:D:599:ARG:NH1	2.23	0.54
2:F:104:DG:H2''	2:F:105:DC:O5'	2.08	0.54
1:G:12:DA:H2''	1:G:13:DG:H8	1.71	0.54
1:G:12:DA:C2'	1:G:13:DG:C8	2.90	0.54
3:B:433:THR:O	3:B:462:MSE:HE2	2.08	0.54
3:B:775:ASN:HD21	3:B:777:ILE:HB	1.73	0.54
3:D:685:ARG:NH1	3:D:688:ILE:HG13	2.23	0.54
1:K:12:DA:H2''	1:K:13:DG:O5'	2.07	0.54
3:D:64:ASN:HD22	3:D:66:ARG:H	1.56	0.54
3:D:637:GLY:HA2	4:D:956:HOH:O	2.07	0.54
1:E:6:DA:H2''	1:E:7:DA:H8	1.69	0.53
3:D:744:ALA:HB2	3:D:767:PHE:CE2	2.43	0.53
2:F:103:DG:H2''	2:F:104:DG:O5'	2.08	0.53
3:A:132:PRO:HD2	4:A:963:HOH:O	2.07	0.53
3:B:251:LYS:HB3	3:B:262:ILE:HG13	1.89	0.53
3:C:15:ILE:HD11	3:C:92:TYR:CZ	2.43	0.53
3:D:111:ALA:HB3	3:D:210:PRO:HB3	1.90	0.53
3:D:582:ASN:O	3:D:586:ILE:HG13	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:105:DC:OP1	2:L:105:DC:C4'	2.57	0.53
3:A:373:LEU:HD12	3:A:380:ILE:HG22	1.90	0.53
3:B:163:SER:N	3:B:318:GLN:HE22	2.06	0.53
3:D:125:GLU:O	3:D:129:ALA:HB2	2.08	0.53
3:D:155:PRO:C	3:D:157:GLY:H	2.12	0.53
3:D:487:GLY:C	4:D:938:HOH:O	2.46	0.53
2:F:112:DT:H2''	2:F:113:DC:O5'	2.08	0.53
2:J:109:DC:H2''	2:J:110:DA:C5'	2.37	0.53
3:A:389:GLN:HB2	4:A:998:HOH:O	2.07	0.53
3:B:645:ASN:OD1	3:B:719:ARG:NH1	2.42	0.53
3:C:526:ILE:HG23	3:C:529:LYS:HD3	1.90	0.53
3:D:459:ASN:HD21	3:D:461:MSE:HB2	1.73	0.53
3:D:524:ASP:HB3	3:D:525:GLU:OE2	2.07	0.53
3:D:642:ARG:H	3:D:646:HIS:CD2	2.26	0.53
3:A:213:LEU:CD1	3:A:223:ILE:HD11	2.37	0.53
3:A:739:LYS:H	3:A:739:LYS:HD2	1.74	0.53
3:B:303:LEU:HB2	3:B:323:TYR:HD1	1.72	0.53
3:C:14:SER:HB3	3:C:32:GLU:OE1	2.09	0.53
3:D:87:ASP:CG	3:D:90:LEU:HD13	2.28	0.53
3:D:533:LEU:HD12	3:D:537:SER:OG	2.08	0.53
3:D:730:LEU:H	3:D:730:LEU:CD2	2.21	0.53
3:D:809:LEU:HA	3:D:812:ASN:ND2	2.23	0.53
2:J:115:DA:OP1	3:C:708:TYR:OH	2.23	0.53
1:K:2:DG:H1'	1:K:3:CTG:O5	2.07	0.53
3:A:552:GLY:O	3:A:555:ALA:HB3	2.09	0.53
3:B:435:LYS:H	3:B:435:LYS:CD	2.21	0.53
3:D:490:LEU:O	3:D:490:LEU:HD23	2.08	0.53
3:A:825:VAL:HG23	3:A:828:GLU:HB2	1.90	0.53
3:D:247:LYS:O	3:D:266:PHE:HB2	2.09	0.53
3:D:679:HIS:O	3:D:680:LEU:HG	2.09	0.53
3:D:700:GLY:CA	3:D:753:LEU:HD22	2.38	0.53
1:G:16:DG:H2''	1:G:17:DC:H5''	1.90	0.53
2:H:107:DG:H8	4:H:306:HOH:O	1.92	0.53
3:A:738:PRO:HD3	3:A:781:SER:HA	1.91	0.53
3:B:154:SER:HB3	3:B:313:ARG:NH1	2.20	0.53
3:C:858:ILE:O	3:C:862:VAL:HG23	2.08	0.53
3:A:254:GLU:CD	3:A:259:SER:HB2	2.29	0.53
3:D:602:ASN:HD21	3:D:617:VAL:HG22	1.74	0.53
3:D:782:VAL:HG12	3:D:783:SER:N	2.24	0.53
3:B:133:ILE:HD12	3:B:198:LEU:HD21	1.90	0.53
3:C:461:MSE:HE3	3:C:581:ARG:HB3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:13:DG:OP1	3:A:800:LYS:HA	2.10	0.52
3:C:351:ALA:O	3:C:352:LYS:HB2	2.08	0.52
3:C:355:ILE:O	3:C:358:VAL:HG13	2.08	0.52
3:C:681:MSE:HE2	3:C:681:MSE:HA	1.92	0.52
2:J:112:DT:H2''	2:J:113:DC:OP2	2.09	0.52
2:L:114:DC:H1'	3:D:706:LYS:HD3	1.90	0.52
3:A:12:GLY:O	3:A:13:ASP:HB2	2.10	0.52
3:A:902:ASP:HA	4:A:1014:HOH:O	2.10	0.52
3:B:465:LYS:HE3	3:B:677:LYS:HA	1.92	0.52
2:F:104:DG:H2'	2:F:105:DC:C6	2.44	0.52
3:A:64:ASN:HD22	3:A:67:ASP:H	1.57	0.52
3:D:47:THR:HG22	3:D:48:LYS:H	1.74	0.52
1:E:7:DA:H2'	1:E:8:DT:H72	1.91	0.52
1:G:6:DA:H2''	1:G:7:DA:OP2	2.10	0.52
2:H:110:DA:H1'	2:H:111:DT:H5''	1.90	0.52
1:K:7:DA:H2'	1:K:8:DT:C6	2.44	0.52
3:A:709:ALA:O	3:A:710:LEU:HD23	2.09	0.52
3:A:739:LYS:H	3:A:739:LYS:CE	2.22	0.52
3:B:791:TYR:HA	4:B:1086:HOH:O	2.10	0.52
3:C:145:ARG:HB2	3:C:147:TYR:CE1	2.45	0.52
3:D:21:ASP:HB3	3:D:23:ASN:OD1	2.09	0.52
3:A:557:ILE:HB	4:A:960:HOH:O	2.10	0.52
3:B:34:LYS:NZ	3:B:61:LEU:HD11	2.24	0.52
3:B:592:MSE:HE1	3:B:674:MSE:HG3	1.91	0.52
3:C:34:LYS:HE3	3:C:63:ALA:HA	1.91	0.52
3:C:369:ILE:HG12	3:C:474:GLU:HG3	1.92	0.52
3:C:898:PHE:O	3:C:899:ASP:HB3	2.09	0.52
1:E:11:DC:H2''	1:E:12:DA:O5'	2.10	0.52
1:K:17:DC:H6	1:K:17:DC:H5'	1.74	0.52
3:A:527:LYS:O	3:A:530:ILE:HG12	2.09	0.52
3:C:221:PHE:C	3:C:224:PRO:HD2	2.29	0.52
3:C:659:MSE:O	3:C:663:ILE:HG13	2.09	0.52
3:A:51:ASP:HB2	4:A:908:HOH:O	2.09	0.52
3:A:346:ASP:HB3	4:A:965:HOH:O	2.10	0.52
3:A:896:SER:HB3	3:A:899:ASP:CG	2.29	0.52
3:B:193:ASN:HD22	3:B:194:GLU:N	2.08	0.52
3:B:727:ILE:HG21	3:B:732:THR:HG21	1.91	0.52
3:D:116:GLU:HB2	3:D:324:ASN:HD22	1.74	0.52
3:B:486:LYS:HA	3:B:556:GLN:OE1	2.09	0.52
3:B:528:GLU:C	3:B:530:ILE:H	2.14	0.52
3:A:486:LYS:CE	3:A:556:GLN:HG2	2.38	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:434:PHE:CE2	3:B:460:GLY:HA2	2.45	0.52
3:C:397:LYS:O	3:C:399:PRO:HD3	2.10	0.52
3:D:364:THR:O	3:D:368:ILE:HG13	2.09	0.52
3:D:713:TRP:CZ3	3:D:723:PRO:HD3	2.45	0.52
1:I:9:DG:H2''	1:I:10:DA:H5'	1.92	0.51
3:C:110:VAL:O	3:C:141:SER:HB3	2.10	0.51
3:C:240:LYS:HD2	3:C:246:ARG:O	2.10	0.51
3:D:50:PHE:HD2	3:D:54:GLY:O	1.93	0.51
3:D:285:GLN:HE21	3:D:286:PRO:HD2	1.75	0.51
3:D:735:SER:HA	4:D:930:HOH:O	2.09	0.51
3:A:822:PRO:HB2	3:A:849:PRO:HG3	1.91	0.51
3:B:641:PHE:HD1	3:B:646:HIS:CD2	2.28	0.51
3:D:218:VAL:HG12	3:D:223:ILE:CG1	2.31	0.51
3:D:410:PHE:O	3:D:624:SER:HA	2.10	0.51
1:E:9:DG:O3'	3:A:874:LYS:HE3	2.11	0.51
3:A:739:LYS:NZ	3:A:780:ALA:O	2.43	0.51
3:C:20:ILE:HA	3:C:25:ARG:O	2.10	0.51
3:C:451:SER:HB3	3:C:456:CYS:SG	2.50	0.51
3:C:594:LEU:O	3:C:597:ILE:HG22	2.10	0.51
3:D:485:HIS:HA	3:D:488:TYR:HD1	1.74	0.51
3:A:458:PRO:HG3	3:A:592:MSE:SE	2.60	0.51
3:A:518:TYR:HE2	3:A:541:MSE:HG3	1.76	0.51
3:D:517:ASP:C	3:D:519:ARG:H	2.12	0.51
1:I:16:DG:H2''	1:I:17:DC:C5'	2.41	0.51
3:B:555:ALA:O	3:B:559:ARG:HD3	2.10	0.51
3:B:597:ILE:HD12	3:B:598:GLU:N	2.26	0.51
3:C:750:ARG:HH22	3:C:755:GLU:CD	2.13	0.51
3:C:811:TYR:CE2	3:C:815:ILE:HD13	2.45	0.51
3:D:757:GLU:HB2	3:D:889:LEU:HD22	1.92	0.51
3:A:757:GLU:HB2	3:A:889:LEU:HD22	1.92	0.51
3:B:75:MSE:HE2	3:B:78:ILE:HG21	1.92	0.51
3:B:401:PRO:O	3:B:402:ASN:HB2	2.11	0.51
3:C:11:ILE:HD13	3:C:247:LYS:HD2	1.92	0.51
3:C:112:ASN:ND2	3:C:332:LEU:HD11	2.17	0.51
3:C:116:GLU:HB2	3:C:135:ALA:HB3	1.92	0.51
3:C:159:VAL:HG21	3:C:317:HIS:CD2	2.45	0.51
3:C:598:GLU:HG3	3:C:617:VAL:HG11	1.92	0.51
3:D:410:PHE:HB3	3:D:683:MSE:HE2	1.93	0.51
3:D:846:ILE:HD13	3:D:862:VAL:HG21	1.93	0.51
3:A:526:ILE:O	3:A:530:ILE:HG23	2.11	0.51
3:B:581:ARG:HD2	4:B:999:HOH:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:137:THR:HG21	3:C:325:ILE:HA	1.92	0.51
3:C:482:ARG:C	3:C:484:GLU:N	2.64	0.51
3:D:485:HIS:CG	4:D:918:HOH:O	2.63	0.51
3:D:489:MSE:HA	4:D:936:HOH:O	2.09	0.51
3:D:494:ARG:O	3:D:494:ARG:HG2	2.10	0.51
3:D:505:ASN:N	3:D:506:PRO:HD3	2.26	0.51
3:D:781:SER:HB2	4:D:957:HOH:O	2.10	0.51
3:B:402:ASN:HA	3:B:886:ALA:O	2.10	0.51
3:B:589:PHE:HE1	3:B:681:MSE:CE	2.24	0.51
3:B:793:VAL:O	3:B:796:PHE:HD2	1.93	0.51
3:C:738:PRO:HG2	3:C:741:VAL:HB	1.93	0.51
3:D:841:PHE:CZ	3:D:861:ASP:HB3	2.44	0.51
1:G:16:DG:H2''	1:G:17:DC:C5'	2.41	0.51
3:B:89:LYS:HB2	3:B:89:LYS:NZ	2.25	0.51
3:B:398:GLU:OE2	3:B:705:LYS:HE3	2.11	0.51
3:C:362:ILE:HD12	3:C:575:PHE:HB2	1.93	0.51
3:C:518:TYR:HA	4:C:1027:HOH:O	2.10	0.51
3:C:620:GLY:HA2	3:C:624:SER:O	2.11	0.51
3:D:354:GLN:HB3	3:D:356:GLN:NE2	2.26	0.51
3:D:599:ARG:O	3:D:603:GLU:HG3	2.11	0.51
3:A:489:MSE:C	3:A:491:ALA:H	2.14	0.51
3:A:700:GLY:HA2	3:A:753:LEU:CD2	2.41	0.51
3:B:241:ARG:NH2	4:B:1087:HOH:O	2.44	0.51
3:C:572:ASN:HD22	3:C:574:TRP:N	2.07	0.51
3:D:599:ARG:HB3	3:D:599:ARG:HH11	1.76	0.51
3:A:298:LEU:O	3:A:299:ASN:HB3	2.11	0.50
3:C:162:TRP:HB3	3:C:188:TYR:CZ	2.46	0.50
3:D:469:GLY:C	3:D:472:PRO:HD2	2.31	0.50
3:D:811:TYR:CZ	3:D:815:ILE:HD11	2.47	0.50
3:D:819:ILE:HG13	3:D:819:ILE:O	2.11	0.50
1:E:7:DA:H2''	1:E:8:DT:O5'	2.12	0.50
2:L:103:DG:H2''	2:L:104:DG:H8	1.74	0.50
3:D:322:SER:O	3:D:326:ILE:HG23	2.11	0.50
3:A:839:ASN:ND2	3:A:841:PHE:HB2	2.26	0.50
3:B:405:LYS:O	3:B:630:ASP:OD2	2.29	0.50
3:B:522:PHE:HB2	3:B:526:ILE:HD12	1.92	0.50
3:C:133:ILE:HD12	3:C:198:LEU:HD21	1.92	0.50
3:D:64:ASN:ND2	3:D:67:ASP:H	2.09	0.50
3:B:658:ARG:HG2	3:D:897:LEU:HD21	1.94	0.50
3:B:790:LYS:HA	4:B:1052:HOH:O	2.10	0.50
3:C:260:ARG:HG2	3:C:260:ARG:HH11	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:182:ILE:O	3:D:186:ILE:HG23	2.11	0.50
3:D:381:PRO:O	3:D:576:ARG:HD2	2.11	0.50
2:J:108:DT:H2''	2:J:109:DC:C5'	2.42	0.50
3:A:171:GLN:HE22	3:A:319:ARG:HH12	1.60	0.50
3:A:526:ILE:HA	3:A:529:LYS:HB3	1.92	0.50
3:B:599:ARG:HA	4:B:1083:HOH:O	2.11	0.50
3:C:284:ASN:HD21	3:C:829:LYS:HZ1	1.58	0.50
3:C:447:ALA:HA	4:C:927:HOH:O	2.11	0.50
1:K:11:DC:H2''	1:K:12:DA:C5'	2.42	0.50
3:A:221:PHE:C	3:A:224:PRO:HD2	2.32	0.50
3:A:730:LEU:HD13	3:A:883:PHE:CE1	2.46	0.50
3:D:487:GLY:O	3:D:491:ALA:N	2.37	0.50
2:F:106:DT:C1'	2:F:107:DG:H5''	2.41	0.50
1:K:1:DC:H4'	3:D:572:ASN:ND2	2.27	0.50
3:A:245:HIS:HE1	4:A:949:HOH:O	1.94	0.50
3:A:733:GLN:N	3:A:733:GLN:HE21	2.09	0.50
3:B:608:VAL:HG11	3:D:897:LEU:HD22	1.94	0.50
3:D:479:PHE:CE1	3:D:563:ILE:HD13	2.47	0.50
1:I:10:DA:OP1	3:C:874:LYS:HD2	2.11	0.50
2:J:101:DG:H2''	2:J:102:DC:C6	2.46	0.50
3:A:236:GLU:HG2	3:A:240:LYS:HE2	1.93	0.50
3:A:439:LEU:HD22	4:A:988:HOH:O	2.12	0.50
3:B:218:VAL:HG22	3:B:223:ILE:HG13	1.94	0.50
3:B:326:ILE:HG23	3:B:330:ARG:HE	1.76	0.50
3:D:488:TYR:O	3:D:552:GLY:HA3	2.11	0.50
2:J:104:DG:H2'	2:J:105:DC:C5	2.47	0.50
1:K:2:DG:OP2	3:D:361:PRO:HD2	2.11	0.50
3:A:653:LYS:HD2	3:A:653:LYS:C	2.32	0.50
3:C:818:ASN:HD22	3:C:819:ILE:N	2.09	0.50
3:D:144:ASP:OD1	3:D:185:LYS:HD3	2.11	0.50
3:D:854:ILE:HD11	3:D:858:ILE:CD1	2.37	0.50
3:B:471:VAL:O	3:B:475:ILE:HG22	2.11	0.49
3:D:213:LEU:HD23	3:D:213:LEU:C	2.32	0.49
3:D:642:ARG:HG2	3:D:646:HIS:CD2	2.46	0.49
3:D:809:LEU:HA	3:D:812:ASN:HD22	1.76	0.49
3:A:154:SER:HB2	3:A:155:PRO:HD2	1.94	0.49
3:A:338:ARG:HB3	3:A:340:PHE:CZ	2.47	0.49
3:C:179:PRO:HB3	3:C:181:GLU:OE1	2.12	0.49
3:D:274:ILE:HG23	3:D:275:ASP:N	2.27	0.49
1:E:14:DC:H5''	1:E:14:DC:H6	1.78	0.49
3:B:797:PRO:HG3	3:B:806:ARG:HH12	1.74	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:51:ASP:HB2	4:D:909:HOH:O	2.13	0.49
3:D:380:ILE:HD12	3:D:577:TYR:OH	2.11	0.49
3:B:355:ILE:N	3:B:355:ILE:HD12	2.26	0.49
3:D:518:TYR:C	3:D:520:PHE:H	2.14	0.49
3:B:116:GLU:CB	3:B:135:ALA:HB3	2.41	0.49
3:B:362:ILE:HD12	3:B:575:PHE:HB2	1.94	0.49
