Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 12:41 PM GMT

PDB ID	:	3RMB
Title	:	Crystal Structure of a replicative DNA polymerase bound to DNA containing Thymine Glycol
Authors	:	Aller, P.; Duclos, S.; Wallace, S.S.; Doublie, S.
Deposited on	:	2011-04-20
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

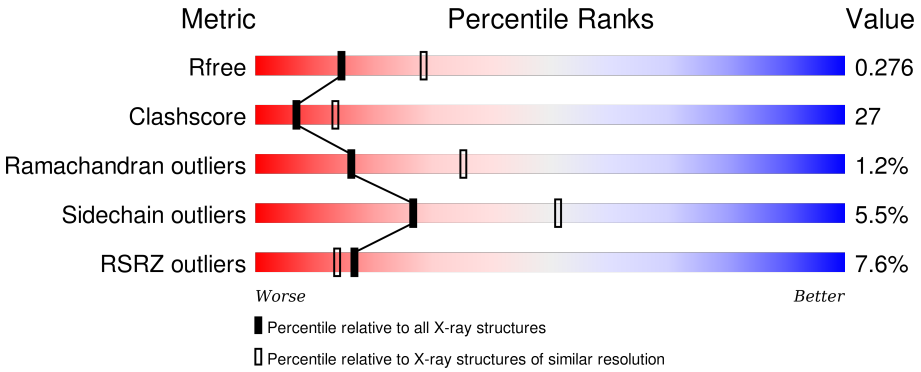
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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}	91344	3152 (2.70-2.62)
Clashscore	102246	3524 (2.70-2.62)
Ramachandran outliers	100387	3469 (2.70-2.62)
Sidechain outliers	100360	3469 (2.70-2.62)
RSRZ outliers	91569	3161 (2.70-2.62)

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

Mol	Chain	Length	Quality of chain
1	A	906	7% 53% 42% 5%
1	B	906	8% 59% 38%
1	C	906	% 61% 36%
1	D	906	15% 49% 47%
2	E	18	6% 11% 89%

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Mol	Chain	Length	Quality of chain
2	G	18	22% 78%
2	I	18	44% 56%
2	K	18	11% 39% 61%
3	F	14	21% 79%
3	H	14	14% 86%
3	J	14	29% 71%
3	L	14	21% 7% 93%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 32166 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 protein called DNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	903	Total	C	N	O	S	4	0	0
			7342	4715	1220	1374	33			
1	B	903	Total	C	N	O	S	0	0	0
			7294	4686	1209	1366	33			
1	C	900	Total	C	N	O	S	0	0	0
			7332	4706	1220	1373	33			
1	D	897	Total	C	N	O	S	0	0	0
			7097	4558	1163	1344	32			

There are 20 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
A	904	HIS	-	EXPRESSION TAG	UNP Q38087
A	905	HIS	-	EXPRESSION TAG	UNP Q38087
A	906	HIS	-	EXPRESSION TAG	UNP Q38087
B	222	ALA	ASP	ENGINEERED MUTATION	UNP Q38087
B	327	ALA	ASP	ENGINEERED MUTATION	UNP Q38087
B	904	HIS	-	EXPRESSION TAG	UNP Q38087
B	905	HIS	-	EXPRESSION TAG	UNP Q38087
B	906	HIS	-	EXPRESSION TAG	UNP Q38087
C	222	ALA	ASP	ENGINEERED MUTATION	UNP Q38087
C	327	ALA	ASP	ENGINEERED MUTATION	UNP Q38087
C	904	HIS	-	EXPRESSION TAG	UNP Q38087
C	905	HIS	-	EXPRESSION TAG	UNP Q38087
C	906	HIS	-	EXPRESSION TAG	UNP Q38087
D	222	ALA	ASP	ENGINEERED MUTATION	UNP Q38087
D	327	ALA	ASP	ENGINEERED MUTATION	UNP Q38087
D	904	HIS	-	EXPRESSION TAG	UNP Q38087
D	905	HIS	-	EXPRESSION TAG	UNP Q38087
D	906	HIS	-	EXPRESSION TAG	UNP Q38087