3:D:202:LEU:HD21	3:D:230:ILE:HD13	1.95	0.49
3:D:428:GLU:N	4:D:953:HOH:O	2.44	0.49
3:D:484:GLU:C	3:D:486:LYS:H	2.14	0.49
3:B:154:SER:CB	3:B:313:ARG:HH12	2.21	0.49
3:B:423:VAL:O	3:B:424:ASN:HB3	2.11	0.49
3:B:486:LYS:O	3:B:489:MSE:HG3	2.12	0.49
3:C:302:LYS:HE2	3:C:326:ILE:HG21	1.94	0.49
3:C:707:ARG:HD3	4:C:905:HOH:O	2.12	0.49
3:D:115:ILE:HD13	3:D:226:VAL:HG23	1.94	0.49
3:A:491:ALA:C	3:A:493:GLN:H	2.15	0.49
3:A:629:ALA:HA	3:A:632:ILE:HD12	1.94	0.49
3:B:183:ILE:CG2	3:B:184:ASP:N	2.76	0.49
3:B:218:VAL:O	3:B:223:ILE:HG13	2.13	0.49
3:B:499:ILE:HG22	4:B:1054:HOH:O	2.12	0.49
3:B:863:LEU:O	3:B:863:LEU:HD23	2.12	0.49
3:C:167:ALA:O	3:C:176:ASP:O	2.31	0.49
3:C:284:ASN:ND2	3:C:829:LYS:HZ1	2.11	0.49
3:D:639:SER:C	3:D:641:PHE:H	2.16	0.49
3:A:415:LEU:O	3:A:419:ILE:HG13	2.13	0.49
3:B:609:CYS:HA	3:B:635:LYS:HE3	1.94	0.49
3:C:272:ASP:OD1	3:C:274:ILE:HG22	2.13	0.49
3:B:645:ASN:HB2	4:B:1063:HOH:O	2.13	0.49
3:B:808:ILE:HD13	3:B:824:VAL:HG11	1.95	0.49
3:D:197:LEU:HD12	3:D:197:LEU:H	1.78	0.49
3:D:285:GLN:NE2	3:D:286:PRO:HD2	2.27	0.49
3:D:399:PRO:HB3	3:D:619:TYR:CD2	2.41	0.49
2:J:104:DG:H2'	2:J:105:DC:H6	1.73	0.49
3:B:193:ASN:ND2	3:B:194:GLU:N	2.61	0.49
3:C:61:LEU:HD23	3:C:62:PHE:N	2.28	0.49
3:D:11:ILE:O	3:D:11:ILE:HG23	2.13	0.49
3:C:52:ILE:HD12	3:C:428:GLU:CG	2.41	0.48
3:C:471:VAL:HB	3:C:472:PRO:HD3	1.95	0.48
3:C:533:LEU:HB2	3:C:537:SER:HB2	1.95	0.48
3:C:880:LEU:HD22	3:C:884:THR:HG23	1.94	0.48
3:D:316:ASN:HD22	3:D:316:ASN:H	1.60	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:824:VAL:HG22	3:D:825:VAL:N	2.28	0.48
1:E:12:DA:O3'	3:A:800:LYS:HA	2.14	0.48
3:B:123:PHE:CD1	3:B:124:PRO:HD2	2.48	0.48
3:B:789:ALA:C	3:B:791:TYR:H	2.16	0.48
3:D:830:VAL:HG22	3:D:831:TYR:N	2.28	0.48
1:G:8:DT:H2''	1:G:9:DG:C8	2.48	0.48
3:A:159:VAL:HG21	3:A:317:HIS:CD2	2.48	0.48
3:A:685:ARG:NH2	3:A:717:GLY:H	2.10	0.48
3:A:739:LYS:H	3:A:739:LYS:HE3	1.78	0.48
3:C:605:LEU:HA	3:C:608:VAL:HG22	1.94	0.48
3:C:347:MSE:HE2	3:C:558:ASN:ND2	2.29	0.48
3:C:410:PHE:HB3	3:C:683:MSE:HG2	1.95	0.48
3:C:416:TYR:HB2	3:C:417:PRO:HD3	1.95	0.48
3:D:116:GLU:CB	3:D:135:ALA:HB3	2.43	0.48
3:A:776:TYR:CD1	3:A:863:LEU:HD11	2.49	0.48
3:B:727:ILE:HG21	3:B:732:THR:CG2	2.43	0.48
3:D:530:ILE:HG12	3:D:531:LYS:N	2.29	0.48
3:A:113:PHE:CE1	3:A:218:VAL:CG2	2.97	0.48
3:A:347:MSE:N	4:A:965:HOH:O	2.46	0.48
3:B:415:LEU:HD11	3:B:419:ILE:HD11	1.95	0.48
3:B:597:ILE:HG21	3:B:667:PHE:CE2	2.49	0.48
3:B:734:LYS:O	3:B:735:SER:OG	2.30	0.48
3:B:901:PHE:HB2	3:D:608:VAL:O	2.13	0.48
3:C:34:LYS:HB3	3:C:61:LEU:HD21	1.96	0.48
3:C:149:PHE:CD1	3:C:149:PHE:N	2.81	0.48
3:C:803:PHE:HA	4:C:922:HOH:O	2.14	0.48
3:D:64:ASN:ND2	3:D:66:ARG:H	2.12	0.48
3:D:213:LEU:HD21	3:D:218:VAL:HG11	1.95	0.48
3:D:804:HIS:CD2	3:D:805:ILE:HG13	2.48	0.48
3:A:347:MSE:CB	3:A:558:ASN:HD21	2.23	0.48
3:A:405:LYS:O	3:A:690:GLY:HA2	2.13	0.48
3:B:900:MSE:SE	3:D:636:VAL:HA	2.64	0.48
3:C:486:LYS:O	3:C:490:LEU:HG	2.12	0.48
3:C:706:LYS:C	3:C:707:ARG:HG2	2.34	0.48
3:D:727:ILE:HG13	3:D:732:THR:HG21	1.96	0.48
3:D:732:THR:HG23	4:D:914:HOH:O	2.13	0.48
1:E:3:CTG:O6	1:E:3:CTG:H2'	2.12	0.48
3:A:158:ASN:HD22	3:A:158:ASN:N	2.12	0.48
3:D:316:ASN:HD22	3:D:316:ASN:N	2.11	0.48
2:L:107:DG:H2'	2:L:108:DT:C6	2.49	0.48
3:A:6:LEU:HD11	3:A:26:GLU:HG3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:211:VAL:HG21	4:A:957:HOH:O	2.14	0.48
3:B:475:ILE:HD13	3:B:475:ILE:C	2.33	0.48
3:B:560:LYS:HE3	4:B:979:HOH:O	2.13	0.48
3:B:642:ARG:H	3:B:646:HIS:CD2	2.31	0.48
3:C:3:GLU:HG2	3:C:22:SER:N	2.29	0.48
3:C:302:LYS:HD2	3:C:323:TYR:CE1	2.48	0.48
3:C:592:MSE:HE1	3:C:674:MSE:HG3	1.96	0.48
3:D:487:GLY:O	3:D:491:ALA:HB3	2.13	0.48
3:D:528:GLU:C	3:D:530:ILE:HD13	2.34	0.48
1:K:10:DA:H3'	4:K:146:HOH:O	2.14	0.48
3:A:636:VAL:O	3:A:640:LYS:HG3	2.14	0.48
3:A:706:LYS:O	3:A:707:ARG:HD3	2.14	0.48
3:B:85:MSE:HA	3:B:380:ILE:HD11	1.96	0.48
3:B:163:SER:HB3	3:B:166:ILE:HD12	1.95	0.48
3:B:471:VAL:HB	3:B:472:PRO:CD	2.44	0.48
3:C:104:ASP:OD1	3:C:107:LYS:HG2	2.14	0.48
3:D:62:PHE:HB3	3:D:67:ASP:OD2	2.12	0.48
3:D:503:LEU:O	3:D:506:PRO:HG3	2.13	0.48
1:I:13:DG:H2''	1:I:14:DC:O5'	2.13	0.47
3:C:481:GLN:HE21	3:C:559:ARG:HD2	1.78	0.47
3:D:484:GLU:C	3:D:486:LYS:N	2.67	0.47
1:E:16:DG:H2''	1:E:17:DC:O5'	2.14	0.47
3:A:502:ALA:O	3:A:506:PRO:HB3	2.14	0.47
3:B:748:CYS:O	3:B:752:MSE:HG3	2.14	0.47
3:C:878:LYS:HB3	3:C:879:PRO:CD	2.45	0.47
3:D:248:THR:HG22	3:D:265:LEU:HA	1.96	0.47
1:G:5:DG:H1'	1:G:6:DA:H5'	1.96	0.47
3:B:858:ILE:O	3:B:862:VAL:HG23	2.13	0.47
3:C:667:PHE:HB3	3:C:679:HIS:HE1	1.77	0.47
2:J:102:DC:H2''	2:J:103:DG:O5'	2.15	0.47
2:J:111:DT:C2'	2:J:112:DT:C5'	2.79	0.47
3:A:790:LYS:HD3	3:A:791:TYR:CE1	2.49	0.47
3:B:403:ARG:NH1	3:B:887:ALA:O	2.47	0.47
3:C:81:GLU:HG2	3:C:83:LEU:CD2	2.44	0.47
3:D:660:GLU:CB	3:D:661:PRO:HD3	2.43	0.47
1:E:5:DG:H2'	1:E:6:DA:H5''	1.97	0.47
3:B:167:ALA:HA	3:B:176:ASP:HB2	1.97	0.47
3:B:664:ASP:OD2	3:B:668:ARG:NH1	2.48	0.47
3:D:197:LEU:C	3:D:199:MSE:H	2.17	0.47
3:D:824:VAL:HG22	3:D:825:VAL:H	1.80	0.47
1:G:3:CTG:O6	1:G:3:CTG:H2'	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:72:ILE:HG22	3:A:76:GLU:OE1	2.15	0.47
3:A:112:ASN:C	3:A:112:ASN:HD22	2.18	0.47
3:B:494:ARG:CB	3:B:494:ARG:NH1	2.77	0.47
3:C:305:TYR:HB3	3:C:323:TYR:OH	2.14	0.47
3:D:82:ALA:N	3:D:382:GLN:OE1	2.43	0.47
3:D:154:SER:HB3	3:D:155:PRO:CD	2.39	0.47
3:D:856:ASP:HA	3:D:859:LYS:CB	2.45	0.47
2:H:112:DT:H2''	2:H:113:DC:OP2	2.15	0.47
3:A:202:LEU:O	3:A:206:GLN:HG2	2.15	0.47
3:A:774:LEU:HB3	4:A:1004:HOH:O	2.14	0.47
3:A:797:PRO:N	3:A:809:LEU:HD13	2.30	0.47
3:B:732:THR:CG2	3:B:733:GLN:N	2.77	0.47
3:B:787:ASN:C	3:B:789:ALA:N	2.68	0.47
3:D:201:TYR:O	3:D:204:PHE:HB3	2.15	0.47
1:I:2:DG:C8	3:C:361:PRO:HG2	2.50	0.47
3:A:822:PRO:HD3	4:A:933:HOH:O	2.15	0.47
3:A:887:ALA:O	3:A:888:LYS:HB2	2.15	0.47
3:D:197:LEU:HD12	3:D:197:LEU:N	2.30	0.47
3:D:399:PRO:O	3:D:401:PRO:HD3	2.15	0.47
3:A:347:MSE:HG2	3:A:358:VAL:HG23	1.96	0.47
3:C:15:ILE:HD11	3:C:92:TYR:CE2	2.49	0.47
3:C:451:SER:OG	3:C:462:MSE:HE3	2.14	0.47
3:D:109:ARG:HD2	3:D:209:THR:O	2.14	0.47
3:D:151:LEU:HD22	3:D:152:LEU:N	2.30	0.47
3:D:170:LEU:HA	3:D:177:GLU:HG2	1.97	0.47
3:D:290:LEU:HD21	3:D:330:ARG:HB2	1.96	0.47
3:D:644:THR:O	3:D:648:VAL:HG23	2.15	0.47
3:D:730:LEU:HD11	3:D:749:ILE:HD13	1.97	0.47
2:H:104:DG:C2'	2:H:105:DC:O5'	2.61	0.47
3:A:197:LEU:HD23	3:A:197:LEU:C	2.35	0.47
3:A:730:LEU:HD22	3:A:883:PHE:HE1	1.80	0.47
3:B:362:ILE:HD13	3:B:569:ALA:HB1	1.96	0.47
3:D:153:ASN:HA	3:D:158:ASN:OD1	2.15	0.47
3:D:752:MSE:HG2	3:D:889:LEU:HD13	1.97	0.47
1:E:15:DC:H2''	1:E:16:DG:C8	2.50	0.46
3:A:412:LEU:HG	3:A:683:MSE:HG2	1.96	0.46
3:A:607:GLU:O	3:A:607:GLU:HG2	2.14	0.46
3:B:818:ASN:ND2	3:B:857:LEU:CD1	2.78	0.46
3:D:202:LEU:HD21	3:D:230:ILE:CD1	2.45	0.46
3:D:808:ILE:HA	3:D:847:ALA:HB3	1.96	0.46
3:B:249:ARG:HG2	3:B:249:ARG:HH11	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:415:LEU:HD22	3:B:623:ASP:HB3	1.97	0.46
3:B:489:MSE:HE2	3:B:490:LEU:HG	1.97	0.46
3:B:787:ASN:O	3:B:789:ALA:N	2.48	0.46
3:D:386:HIS:HB3	3:D:387:PRO:HD2	1.96	0.46
3:A:875:THR:HA	4:A:955:HOH:O	2.15	0.46
3:B:641:PHE:HA	3:B:646:HIS:HD2	1.80	0.46
3:D:151:LEU:HD13	3:D:151:LEU:C	2.35	0.46
3:D:416:TYR:HB2	3:D:417:PRO:HD3	1.96	0.46
3:D:511:ASP:C	3:D:533:LEU:HD11	2.35	0.46
3:A:482:ARG:HH11	3:A:483:LYS:NZ	2.13	0.46
3:C:138:HIS:C	3:C:138:HIS:CD2	2.88	0.46
3:C:412:LEU:HD13	3:C:415:LEU:CD1	2.43	0.46
3:C:482:ARG:HD2	3:C:556:GLN:HE21	1.79	0.46
3:C:514:LEU:HD23	3:C:541:MSE:HE1	1.98	0.46
3:D:33:TYR:HB3	3:D:65:MSE:CE	2.45	0.46
3:D:517:ASP:C	3:D:519:ARG:N	2.69	0.46
3:D:730:LEU:O	3:D:731:GLU:HB2	2.15	0.46
1:K:16:DG:H2''	1:K:17:DC:C5'	2.43	0.46
3:B:312:LEU:HD12	3:B:320:TYR:CB	2.45	0.46
3:B:319:ARG:HA	3:B:319:ARG:HD3	1.73	0.46
3:B:347:MSE:HB2	3:B:558:ASN:HD21	1.80	0.46
3:B:793:VAL:C	3:B:795:GLY:H	2.18	0.46
3:C:579:ASP:HB3	3:C:582:ASN:HB2	1.96	0.46
1:E:13:DG:P	3:A:800:LYS:HA	2.56	0.46
1:E:14:DC:H2'	1:E:15:DC:C5	2.50	0.46
3:A:326:ILE:O	3:A:330:ARG:HG2	2.15	0.46
3:A:523:SER:HB3	3:A:526:ILE:HG12	1.96	0.46
3:B:285:GLN:HG3	3:B:292:TYR:HE2	1.80	0.46
3:B:386:HIS:HD2	4:B:1064:HOH:O	1.98	0.46
3:C:162:TRP:HB3	3:C:188:TYR:CE1	2.50	0.46
3:D:10:GLN:H	3:D:89:LYS:HE2	1.80	0.46
3:D:730:LEU:HG	3:D:732:THR:H	1.80	0.46
2:H:105:DC:H2''	2:H:106:DT:H5'	1.98	0.46
3:A:797:PRO:HD3	3:A:809:LEU:HD13	1.98	0.46
3:C:881:GLU:HG3	3:C:891:TYR:CE1	2.44	0.46
3:D:391:TYR:CZ	3:D:583:ALA:HB1	2.51	0.46
3:D:490:LEU:HD23	3:D:490:LEU:C	2.36	0.46
3:D:660:GLU:HB3	3:D:661:PRO:HD3	1.96	0.46
1:E:14:DC:H2''	1:E:15:DC:C5'	2.46	0.46
1:K:7:DA:H2'	1:K:8:DT:H6	1.81	0.46
1:K:16:DG:C2'	1:K:17:DC:H5''	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:101:DG:N3	2:L:102:DC:C5	2.84	0.46
3:A:824:VAL:HG22	3:A:849:PRO:HD3	1.98	0.46
3:B:75:MSE:HE2	3:B:78:ILE:CG2	2.46	0.46
3:B:492:ALA:HB1	3:B:545:ALA:O	2.14	0.46
3:B:702:TRP:CD1	3:B:708:TYR:HB3	2.51	0.46
3:B:811:TYR:O	3:B:815:ILE:HG12	2.16	0.46
3:C:127:SER:HA	3:C:228:ASN:ND2	2.31	0.46
3:C:154:SER:C	3:C:156:TYR:H	2.18	0.46
2:J:101:DG:H2''	2:J:102:DC:O5'	2.16	0.46
3:A:514:LEU:HB3	3:A:541:MSE:SE	2.65	0.46
3:B:252:VAL:HG23	3:B:252:VAL:O	2.15	0.46
3:B:747:GLU:OE2	3:B:750:ARG:NH2	2.49	0.46
3:C:526:ILE:HG22	3:C:526:ILE:O	2.15	0.46
3:D:183:ILE:O	3:D:186:ILE:HG12	2.15	0.46
3:D:216:TRP:CZ3	3:D:274:ILE:HD12	2.51	0.46
3:D:394:ALA:HB1	4:D:945:HOH:O	2.15	0.46
1:G:16:DG:H2''	1:G:17:DC:O5'	2.16	0.46
3:A:205:TRP:CE2	3:A:242:LEU:HD12	2.51	0.46
3:A:455:SER:OG	3:A:676:ASN:HA	2.15	0.46
3:A:758:GLU:O	3:A:762:GLU:HG3	2.16	0.46
3:B:9:GLU:HA	3:B:89:LYS:HD2	1.98	0.46
3:B:415:LEU:O	3:B:419:ILE:HG13	2.16	0.46
3:C:347:MSE:CE	3:C:562:LEU:HD13	2.46	0.46
3:C:491:ALA:HB1	3:C:521:ASP:N	2.31	0.46
3:D:136:ILE:HD11	3:D:201:TYR:CE2	2.51	0.46
3:D:293:ILE:HG13	3:D:294:SER:N	2.31	0.46
3:D:546:GLN:O	3:D:550:VAL:HG23	2.16	0.46
1:E:12:DA:H61	2:F:106:DT:H3	1.64	0.45
3:A:691:PRO:HD3	3:A:699:GLY:HA2	1.98	0.45
3:B:347:MSE:SE	3:B:562:LEU:HG	2.66	0.45