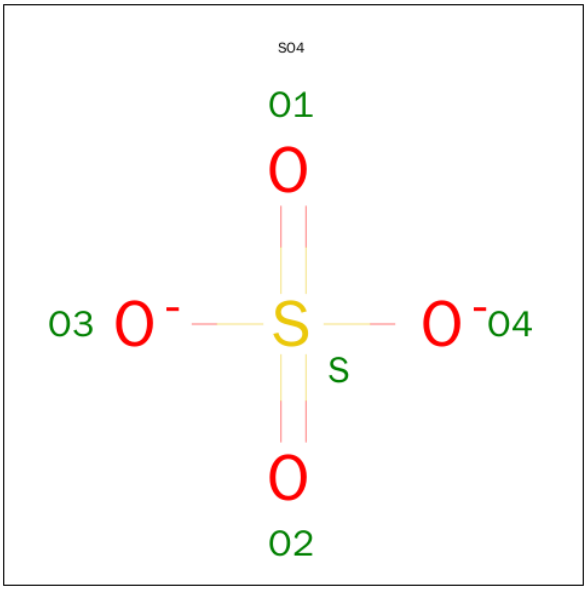
- Molecule 2 is a DNA chain called DNA (5'-D(*CP*GP*CP*(CTG)P*GP*AP*AP*TP*GP *AP*CP*AP*GP*CP*CP*GP*CP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	18	Total	C	N	O	P	0	0	0
			369	174	72	106	17			
2	G	18	Total	C	N	O	P	0	0	0
			369	174	72	106	17			
2	I	18	Total	C	N	O	P	0	0	0
			369	174	72	106	17			
2	K	18	Total	C	N	O	P	0	0	0
			369	174	72	106	17			

- Molecule 3 is a DNA chain called DNA (5'-D(*GP*CP*GP*GP*CP*TP*GP*TP*CP*AP* TP*TP*CP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	14	Total	C	N	O	P	0	0	0
			280	134	50	83	13			
3	H	14	Total	C	N	O	P	0	0	0
			280	134	50	83	13			
3	J	14	Total	C	N	O	P	0	0	0
			280	134	50	83	13			
3	L	14	Total	C	N	O	P	0	0	0
			280	134	50	83	13			

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total O S 5 4 1	0	0

- Molecule 5 is water.