3:D:226:VAL:O	3:D:230:ILE:HG13	2.16	0.45
3:D:428:GLU:OE2	3:D:470:VAL:HG12	2.15	0.45
3:D:775:ASN:OD1	3:D:777:ILE:HG12	2.16	0.45
3:A:308:PRO:CG	3:A:311:LYS:HD2	2.47	0.45
3:C:167:ALA:HA	3:C:176:ASP:HB3	1.98	0.45
3:C:239:ALA:C	3:C:241:ARG:H	2.20	0.45
3:C:738:PRO:HG2	3:C:741:VAL:CG2	2.46	0.45
3:C:854:ILE:CG2	3:C:859:LYS:HD3	2.47	0.45
3:D:37:LEU:HD11	3:D:72:ILE:HD11	1.97	0.45
3:D:113:PHE:HE1	3:D:213:LEU:HD21	1.81	0.45
3:D:429:THR:O	3:D:463:TYR:HA	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:443:ILE:HD13	3:D:595:GLN:CB	2.46	0.45
3:A:495:ASN:ND2	3:A:521:ASP:HA	2.21	0.45
3:B:14:SER:HG	3:B:16:PHE:HE1	1.62	0.45
3:B:369:ILE:HG12	3:B:474:GLU:HG3	1.98	0.45
3:B:897:LEU:O	3:B:900:MSE:HG3	2.16	0.45
3:D:410:PHE:CB	3:D:683:MSE:HE2	2.46	0.45
1:I:5:DG:C2'	1:I:6:DA:H5''	2.46	0.45
3:A:642:ARG:HG3	3:A:646:HIS:CD2	2.52	0.45
3:B:835:LEU:HD23	3:B:866:MSE:HA	1.98	0.45
3:B:873:GLU:HA	3:B:877:ILE:HG13	1.98	0.45
3:D:155:PRO:O	3:D:156:TYR:HB2	2.16	0.45
3:D:433:THR:N	3:D:462:MSE:HE2	2.31	0.45
3:A:422:GLN:NE2	3:A:680:LEU:H	2.14	0.45
3:A:481:GLN:HA	3:A:484:GLU:HG2	1.99	0.45
3:B:273:TYR:OH	3:B:335:ASP:HA	2.16	0.45
3:B:516:VAL:H	3:B:544:ARG:CZ	2.29	0.45
3:B:548:THR:C	3:B:550:VAL:H	2.19	0.45
3:B:818:ASN:ND2	3:B:857:LEU:HD12	2.32	0.45
1:E:13:DG:O4'	3:A:800:LYS:HD3	2.16	0.45
3:A:843:ASP:HA	4:A:1009:HOH:O	2.16	0.45
3:A:769:LYS:HD2	4:A:994:HOH:O	2.16	0.45
3:A:810:THR:HG22	4:A:999:HOH:O	2.16	0.45
3:B:221:PHE:C	3:B:224:PRO:HD2	2.37	0.45
3:D:127:SER:C	3:D:129:ALA:H	2.20	0.45
3:D:412:LEU:HD23	3:D:683:MSE:HG2	1.99	0.45
3:A:732:THR:C	3:A:733:GLN:HE21	2.18	0.45
3:B:413:THR:O	3:B:414:SER:C	2.55	0.45
3:C:109:ARG:NH1	3:C:140:ASP:OD2	2.40	0.45
3:C:660:GLU:HB2	3:C:661:PRO:CD	2.39	0.45
1:E:4:DG:OP1	3:A:390:PRO:HA	2.16	0.45
3:A:594:LEU:HD21	3:A:621:ASP:H	1.82	0.45
3:A:810:THR:HG23	3:A:841:PHE:O	2.17	0.45
3:B:193:ASN:ND2	3:B:195:LYS:H	2.14	0.45
3:B:435:LYS:O	3:B:435:LYS:CG	2.64	0.45
3:D:533:LEU:HD12	3:D:537:SER:CB	2.47	0.45
3:D:692:PRO:HG3	3:D:713:TRP:HZ2	1.82	0.45
3:D:858:ILE:O	3:D:862:VAL:HG23	2.16	0.45
2:J:104:DG:H2''	2:J:105:DC:O5'	2.17	0.45
1:K:18:DG:O4'	3:A:36:SER:HB2	2.17	0.45
3:A:402:ASN:HA	3:A:886:ALA:O	2.17	0.45
3:A:471:VAL:HG11	3:A:570:LEU:HD11	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:901:PHE:HD2	3:D:635:LYS:HG2	1.82	0.45
3:D:709:ALA:HB1	3:D:727:ILE:HG22	1.99	0.45
3:D:786:ASN:OD1	3:D:805:ILE:HD11	2.17	0.45
1:G:5:DG:H2''	1:G:6:DA:O5'	2.17	0.44
1:I:7:DA:H2'	1:I:8:DT:H71	1.98	0.44
3:A:71:TRP:CZ2	3:A:75:MSE:HE2	2.53	0.44
3:B:113:PHE:CE1	3:B:218:VAL:CG2	3.00	0.44
3:B:735:SER:HB2	3:B:737:THR:HG23	1.97	0.44
3:C:425:ILE:HG23	3:C:463:TYR:CE2	2.52	0.44
3:D:289:SER:HB2	3:D:292:TYR:CB	2.47	0.44
3:D:470:VAL:HG13	3:D:471:VAL:H	1.81	0.44
1:I:11:DC:H2''	1:I:12:DA:O5'	2.18	0.44
2:J:109:DC:O4'	3:C:800:LYS:NZ	2.50	0.44
3:A:747:GLU:HA	4:A:916:HOH:O	2.16	0.44
3:B:435:LYS:HG3	4:B:1082:HOH:O	2.16	0.44
3:B:751:ARG:NE	3:B:763:TYR:HB2	2.33	0.44
3:B:872:LEU:HD12	3:B:876:PHE:HB3	1.99	0.44
3:D:240:LYS:HE2	3:D:248:THR:OG1	2.16	0.44
3:D:250:VAL:HG22	3:D:263:ILE:HG23	2.00	0.44
2:F:111:DT:H2''	2:F:112:DT:H5''	1.99	0.44
2:F:112:DT:H1'	2:F:113:DC:H5'	1.99	0.44
3:A:15:ILE:HG12	3:A:65:MSE:HE1	2.00	0.44
3:B:421:ARG:HB3	3:B:680:LEU:CD1	2.47	0.44
3:B:608:VAL:HG13	3:D:897:LEU:HB2	1.99	0.44
3:C:214:THR:OG1	3:C:215:GLY:N	2.50	0.44
3:D:33:TYR:HB3	3:D:65:MSE:HE1	1.99	0.44
3:D:741:VAL:O	3:D:745:LEU:HD13	2.18	0.44
2:H:111:DT:H2''	2:H:112:DT:C5'	2.47	0.44
3:B:408:MSE:CE	3:B:655:ALA:HB2	2.45	0.44
3:B:792:ASP:CG	3:B:793:VAL:H	2.20	0.44
3:C:469:GLY:C	3:C:472:PRO:HD2	2.38	0.44
3:C:558:ASN:HD22	3:C:558:ASN:HA	1.62	0.44
3:C:738:PRO:HB3	3:C:780:ALA:O	2.18	0.44
3:D:150:ASP:HB3	3:D:188:TYR:CE1	2.53	0.44
3:D:434:PHE:CE1	3:D:460:GLY:HA2	2.53	0.44
3:A:176:ASP:OD2	3:A:318:GLN:NE2	2.51	0.44
3:A:406:TYR:CD2	3:A:633:ILE:HG13	2.53	0.44
3:A:507:ASN:O	3:A:508:LEU:HD22	2.17	0.44
3:A:553:MSE:HA	3:A:556:GLN:OE1	2.18	0.44
3:A:641:PHE:HA	3:A:646:HIS:CD2	2.52	0.44
3:A:715:MSE:O	3:A:716:GLU:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:257:TYR:CD2	3:B:257:TYR:N	2.85	0.44
3:D:290:LEU:HD23	3:D:290:LEU:O	2.16	0.44
3:D:873:GLU:HB3	3:D:877:ILE:HD11	2.00	0.44
3:A:787:ASN:N	3:A:826:GLU:OE1	2.47	0.44
3:A:854:ILE:HG23	3:A:859:LYS:HB2	2.00	0.44
3:B:193:ASN:ND2	3:B:193:ASN:C	2.71	0.44
3:D:434:PHE:CE2	3:D:450:PRO:HB3	2.53	0.44
3:A:539:ASN:HD22	3:A:539:ASN:HA	1.61	0.44
3:A:800:LYS:HB2	3:A:800:LYS:HZ2	1.82	0.44
3:B:270:VAL:O	3:B:271:LEU:HD12	2.18	0.44
3:B:818:ASN:HD22	3:B:857:LEU:HD13	1.82	0.44
3:B:825:VAL:HB	3:B:828:GLU:CD	2.38	0.44
3:C:198:LEU:O	3:C:202:LEU:HB2	2.18	0.44
3:C:71:TRP:O	3:C:75:MSE:HG2	2.17	0.44
3:C:83:LEU:HB3	3:C:379:VAL:CG1	2.48	0.44
3:C:154:SER:O	3:C:156:TYR:N	2.51	0.44
3:C:284:ASN:ND2	3:C:829:LYS:NZ	2.66	0.44
3:C:491:ALA:O	3:C:495:ASN:HB2	2.18	0.44
3:D:151:LEU:HD23	3:D:191:PHE:O	2.18	0.44
1:I:15:DC:H2''	1:I:16:DG:C8	2.53	0.44
2:L:112:DT:H2''	2:L:113:DC:C4'	2.47	0.44
3:A:777:ILE:HD13	3:A:848:TRP:HZ2	1.83	0.44
3:C:482:ARG:O	3:C:484:GLU:N	2.50	0.44
3:D:8:VAL:HG11	3:D:93:LEU:CD1	2.46	0.44
3:D:314:GLU:HG3	3:D:314:GLU:O	2.18	0.44
3:D:481:GLN:HB3	3:D:559:ARG:HE	1.83	0.44
3:D:749:ILE:O	3:D:753:LEU:HG	2.18	0.44
3:D:848:TRP:CB	4:D:932:HOH:O	2.65	0.44
2:F:113:DC:H2''	2:F:114:DC:OP2	2.18	0.43
1:G:15:DC:H5'	1:G:15:DC:H6	1.81	0.43
2:J:105:DC:H2''	2:J:106:DT:O5'	2.17	0.43
3:B:686:GLU:HG3	3:B:715:MSE:SE	2.68	0.43
3:D:499:ILE:O	3:D:502:ALA:HB3	2.18	0.43
3:D:602:ASN:HD21	3:D:617:VAL:CG2	2.31	0.43
3:D:685:ARG:HD2	3:D:686:GLU:N	2.33	0.43
3:D:849:PRO:HG2	3:D:852:THR:OG1	2.18	0.43
3:D:853:GLU:O	3:D:854:ILE:HB	2.18	0.43
3:A:218:VAL:HG23	3:A:222:ALA:CB	2.46	0.43
3:A:734:LYS:HG2	3:A:736:SER:OG	2.17	0.43
3:A:814:ALA:HB1	3:A:858:ILE:HG21	2.00	0.43
3:B:494:ARG:NH1	3:B:494:ARG:HB2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:606:ASN:HA	3:B:611:THR:OG1	2.19	0.43
3:B:703:THR:HG1	3:B:707:ARG:HD3	1.82	0.43
3:C:455:SER:HG	3:C:676:ASN:HA	1.83	0.43
3:A:516:VAL:HG22	3:A:517:ASP:N	2.33	0.43
3:A:737:THR:O	3:A:742:GLN:NE2	2.51	0.43
3:B:901:PHE:CD2	3:D:635:LYS:HG2	2.53	0.43
3:C:283:THR:HG23	3:C:283:THR:O	2.17	0.43
3:C:818:ASN:C	3:C:818:ASN:ND2	2.71	0.43
3:C:864:HIS:HD2	3:C:865:TRP:NE1	2.16	0.43
3:D:147:TYR:HA	3:D:187:ILE:CG2	2.48	0.43
3:D:438:PRO:HG2	3:D:441:ASP:CG	2.37	0.43
3:D:487:GLY:HA2	3:D:490:LEU:HB3	2.00	0.43
3:B:791:TYR:CD1	3:B:809:LEU:HD22	2.53	0.43
3:C:227:TYR:HD1	3:C:242:LEU:HD12	1.82	0.43
3:D:503:LEU:HA	3:D:538:LEU:HD13	2.01	0.43
3:D:700:GLY:HA2	3:D:753:LEU:CD2	2.44	0.43
3:A:83:LEU:HD12	3:A:83:LEU:N	2.31	0.43
3:A:401:PRO:O	3:A:402:ASN:HB2	2.17	0.43
3:B:604:TYR:O	3:B:608:VAL:HG23	2.17	0.43
3:B:643:ASP:OD2	3:B:646:HIS:HB2	2.18	0.43
3:B:660:GLU:CB	3:B:661:PRO:HD3	2.47	0.43
3:B:878:LYS:HB3	3:B:879:PRO:CD	2.48	0.43
3:D:485:HIS:N	4:D:918:HOH:O	2.51	0.43
3:D:514:LEU:C	3:D:516:VAL:H	2.21	0.43
3:D:730:LEU:HB2	3:D:883:PHE:CE2	2.54	0.43
3:D:744:ALA:HB1	3:D:876:PHE:CE1	2.54	0.43
2:H:105:DC:H2'	2:H:106:DT:C6	2.53	0.43
3:A:36:SER:O	3:A:37:LEU:HD12	2.19	0.43
3:B:643:ASP:HB2	4:B:1024:HOH:O	2.18	0.43
3:B:834:PRO:O	3:B:866:MSE:HA	2.19	0.43
3:D:181:GLU:O	3:D:185:LYS:HD2	2.18	0.43
3:D:437:ALA:HB3	3:D:442:TYR:CE2	2.54	0.43
2:H:105:DC:H2''	2:H:106:DT:C5'	2.49	0.43
1:I:2:DG:P	3:C:361:PRO:HD2	2.59	0.43
3:A:606:ASN:OD1	3:A:616:PHE:CE1	2.69	0.43
3:B:668:ARG:HG3	3:B:668:ARG:NH1	2.30	0.43
3:C:25:ARG:HH21	3:C:27:ARG:HG2	1.84	0.43
3:D:228:ASN:HA	3:D:231:LYS:HD3	2.00	0.43
3:D:408:MSE:HE1	3:D:659:MSE:SE	2.69	0.43
3:D:738:PRO:HG2	3:D:741:VAL:HG23	2.00	0.43
3:D:846:ILE:HG21	3:D:862:VAL:CG1	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:6:DA:H5''	3:D:705:LYS:HD3	1.99	0.43
3:A:386:HIS:HA	3:A:387:PRO:HD3	1.88	0.43
3:A:830:VAL:HG12	3:A:849:PRO:HA	2.01	0.43
3:B:145:ARG:HA	3:B:145:ARG:HD3	1.75	0.43
3:B:656:ARG:HD3	4:B:970:HOH:O	2.18	0.43
3:C:112:ASN:ND2	3:C:332:LEU:CD1	2.80	0.43
3:D:140:ASP:OD2	3:D:142:ILE:HD11	2.18	0.43
3:D:641:PHE:HB3	3:D:646:HIS:HB3	2.00	0.43
3:D:835:LEU:HA	3:D:865:TRP:O	2.19	0.43
3:A:41:CYS:O	3:A:56:PRO:HG2	2.19	0.43
3:A:199:MSE:HG2	3:A:234:PHE:CZ	2.53	0.43
3:A:353:ILE:HG21	3:A:367:ALA:HB2	2.01	0.43
3:B:541:MSE:CE	3:B:544:ARG:NH2	2.82	0.43
3:B:782:VAL:HG12	3:B:783:SER:N	2.33	0.43
3:C:818:ASN:ND2	3:C:820:ASP:H	2.16	0.43
3:C:878:LYS:HB3	3:C:879:PRO:HD3	2.00	0.43
3:D:421:ARG:HD2	3:D:475:ILE:HG23	2.01	0.43
2:J:101:DG:H8	2:J:101:DG:O5'	2.02	0.43
3:A:489:MSE:C	3:A:491:ALA:N	2.71	0.43
3:B:643:ASP:HA	3:B:693:LEU:HD23	2.00	0.43
3:B:698:ILE:HG12	3:B:752:MSE:O	2.19	0.43
3:C:240:LYS:O	3:C:246:ARG:HA	2.18	0.43
3:D:214:THR:CG2	3:D:215:GLY:N	2.78	0.43
3:D:312:LEU:HG	3:D:320:TYR:CD2	2.54	0.43
3:D:511:ASP:OD1	3:D:536:LYS:HG2	2.18	0.43
3:D:642:ARG:H	3:D:646:HIS:HD2	1.67	0.43
3:D:710:LEU:HA	3:D:753:LEU:HD13	2.01	0.43
1:E:15:DC:H2''	1:E:16:DG:O5'	2.18	0.42
2:H:107:DG:H1'	2:H:108:DT:H5'	2.01	0.42
1:K:4:DG:H2'	1:K:5:DG:H8	1.84	0.42
2:L:113:DC:H2''	2:L:114:DC:O5'	2.19	0.42
3:A:17:GLU:O	3:A:28:THR:HA	2.19	0.42
3:A:422:GLN:HG3	3:A:678:GLN:O	2.19	0.42
3:A:785:ALA:HB2	3:A:808:ILE:HD11	1.99	0.42
3:B:19:TYR:HE1	3:B:29:ARG:HG2	1.84	0.42
3:B:423:VAL:O	3:B:424:ASN:CB	2.67	0.42
3:C:123:PHE:CD1	3:C:124:PRO:HD2	2.54	0.42
3:D:499:ILE:HD11	3:D:522:PHE:CE1	2.54	0.42
3:D:747:GLU:OE2	3:D:747:GLU:HA	2.19	0.42
2:J:107:DG:H2''	2:J:108:DT:O5'	2.19	0.42
2:J:113:DC:H2'	2:J:114:DC:C6	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:388:VAL:O	3:A:388:VAL:HG23	2.19	0.42
3:A:411:ASP:O	3:A:683:MSE:HA	2.19	0.42
3:A:532:LYS:O	3:A:533:LEU:HD22	2.18	0.42
3:A:728:MSE:HE2	3:A:728:MSE:HA	2.01	0.42
3:C:3:GLU:HG2	3:C:21:ASP:C	2.38	0.42
3:D:564:ASN:N	3:D:564:ASN:HD22	2.15	0.42
3:D:715:MSE:O	3:D:716:GLU:HB2	2.18	0.42
1:E:2:DG:H2''	1:E:3:CTG:OP2	2.19	0.42
1:E:9:DG:N2	4:E:449:HOH:O	2.52	0.42
2:H:111:DT:H2''	2:H:112:DT:O5'	2.19	0.42
3:A:3:GLU:CG	3:A:21:ASP:HA	2.49	0.42
3:A:514:LEU:HD23	3:A:533:LEU:HD21	2.00	0.42
3:A:802:PRO:HG2	3:A:805:ILE:HD12	2.01	0.42
3:A:836:ARG:HG3	3:A:836:ARG:HH11	1.84	0.42
3:C:200:GLU:OE2	3:C:200:GLU:HA	2.19	0.42
3:C:350:TYR:OH	3:C:481:GLN:NE2	2.43	0.42
3:D:423:VAL:HG12	3:D:423:VAL:O	2.19	0.42
3:D:500:LYS:HA	4:D:942:HOH:O	2.19	0.42
3:D:743:LYS:HA	4:D:951:HOH:O	2.19	0.42
1:E:6:DA:OP1	3:A:705:LYS:NZ	2.52	0.42
1:K:14:DC:C4	1:K:15:DC:N4	2.88	0.42
3:A:10:GLN:HG3	3:A:65:MSE:SE	2.68	0.42
3:A:597:ILE:HD12	3:A:597:ILE:HA	1.82	0.42
3:C:176:ASP:OD1	3:C:318:GLN:HG3	2.20	0.42
3:C:799:PRO:HD2	4:C:952:HOH:O	2.19	0.42
3:D:707:ARG:HA	3:D:729:GLY:HA3	2.02	0.42
3:D:785:ALA:HB3	3:D:827:GLY:H	1.84	0.42
1:K:5:DG:P	3:D:393:GLY:H	2.43	0.42
3:A:573:VAL:HG12	3:A:578:TYR:CZ	2.54	0.42
3:B:75:MSE:CE	3:B:80:LEU:HD12	2.50	0.42
3:B:857:LEU:O	3:B:857:LEU:HD23	2.18	0.42
3:C:402:ASN:HA	3:C:886:ALA:O	2.20	0.42
3:D:323:TYR:HA	3:D:326:ILE:HG12	2.02	0.42
3:D:472:PRO:O	3:D:475:ILE:HG22	2.20	0.42
3:D:810:THR:HG23	3:D:841:PHE:O	2.19	0.42
3:A:413:THR:O	3:A:414:SER:C	2.57	0.42
3:A:476:THR:HG22	3:A:480:ASN:ND2	2.34	0.42
3:A:519:ARG:HA	3:A:548:THR:HG21	2.01	0.42
3:B:238:THR:O	3:B:241:ARG:HB2	2.20	0.42
3:B:362:ILE:CD1	3:B:575:PHE:HB2	2.49	0.42
3:B:515:ASP:HA	3:B:544:ARG:HH12	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:725:LEU:HD11	3:B:750:ARG:HG2	2.02	0.42
3:C:85:MSE:HA	3:C:380:ILE:HD11	2.00	0.42
3:C:354:GLN:HB3	3:C:356:GLN:OE1	2.18	0.42
3:C:642:ARG:HG3	3:C:646:HIS:CD2	2.55	0.42
3:D:6:LEU:HB2	3:D:18:ARG:O	2.19	0.42
3:D:6:LEU:HD21	3:D:108:ILE:HG12	2.00	0.42
3:D:298:LEU:HD13	3:D:333:GLN:OE1	2.20	0.42
3:D:685:ARG:HD2	3:D:685:ARG:C	2.40	0.42
3:D:824:VAL:HG13	3:D:826:GLU:H	1.84	0.42
1:E:13:DG:P	3:A:800:LYS:HG2	2.60	0.42
2:H:101:DG:H2''	2:H:102:DC:O5'	2.18	0.42
1:I:9:DG:H1'	1:I:10:DA:H5''	2.01	0.42
3:B:113:PHE:CE1	3:B:218:VAL:HG21	2.54	0.42
3:B:421:ARG:HG2	3:B:421:ARG:HH11	1.85	0.42
3:B:479:PHE:CE2	3:B:563:ILE:HD13	2.54	0.42
3:C:83:LEU:HD22	3:C:83:LEU:N	2.34	0.42
3:C:392:PRO:C	3:C:587:THR:HG21	2.39	0.42
3:C:472:PRO:O	3:C:475:ILE:HG22	2.20	0.42
3:C:656:ARG:HA	3:C:660:GLU:CG	2.48	0.42
3:D:205:TRP:HH2	3:D:213:LEU:HD12	1.84	0.42
3:D:373:LEU:HD12	3:D:380:ILE:CD1	2.49	0.42
3:D:456:CYS:SG	3:D:462:MSE:HG2	2.60	0.42
3:D:770:GLU:O	3:D:774:LEU:HD23	2.19	0.42
3:D:811:TYR:O	3:D:814:ALA:HB3	2.20	0.42
1:I:11:DC:H5'	1:I:11:DC:H6	1.85	0.42
3:B:283:THR:HG23	3:B:283:THR:O	2.20	0.42
3:B:655:ALA:HA	3:B:659:MSE:HB2	2.01	0.42
3:C:423:VAL:HB	3:C:425:ILE:HG13	2.02	0.42
3:C:529:LYS:HE3	4:C:1047:HOH:O	2.20	0.42
1:G:15:DC:H2''	1:G:16:DG:O5'	2.20	0.42
3:A:254:GLU:OE1	3:A:259:SER:HB2	2.20	0.42
3:A:357:SER:C	3:A:359:PHE:N	2.72	0.42
3:A:494:ARG:NH2	3:A:521:ASP:OD1	2.53	0.42
3:A:789:ALA:HA	3:A:792:ASP:HB3	2.01	0.42
3:B:787:ASN:C	3:B:789:ALA:H	2.21	0.42
3:C:482:ARG:CD	3:C:556:GLN:HE21	2.33	0.42
3:C:605:LEU:HD21	3:C:659:MSE:HE3	2.02	0.42
3:C:898:PHE:N	3:C:898:PHE:CD2	2.83	0.42
3:D:262:ILE:N	3:D:262:ILE:CD1	2.82	0.42
3:D:818:ASN:C	3:D:820:ASP:H	2.22	0.42
3:D:859:LYS:O	3:D:863:LEU:HD13	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:775:ASN:HB3	3:A:778:SER:OG	2.20	0.42
3:B:466:ASP:OD1	3:B:466:ASP:N	2.53	0.42
3:B:790:LYS:HE2	3:B:801:CYS:HA	2.02	0.42
3:C:38:PHE:CD1	3:C:38:PHE:N	2.87	0.42
3:D:72:ILE:HG22	3:D:76:GLU:OE2	2.20	0.42
3:D:148:VAL:HG21	3:D:325:ILE:CD1	2.50	0.42
3:D:431:ALA:HA	3:D:464:TYR:CE1	2.55	0.42
2:F:109:DC:H2''	2:F:110:DA:O5'	2.20	0.41
2:H:113:DC:O5'	3:B:734:LYS:O	2.37	0.41
3:A:338:ARG:HD2	3:A:340:PHE:CZ	2.54	0.41
3:B:119:SER:HA	3:B:120:PRO:HD2	1.91	0.41
3:B:326:ILE:HG22	3:B:330:ARG:HG2	2.02	0.41
3:C:448:GLU:O	3:C:449:ARG:C	2.57	0.41
3:C:503:LEU:HD21	3:C:538:LEU:CB	2.50	0.41
3:D:96:THR:HB	3:D:97:TYR:CD1	2.54	0.41
3:D:214:THR:CG2	3:D:215:GLY:H	2.11	0.41
3:D:352:LYS:O	3:D:353:ILE:HG23	2.19	0.41
3:D:368:ILE:CD1	3:D:562:LEU:HD21	2.50	0.41
3:D:489:MSE:CE	3:D:490:LEU:HB2	2.39	0.41
3:D:492:ALA:HA	3:D:495:ASN:HB2	2.02	0.41
3:D:779:ILE:CD1	3:D:866:MSE:HE1	2.45	0.41
1:G:6:DA:H1'	1:G:7:DA:C8	2.55	0.41
3:C:510:VAL:O	3:C:533:LEU:HB3	2.19	0.41
3:D:433:THR:OG1	3:D:434:PHE:N	2.53	0.41
3:A:120:PRO:HG2	3:A:156:TYR:CE1	2.55	0.41
3:B:195:LYS:O	3:B:199:MSE:HB2	2.20	0.41
3:B:355:ILE:N	3:B:355:ILE:CD1	2.83	0.41
3:C:239:ALA:O	3:C:241:ARG:N	2.53	0.41
3:A:51:ASP:HA	3:A:379:VAL:HG22	2.01	0.41
3:A:101:ILE:CG2	3:A:349:TYR:HB3	2.50	0.41
3:A:382:GLN:HE21	3:A:382:GLN:HB3	1.62	0.41
3:A:797:PRO:CD	3:A:809:LEU:HD13	2.50	0.41
3:A:811:TYR:HH	3:A:822:PRO:HG2	1.83	0.41
3:B:380:ILE:HD12	3:B:576:ARG:CZ	2.50	0.41
3:B:404:TYR:CD1	3:B:618:LEU:HD22	2.55	0.41
3:B:489:MSE:SE	3:B:553:MSE:SE	3.38	0.41
3:C:458:PRO:CG	3:C:592:MSE:SE	3.18	0.41
3:D:5:TYR:HB3	3:D:97:TYR:CE1	2.55	0.41
3:D:146:PHE:CE2	3:D:182:ILE:HG13	2.55	0.41
3:A:423:VAL:O	3:A:423:VAL:HG12	2.19	0.41
3:A:478:VAL:HG13	3:A:559:ARG:HD2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:702:TRP:NE1	3:A:708:TYR:CD1	2.88	0.41
3:B:291:ASP:HA	3:B:302:LYS:HG3	2.02	0.41
3:B:579:ASP:OD1	3:B:581:ARG:HB2	2.20	0.41
3:C:364:THR:O	3:C:368:ILE:HG13	2.21	0.41
3:C:413:THR:O	3:C:414:SER:C	2.59	0.41
3:C:467:ARG:H	3:C:467:ARG:CD	2.31	0.41
3:D:827:GLY:HA2	4:D:921:HOH:O	2.21	0.41
2:F:102:DC:H1'	2:F:103:DG:C8	2.55	0.41
1:G:15:DC:H2''	1:G:16:DG:C8	2.55	0.41
2:L:104:DG:H1'	2:L:105:DC:O4'	2.20	0.41
3:A:100:GLU:CG	3:A:102:LYS:HE2	2.44	0.41
3:A:104:ASP:OD2	3:A:106:THR:HB	2.20	0.41
3:A:129:ALA:HA	3:A:225:TYR:CZ	2.55	0.41
3:A:212:ILE:HD13	3:A:269:SER:HB2	2.02	0.41
3:A:466:ASP:N	3:A:466:ASP:OD2	2.53	0.41
3:A:804:HIS:O	3:A:808:ILE:HG13	2.20	0.41
3:B:516:VAL:HB	3:B:544:ARG:NH2	2.36	0.41
3:C:414:SER:O	3:C:415:LEU:C	2.59	0.41
3:C:546:GLN:O	3:C:550:VAL:HG23	2.21	0.41
3:C:854:ILE:HD13	3:C:862:VAL:HG21	2.03	0.41
3:D:621:ASP:O	3:D:622:THR:HB	2.19	0.41
3:B:82:ALA:O	3:B:382:GLN:HG3	2.21	0.41
3:B:209:THR:HA	3:B:210:PRO:HD3	1.94	0.41
3:B:444:ASN:HA	3:B:599:ARG:NE	2.35	0.41
3:C:9:GLU:OE2	3:C:266:PHE:HA	2.20	0.41
3:C:802:PRO:HB2	3:C:805:ILE:HG12	2.03	0.41
2:F:101:DG:H2''	2:F:102:DC:C6	2.55	0.41
3:A:216:TRP:O	3:A:217:ASN:HB2	2.21	0.41
3:A:739:LYS:CD	3:A:778:SER:HA	2.42	0.41
3:A:811:TYR:O	3:A:815:ILE:HG12	2.20	0.41
3:B:109:ARG:HB2	3:B:109:ARG:HH11	1.86	0.41
3:B:435:LYS:N	3:B:435:LYS:CD	2.82	0.41
3:B:492:ALA:HB1	3:B:549:GLU:HB2	2.02	0.41
3:C:432:GLY:C	3:C:433:THR:HG23	2.40	0.41
3:C:458:PRO:HG2	3:C:592:MSE:SE	2.71	0.41
3:D:6:LEU:CD2	3:D:108:ILE:HG12	2.51	0.41
3:D:429:THR:O	3:D:464:TYR:HD1	2.03	0.41
3:A:21:ASP:OD1	3:A:25:ARG:HG2	2.20	0.41
3:A:41:CYS:HB3	3:A:58:THR:HG22	2.01	0.41
3:A:273:TYR:OH	3:A:335:ASP:HA	2.20	0.41
3:A:308:PRO:HG3	3:A:311:LYS:HD2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:25:ARG:O	3:B:27:ARG:HG2	2.21	0.41
3:B:257:TYR:HE1	3:B:786:ASN:CG	2.24	0.41
3:B:294:SER:CB	3:B:301:GLY:HA2	2.49	0.41
3:B:485:HIS:HA	3:B:488:TYR:CD2	2.56	0.41
3:B:517:ASP:C	3:B:519:ARG:H	2.24	0.41
3:B:731:GLU:OE2	3:B:731:GLU:N	2.38	0.41
3:C:82:ALA:O	3:C:382:GLN:HB2	2.21	0.41
3:C:891:TYR:CD2	3:C:892:GLU:HG3	2.55	0.41
3:D:228:ASN:HD22	3:D:231:LYS:HD3	1.86	0.41
3:D:657:GLU:O	3:D:661:PRO:HG2	2.21	0.41
2:F:105:DC:H2'	2:F:106:DT:H72	2.03	0.41
1:I:8:DT:P	4:I:192:HOH:O	2.79	0.41
1:I:12:DA:H2''	1:I:13:DG:N7	2.35	0.41
3:A:125:GLU:HA	3:A:126:PRO:HD3	1.91	0.41
3:A:204:PHE:CE1	3:A:208:LYS:HD2	2.56	0.41
3:A:395:PHE:CE2	3:A:595:GLN:HG2	2.56	0.41
3:B:19:TYR:CE1	3:B:29:ARG:HG2	2.56	0.41
3:B:320:TYR:O	3:B:323:TYR:HB3	2.21	0.41
3:B:528:GLU:C	3:B:530:ILE:N	2.74	0.41
3:B:554:THR:O	3:B:558:ASN:HB2	2.21	0.41
3:B:818:ASN:HD22	3:B:821:ALA:HB2	1.83	0.41
3:C:9:GLU:HG3	3:C:267:GLY:N	2.36	0.41
3:C:21:ASP:CG	3:C:25:ARG:HG3	2.40	0.41
3:D:346:ASP:OD2	3:D:554:THR:HG22	2.22	0.41
3:D:668:ARG:HB2	3:D:668:ARG:CZ	2.51	0.41
3:A:405:LYS:O	3:A:699:GLY:HA3	2.22	0.40
3:B:33:TYR:O	3:B:35:PRO:HD3	2.21	0.40
3:B:412:LEU:HA	3:B:682:PHE:O	2.21	0.40
3:B:792:ASP:CG	3:B:793:VAL:N	2.75	0.40
3:C:109:ARG:HD2	3:C:209:THR:O	2.21	0.40
3:C:202:LEU:O	3:C:206:GLN:HG2	2.20	0.40
3:C:433:THR:O	3:C:462:MSE:SE	2.88	0.40
3:C:505:ASN:N	3:C:506:PRO:HD3	2.36	0.40
3:D:426:SER:C	3:D:428:GLU:H	2.25	0.40
3:D:702:TRP:NE1	3:D:708:TYR:HB3	2.35	0.40
1:G:12:DA:H2''	1:G:13:DG:O5'	2.21	0.40
1:K:6:DA:C2	1:K:7:DA:N6	2.90	0.40
3:A:176:ASP:HA	3:A:319:ARG:NH2	2.27	0.40
3:A:294:SER:HB3	3:A:301:GLY:HA2	2.03	0.40
3:B:379:VAL:O	3:B:379:VAL:HG13	2.21	0.40
3:B:593:ALA:HB2	3:B:681:MSE:HE3	2.00	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:454:TYR:HD2	3:C:462:MSE:CE	2.27	0.40
3:D:508:LEU:N	3:D:508:LEU:HD22	2.36	0.40
1:K:8:DT:C2'	1:K:9:DG:C8	2.99	0.40
2:L:101:DG:H2'	2:L:102:DC:C5	2.57	0.40
3:A:457:SER:HA	3:A:458:PRO:HD3	1.94	0.40
3:C:614:GLU:HB2	3:C:616:PHE:HE1	1.86	0.40
1:G:8:DT:H5'	1:G:8:DT:H6	1.86	0.40
1:I:15:DC:C2'	1:I:16:DG:H5'	2.33	0.40
3:A:494:ARG:HE	3:A:494:ARG:HB2	1.75	0.40
3:A:514:LEU:HD13	3:A:515:ASP:N	2.36	0.40
3:A:660:GLU:HB2	3:A:661:PRO:CD	2.42	0.40
3:B:901:PHE:HB2	3:B:902:ASP:H	1.65	0.40
3:C:257:TYR:CD2	3:C:257:TYR:N	2.86	0.40
3:C:302:LYS:HD2	3:C:323:TYR:CD1	2.56	0.40
3:C:578:TYR:CD1	3:C:578:TYR:C	2.95	0.40
3:D:157:GLY:O	3:D:158:ASN:HB3	2.21	0.40
3:D:433:THR:O	3:D:462:MSE:HE2	2.21	0.40
3:D:730:LEU:N	4:D:925:HOH:O	2.54	0.40
2:H:110:DA:C2'	2:H:111:DT:C5'	2.98	0.40
1:K:11:DC:N3	2:L:107:DG:O6	2.55	0.40
3:A:397:LYS:O	3:A:399:PRO:HD3	2.21	0.40
3:B:158:ASN:N	3:B:158:ASN:ND2	2.68	0.40
3:B:397:LYS:O	3:B:399:PRO:HD3	2.21	0.40
3:B:518:TYR:CB	3:B:544:ARG:HG2	2.52	0.40
3:B:597:ILE:HD13	3:B:625:ILE:HD13	2.02	0.40
3:B:857:LEU:CD2	3:B:858:ILE:HG23	2.52	0.40
3:C:209:THR:HA	3:C:210:PRO:HD3	1.85	0.40
3:C:392:PRO:O	3:C:587:THR:CG2	2.62	0.40
3:C:772:ARG:HH11	3:C:772:ARG:HG3	1.87	0.40
3:D:188:TYR:CE2	3:D:190:PRO:HD3	2.55	0.40
3:D:887:ALA:C	3:D:889:LEU:H	2.25	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	A	900/903 (100%)	804 (89%)	84 (9%)	12 (1%)	12	18
3	B	884/903 (98%)	802 (91%)	70 (8%)	12 (1%)	11	16
3	C	898/903 (99%)	830 (92%)	56 (6%)	12 (1%)	12	18
3	D	886/903 (98%)	701 (79%)	131 (15%)	54 (6%)	1	1
All	All	3568/3612 (99%)	3137 (88%)	341 (10%)	90 (2%)	5	7