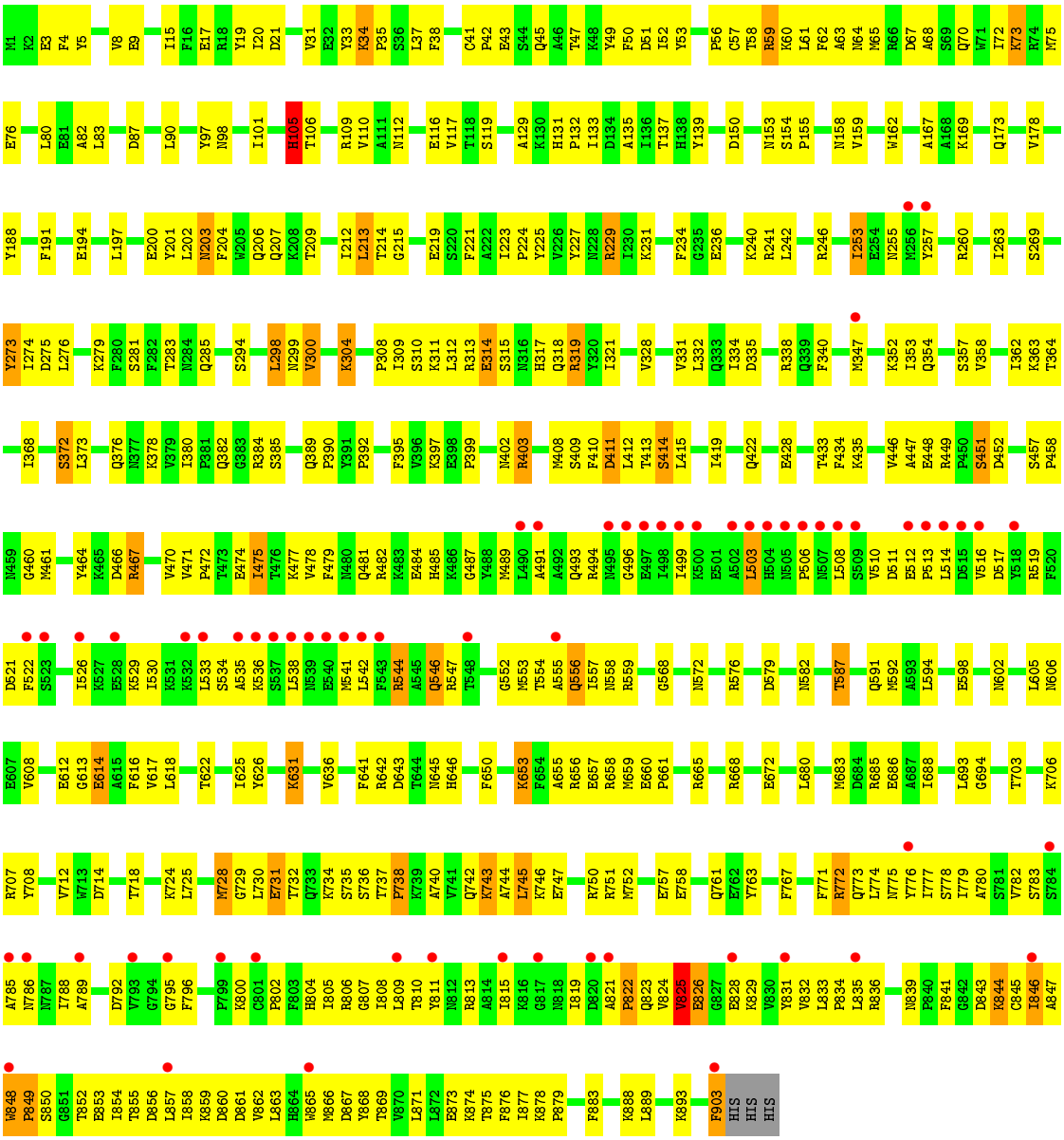
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	111	Total O 111 111	0	0
5	B	129	Total O 129 129	0	0
5	C	178	Total O 178 178	0	0
5	D	33	Total O 33 33	0	0
5	E	5	Total O 5 5	0	0
5	F	4	Total O 4 4	0	0
5	G	11	Total O 11 11	0	0
5	H	4	Total O 4 4	0	0
5	I	13	Total O 13 13	0	0
5	J	7	Total O 7 7	0	0
5	K	3	Total O 3 3	0	0
5	L	2	Total O 2 2	0	0