All (90) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	519	ARG
3	A	611	THR
3	A	621	ASP
3	B	177	GLU
3	C	256	MSE
3	C	458	PRO
3	C	899	ASP
3	D	44	SER
3	D	170	LEU
3	D	265	LEU
3	D	489	MSE
3	D	498	ILE
3	D	521	ASP
3	D	532	LYS
3	D	731	GLU
3	D	736	SER
3	D	815	ILE
3	D	853	GLU
3	A	12	GLY
3	A	121	ASP
3	A	300	VAL
3	B	45	GLN
3	D	127	SER
3	D	155	PRO
3	D	165	GLU
3	D	179	PRO
3	D	221	PHE
3	D	387	PRO
3	D	427	PRO
3	D	506	PRO

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Mol	Chain	Res	Type
3	D	523	SER
3	D	533	LEU
3	D	536	LYS
3	D	695	SER
3	D	800	LYS
3	D	817	GLY
3	D	836	ARG
3	D	854	ILE
3	A	303	LEU
3	B	352	LYS
3	B	406	TYR
3	B	518	TYR
3	B	795	GLY
3	C	432	GLY
3	C	483	LYS
3	C	533	LEU
3	C	622	THR
3	D	45	GLN
3	D	140	ASP
3	D	315	SER
3	D	415	LEU
3	D	622	THR
3	D	843	ASP
3	D	874	LYS
3	A	338	ARG
3	A	490	LEU
3	A	509	SER
3	B	520	PHE
3	B	734	LYS
3	B	793	VAL
3	B	896	SER
3	C	174	GLY
3	C	415	LEU
3	C	506	PRO
3	D	198	LEU
3	D	262	ILE
3	D	272	ASP
3	D	401	PRO
3	D	512	GLU
3	D	640	LYS
3	D	730	LEU
3	D	783	SER

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Mol	Chain	Res	Type
3	D	849	PRO
3	D	889	LEU
3	C	240	LYS
3	D	182	ILE
3	D	269	SER
3	D	391	TYR
3	D	395	PHE
3	D	510	VAL
3	A	622	THR
3	B	302	LYS
3	B	529	LYS
3	D	157	GLY
3	D	35	PRO
3	D	799	PRO
3	C	175	GLY
3	A	388	VAL
3	D	166	ILE
3	D	779	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	A	785/775 (101%)	739 (94%)	46 (6%)	19	30
3	B	767/775 (99%)	722 (94%)	45 (6%)	19	30
3	C	786/775 (101%)	744 (95%)	42 (5%)	22	35
3	D	711/775 (92%)	675 (95%)	36 (5%)	24	37
All	All	3049/3100 (98%)	2880 (94%)	169 (6%)	21	33

All (169) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	14	SER
3	A	29	ARG
3	A	32	GLU

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Mol	Chain	Res	Type
3	A	58	THR
3	A	64	ASN
3	A	66	ARG
3	A	75	MSE
3	A	86	ASP
3	A	112	ASN
3	A	116	GLU
3	A	121	ASP
3	A	181	GLU
3	A	213	LEU
3	A	229	ARG
3	A	242	LEU
3	A	273	TYR
3	A	291	ASP
3	A	304	LYS
3	A	318	GLN
3	A	332	LEU
3	A	346	ASP
3	A	382	GLN
3	A	403	ARG
3	A	411	ASP
3	A	467	ARG
3	A	483	LYS
3	A	503	LEU
3	A	514	LEU
3	A	539	ASN
3	A	561	LEU
3	A	587	THR
3	A	612	GLU
3	A	618	LEU
3	A	631	LYS
3	A	646	HIS
3	A	653	LYS
3	A	656	ARG
3	A	658	ARG
3	A	659	MSE
3	A	702	TRP
3	A	733	GLN
3	A	736	SER
3	A	739	LYS
3	A	773	GLN
3	A	818	ASN

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Mol	Chain	Res	Type
3	A	861	ASP
3	B	26	GLU
3	B	66	ARG
3	B	75	MSE
3	B	89	LYS
3	B	93	LEU
3	B	98	ASN
3	B	109	ARG
3	B	112	ASN
3	B	113	PHE
3	B	116	GLU
3	B	154	SER
3	B	164	ILE
3	B	193	ASN
3	B	217	ASN
3	B	256	MSE
3	B	257	TYR
3	B	259	SER
3	B	260	ARG
3	B	273	TYR
3	B	316	ASN
3	B	324	ASN
3	B	403	ARG
3	B	411	ASP
3	B	421	ARG
3	B	435	LYS
3	B	475	ILE
3	B	489	MSE
3	B	539	ASN
3	B	573	VAL
3	B	658	ARG
3	B	681	MSE
3	B	684	ASP
3	B	685	ARG
3	B	702	TRP
3	B	707	ARG
3	B	728	MSE
3	B	737	THR
3	B	739	LYS
3	B	766	GLU
3	B	787	ASN
3	B	791	TYR

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Mol	Chain	Res	Type
3	B	819	ILE
3	B	861	ASP
3	B	878	LYS
3	B	901	PHE
3	C	43	GLU
3	C	98	ASN
3	C	138	HIS
3	C	141	SER
3	C	257	TYR
3	C	273	TYR
3	C	276	LEU
3	C	284	ASN
3	C	332	LEU
3	C	337	LYS
3	C	356	GLN
3	C	411	ASP
3	C	426	SER
3	C	428	GLU
3	C	439	LEU
3	C	449	ARG
3	C	456	CYS
3	C	467	ARG
3	C	468	ASP
3	C	479	PHE
3	C	525	GLU
3	C	536	LYS
3	C	558	ASN
3	C	559	ARG
3	C	561	LEU
3	C	562	LEU
3	C	580	LEU
3	C	587	THR
3	C	618	LEU
3	C	642	ARG
3	C	702	TRP
3	C	722	GLU
3	C	728	MSE
3	C	747	GLU
3	C	760	LEU
3	C	818	ASN
3	C	843	ASP
3	C	859	LYS

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Mol	Chain	Res	Type
3	C	880	LEU
3	C	881	GLU
3	C	896	SER
3	C	898	PHE
3	D	10	GLN
3	D	47	THR
3	D	58	THR
3	D	86	ASP
3	D	134	ASP
3	D	162	TRP
3	D	216	TRP
3	D	266	PHE
3	D	273	TYR
3	D	303	LEU
3	D	306	ASP
3	D	316	ASN
3	D	356	GLN
3	D	391	TYR
3	D	441	ASP
3	D	479	PHE
3	D	489	MSE
3	D	498	ILE
3	D	519	ARG
3	D	520	PHE
3	D	530	ILE
3	D	556	GLN
3	D	558	ASN
3	D	576	ARG
3	D	591	GLN
3	D	657	GLU
3	D	660	GLU
3	D	702	TRP
3	D	719	ARG
3	D	730	LEU
3	D	755	GLU
3	D	772	ARG
3	D	828	GLU
3	D	844	LYS
3	D	856	ASP
3	D	860	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (92) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	64	ASN
3	A	153	ASN
3	A	158	ASN
3	A	206	GLN
3	A	245	HIS
3	A	284	ASN
3	A	285	GLN
3	A	376	GLN
3	A	382	GLN
3	A	422	GLN
3	A	480	ASN
3	A	485	HIS
3	A	493	GLN
3	A	495	ASN
3	A	505	ASN
3	A	539	ASN
3	A	556	GLN
3	A	558	ASN
3	A	602	ASN
3	A	606	ASN
3	A	646	HIS
3	A	678	GLN
3	A	733	GLN
3	A	742	GLN
3	A	773	GLN
3	A	775	ASN
3	B	70	GLN
3	B	98	ASN
3	B	153	ASN
3	B	158	ASN
3	B	193	ASN
3	B	203	ASN
3	B	217	ASN
3	B	245	HIS
3	B	316	ASN
3	B	318	GLN
3	B	324	ASN
3	B	376	GLN
3	B	382	GLN
3	B	389	GLN
3	B	493	GLN
3	B	646	HIS
3	B	733	GLN

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Mol	Chain	Res	Type
3	B	742	GLN
3	B	775	ASN
3	B	818	ASN
3	C	45	GLN
3	C	98	ASN
3	C	112	ASN
3	C	131	HIS
3	C	153	ASN
3	C	158	ASN
3	C	171	GLN
3	C	173	GLN
3	C	203	ASN
3	C	207	GLN
3	C	284	ASN
3	C	285	GLN
3	C	376	GLN
3	C	481	GLN
3	C	495	ASN
3	C	539	ASN
3	C	556	GLN
3	C	558	ASN
3	C	572	ASN
3	C	675	ASN
3	C	676	ASN
3	C	678	GLN
3	C	679	HIS
3	C	711	ASN
3	C	818	ASN
3	C	864	HIS
3	D	10	GLN
3	D	64	ASN
3	D	70	GLN
3	D	228	ASN
3	D	285	GLN
3	D	316	ASN
3	D	339	GLN
3	D	342	ASN
3	D	356	GLN
3	D	440	HIS
3	D	444	ASN
3	D	485	HIS
3	D	495	ASN

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Mol	Chain	Res	Type
3	D	505	ASN
3	D	564	ASN
3	D	591	GLN
3	D	646	HIS
3	D	742	GLN
3	D	761	GLN
3	D	812	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	CTG	K	3	1	19,23,24	1.01	1 (5%)	21,35,38	1.04	2 (9%)
1	CTG	E	3	2,1	19,23,24	0.74	0	21,35,38	1.03	2 (9%)
1	CTG	I	3	2,1	19,23,24	0.88	1 (5%)	21,35,38	1.09	2 (9%)
1	CTG	G	3	2,1	19,23,24	0.86	1 (5%)	21,35,38	1.03	1 (4%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CTG	K	3	1	-	0/7/45/46	0/2/2/2
1	CTG	E	3	2,1	-	2/7/45/46	0/2/2/2
1	CTG	I	3	2,1	-	2/7/45/46	0/2/2/2
1	CTG	G	3	2,1	-	0/7/45/46	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	3	CTG	C5-C4	2.82	1.55	1.52
1	I	3	CTG	C1'-N1	2.41	1.48	1.45
1	G	3	CTG	C1'-N1	2.04	1.48	1.45

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	3	CTG	O3'-C3'-C2'	2.77	120.79	110.90
1	E	3	CTG	O3'-C3'-C2'	2.52	119.92	110.90
1	G	3	CTG	N3-C2-N1	-2.40	114.20	116.69
1	K	3	CTG	N3-C2-N1	-2.32	114.28	116.69
1	K	3	CTG	O3'-C3'-C2'	2.25	118.95	110.90
1	E	3	CTG	N3-C2-N1	-2.14	114.48	116.69
1	I	3	CTG	N3-C2-N1	-2.07	114.54	116.69

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	E	3	CTG	O4'-C4'-C5'-O5'
1	E	3	CTG	C3'-C4'-C5'-O5'
1	I	3	CTG	O4'-C4'-C5'-O5'
1	I	3	CTG	C3'-C4'-C5'-O5'

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	K	3	CTG	3	0
1	E	3	CTG	2	0
1	I	3	CTG	1	0
1	G	3	CTG	1	0

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	E	16/18 (88%)	0.73	2 (12%) 3 2	87, 109, 126, 131	0
1	G	17/18 (94%)	-0.26	0 100 100	34, 47, 76, 79	0
1	I	17/18 (94%)	-0.06	0 100 100	35, 50, 84, 91	0
1	K	17/18 (94%)	1.92	8 (47%) 0 0	65, 80, 81, 81	0
2	F	14/15 (93%)	1.08	3 (21%) 0 1	106, 125, 133, 135	0
2	H	15/15 (100%)	-0.36	0 100 100	36, 49, 100, 100	0
2	J	15/15 (100%)	-0.09	0 100 100	33, 65, 112, 113	0
2	L	15/15 (100%)	2.30	9 (60%) 0 0	78, 80, 82, 82	0
3	A	877/903 (97%)	0.20	51 (5%) 23 19	23, 51, 125, 141	0
3	B	863/903 (95%)	0.04	41 (4%) 30 27	16, 44, 116, 139	0
3	C	875/903 (96%)	0.07	36 (4%) 37 33	17, 47, 114, 142	0
3	D	867/903 (96%)	0.90	145 (16%) 1 1	54, 102, 140, 153	0
All	All	3608/3744 (96%)	0.32	295 (8%) 11 9	16, 58, 131, 153	0

All (295) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	503	LEU	9.4
3	C	503	LEU	9.2
3	D	309	ILE	9.1
3	D	498	ILE	8.8
3	D	135	ALA	8.7
3	D	534	SER	8.4
3	D	313	ARG	8.0
3	A	504	HIS	7.8
3	C	510	VAL	7.7
3	A	532	LYS	7.6
3	B	538	LEU	6.8

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Mol	Chain	Res	Type	RSRZ
3	D	118	THR	6.8
3	A	505	ASN	6.7
3	A	502	ALA	6.6
3	B	497	GLU	6.5
3	B	258	GLY	6.5
3	D	303	LEU	6.5
3	A	511	ASP	6.3
3	C	531	LYS	6.2
3	A	509	SER	6.2
3	D	535	ALA	6.1
3	C	505	ASN	6.1
3	D	115	ILE	6.0
3	D	514	LEU	6.0
3	D	315	SER	6.0
3	B	794	GLY	6.0
3	D	542	LEU	5.9
3	C	511	ASP	5.8
3	D	829	LYS	5.8
3	D	164	ILE	5.8
3	A	499	ILE	5.7
3	D	305	TYR	5.7
3	A	506	PRO	5.7
3	A	846	ILE	5.6
3	D	526	ILE	5.6
3	D	538	LEU	5.6
3	D	517	ASP	5.5
2	L	108	DT	5.4
3	A	496	GLY	5.4
3	D	875	THR	5.4
3	B	793	VAL	5.3
3	A	508	LEU	5.3
3	C	495	ASN	5.2
3	C	504	HIS	5.2
3	B	498	ILE	5.2
2	L	109	DC	5.2
3	D	522	PHE	5.1
3	D	817	GLY	5.1
3	B	792	ASP	5.1
3	C	498	ILE	5.0
3	C	507	ASN	4.8
3	A	536	LYS	4.8
3	D	121	ASP	4.8

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Mol	Chain	Res	Type	RSRZ
3	B	791	TYR	4.7
3	C	512	GLU	4.6
3	C	508	LEU	4.6
3	D	523	SER	4.6
3	D	314	GLU	4.6
3	A	257	TYR	4.6
3	D	730	LEU	4.5
3	D	230	ILE	4.5
3	C	509	SER	4.5
3	D	491	ALA	4.4
3	A	500	LYS	4.4
3	A	530	ILE	4.4
3	C	522	PHE	4.3
3	D	252	VAL	4.3
3	D	782	VAL	4.3
3	A	514	LEU	4.3
3	D	508	LEU	4.3
3	B	524	ASP	4.2
3	B	819	ILE	4.2
3	C	530	ILE	4.2
3	A	510	VAL	4.2
3	D	320	TYR	4.1
3	A	498	ILE	4.1
3	C	499	ILE	4.1
3	B	542	LEU	4.1
3	C	506	PRO	4.1
3	D	539	ASN	4.0
2	L	101	DG	4.0
3	D	529	LYS	4.0
3	C	496	GLY	3.9
3	A	497	GLU	3.9
3	C	527	LYS	3.9
3	D	787	ASN	3.9
3	D	818	ASN	3.9
3	B	820	ASP	3.8
3	D	150	ASP	3.8
3	D	159	VAL	3.8
3	A	513	PRO	3.8
3	D	203	ASN	3.8
3	D	216	TRP	3.8
3	D	321	ILE	3.7
1	K	2	DG	3.7

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Mol	Chain	Res	Type	RSRZ
3	D	794	GLY	3.7
3	B	259	SER	3.7
3	D	134	ASP	3.6
3	D	78	ILE	3.6
3	A	535	ALA	3.6
3	D	133	ILE	3.6
2	L	107	DG	3.6
3	C	502	ALA	3.6
3	D	789	ALA	3.5
3	A	534	SER	3.5
3	D	537	SER	3.5
3	D	225	TYR	3.5
3	D	136	ILE	3.5
3	A	538	LEU	3.5
3	B	533	LEU	3.5
3	D	306	ASP	3.5
3	B	253	ILE	3.5
3	D	263	ILE	3.4
3	D	191	PHE	3.4
3	A	507	ASN	3.4
3	A	799	PRO	3.4
3	D	234	PHE	3.4
3	B	523	SER	3.4
3	D	518	TYR	3.3
3	D	779	ILE	3.3
3	D	821	ALA	3.3
3	D	126	PRO	3.3
3	A	539	ASN	3.3
3	B	525	GLU	3.2
3	A	528	GLU	3.2
3	D	798	GLY	3.2
3	A	501	GLU	3.2
3	D	876	PHE	3.2
3	B	734	LYS	3.2
3	D	160	GLU	3.2
3	D	190	PRO	3.2
3	D	304	LYS	3.1
3	C	513	PRO	3.1
1	K	15	DC	3.1
3	D	545	ALA	3.1
3	A	533	LEU	3.1
3	C	538	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
3	D	15	ILE	3.1
3	A	537	SER	3.1
3	D	223	ILE	3.1
3	D	497	GLU	3.1
3	D	741	VAL	3.1
3	D	735	SER	3.1
3	D	745	LEU	3.1
3	B	536	LYS	3.1
3	D	201	TYR	3.0
3	D	152	LEU	3.0
3	D	124	PRO	3.0
3	D	873	GLU	3.0
3	B	495	ASN	3.0
3	D	793	VAL	3.0
3	D	229	ARG	3.0
3	C	523	SER	3.0
3	D	506	PRO	3.0
3	D	161	GLU	2.9
3	C	528	GLU	2.9
3	A	254	GLU	2.9
3	C	544	ARG	2.9
3	D	215	GLY	2.9
3	C	175	GLY	2.9
3	A	518	TYR	2.8
3	D	120	PRO	2.8
3	A	857	LEU	2.8
3	D	62	PHE	2.8
3	D	515	ASP	2.8
3	D	857	LEU	2.8
3	A	788	ILE	2.8
3	B	902	ASP	2.8
3	D	61	LEU	2.8
3	A	258	GLY	2.8
3	A	495	ASN	2.8
3	D	113	PHE	2.8
3	D	511	ASP	2.8
3	D	499	ILE	2.8
3	A	516	VAL	2.8
3	D	129	ALA	2.7
3	D	162	TRP	2.7
3	B	526	ILE	2.7
3	D	788	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
3	D	310	SER	2.7
3	D	488	TYR	2.7
3	D	771	PHE	2.7
3	D	394	ALA	2.7
3	D	117	VAL	2.7
1	K	13	DG	2.7
3	D	213	LEU	2.7
3	C	532	LYS	2.7
3	D	198	LEU	2.7
3	D	889	LEU	2.7
3	B	818	ASN	2.7
2	F	111	DT	2.7
3	B	518	TYR	2.7
3	B	530	ILE	2.6
3	D	831	TYR	2.6
3	A	542	LEU	2.6
3	D	122	GLY	2.6
3	D	183	ILE	2.6
3	B	255	ASN	2.6
3	C	526	ILE	2.6
3	D	891	TYR	2.6
3	D	790	LYS	2.6
3	D	167	ALA	2.6
3	A	902	ASP	2.6
3	D	863	LEU	2.6
2	L	106	DT	2.6
3	D	221	PHE	2.5
3	A	786	ASN	2.5
1	K	12	DA	2.5
3	D	233	ILE	2.5
3	B	496	GLY	2.5
3	C	537	SER	2.5
3	B	499	ILE	2.5
3	D	242	LEU	2.5
3	D	391	TYR	2.5
3	B	552	GLY	2.5
3	C	534	SER	2.5
3	B	260	ARG	2.5
3	D	179	PRO	2.5
3	D	513	PRO	2.5
3	D	799	PRO	2.5
3	D	237	SER	2.5

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Mol	Chain	Res	Type	RSRZ
3	A	785	ALA	2.5
2	L	110	DA	2.4
3	D	528	GLU	2.4
1	K	4	DG	2.4
3	B	797	PRO	2.4
3	B	545	ALA	2.4
3	D	325	ILE	2.4
3	B	787	ASN	2.4
3	D	390	PRO	2.4
3	B	521	ASP	2.4
3	D	776	TYR	2.4
3	A	512	GLU	2.4
3	C	514	LEU	2.4
3	C	524	ASP	2.4
3	A	490	LEU	2.4
3	D	781	SER	2.4
3	D	20	ILE	2.4
3	D	175	GLY	2.4
3	D	287	SER	2.3
2	F	107	DG	2.3
1	K	5	DG	2.3
3	A	492	ALA	2.3
3	B	809	LEU	2.3
3	A	493	GLN	2.3
2	L	114	DC	2.3
3	D	729	GLY	2.3
2	F	109	DC	2.3
3	D	800	LYS	2.3
1	K	16	DG	2.3
3	D	338	ARG	2.3
3	D	864	HIS	2.3
3	D	791	TYR	2.3
3	D	731	GLU	2.3
3	A	522	PHE	2.3
3	D	740	ALA	2.3
3	B	522	PHE	2.3
3	B	178	VAL	2.2
3	A	531	LYS	2.2
3	D	780	ALA	2.2
3	D	823	GLN	2.2
3	B	537	SER	2.2
1	E	13	DG	2.2

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Mol	Chain	Res	Type	RSRZ
3	A	523	SER	2.2
3	D	530	ILE	2.2
3	D	312	LEU	2.2
2	L	115	DA	2.2
2	L	105	DC	2.2
3	D	64	ASN	2.2
3	D	768	GLU	2.2
3	D	520	PHE	2.2
3	A	793	VAL	2.1
3	D	224	PRO	2.1
3	D	290	LEU	2.1
3	D	503	LEU	2.1
3	C	535	ALA	2.1
3	D	395	PHE	2.1
3	C	436	VAL	2.1
1	K	14	DC	2.1
3	D	188	TYR	2.1
3	B	532	LYS	2.1
3	D	622	THR	2.1
3	D	178	VAL	2.1
3	D	241	ARG	2.1
3	C	501	GLU	2.1
3	D	833	LEU	2.1
3	C	464	TYR	2.1
3	A	847	ALA	2.0
3	B	535	ALA	2.0
3	D	205	TRP	2.0
1	E	2	DG	2.0
3	D	11	ILE	2.0
3	B	531	LYS	2.0
3	C	500	LYS	2.0
3	D	302	LYS	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	CTG	K	3	22/23	0.81	0.42	75,79,85,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
1	CTG	E	3	22/23	0.82	0.23	110,111,113,114	0
1	CTG	I	3	22/23	0.96	0.17	58,61,62,63	0
1	CTG	G	3	22/23	0.98	0.13	32,41,42,43	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.