3 Residue-property plots (i)

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

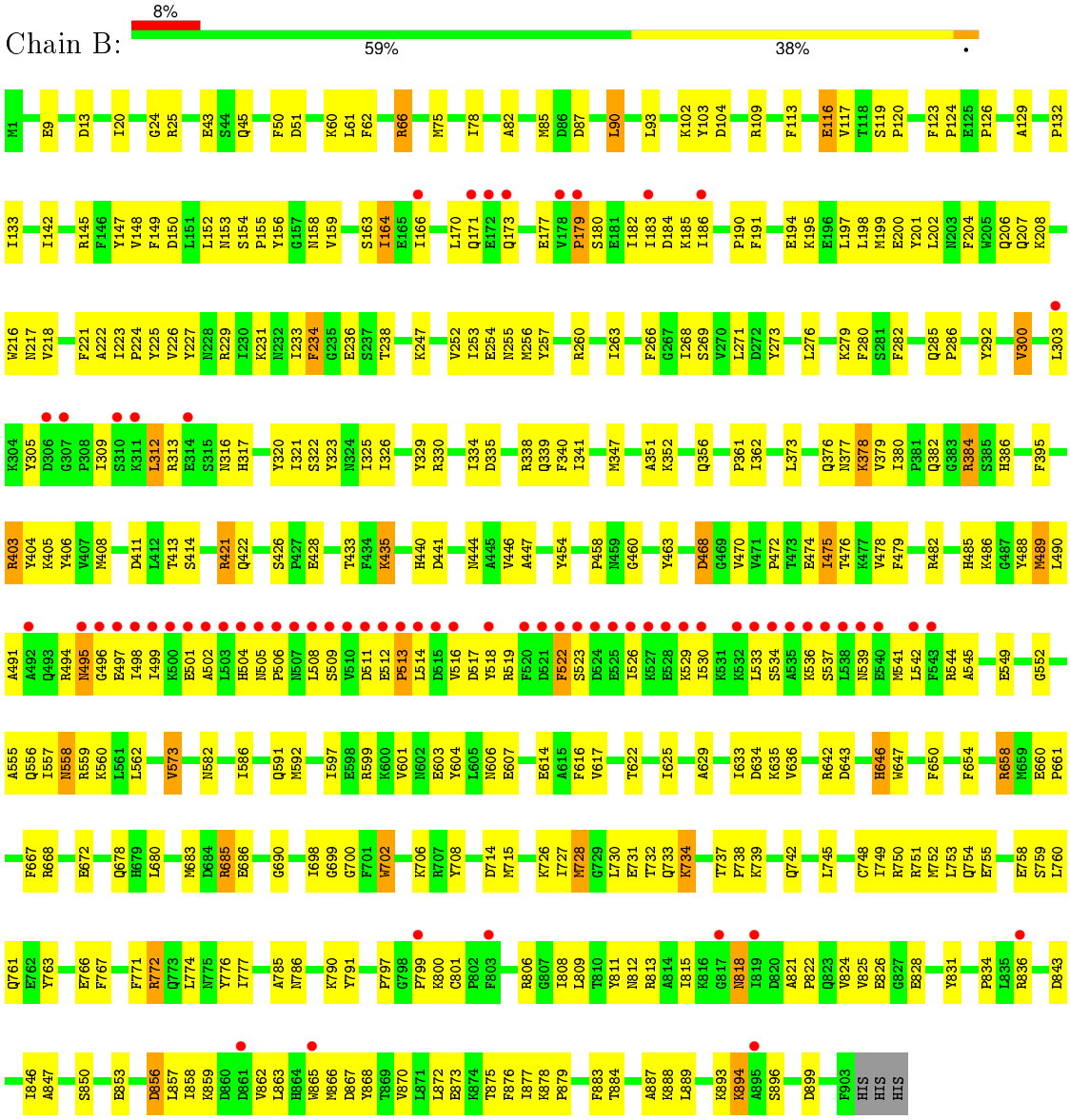
- Molecule 1: DNA polymerase

Chain A:



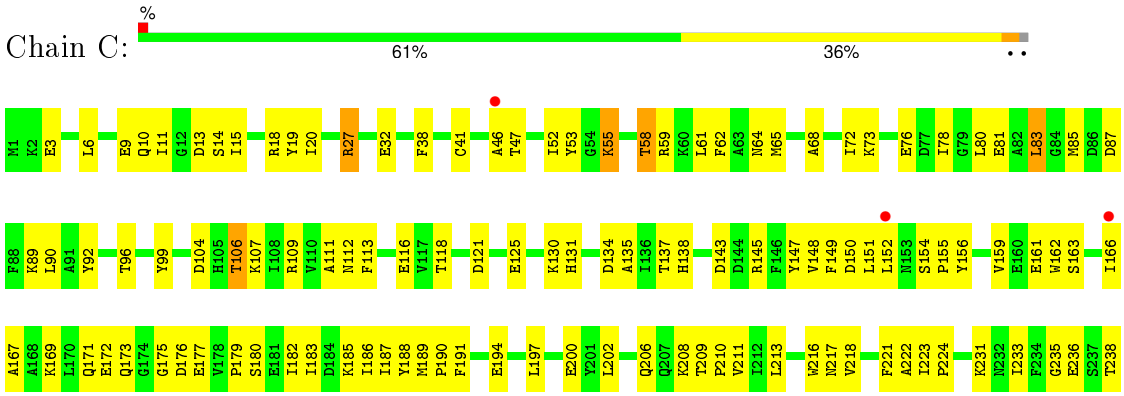
• Molecule 1: DNA polymerase

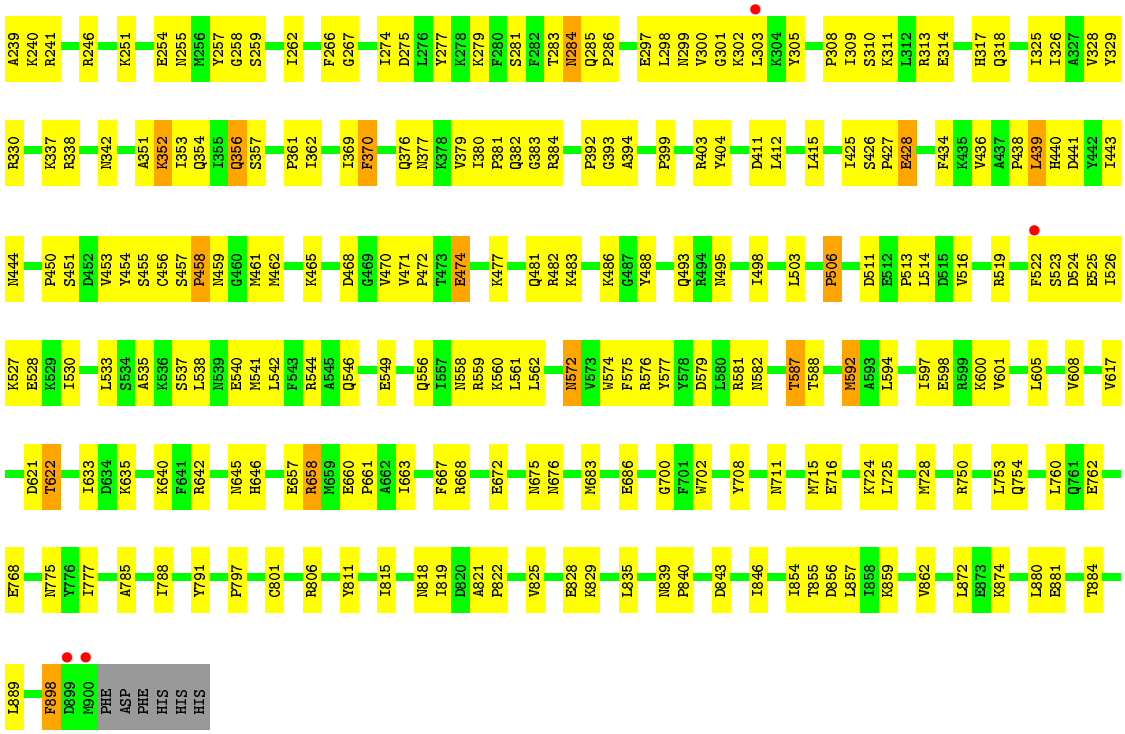
Chain B:



• Molecule 1: DNA polymerase

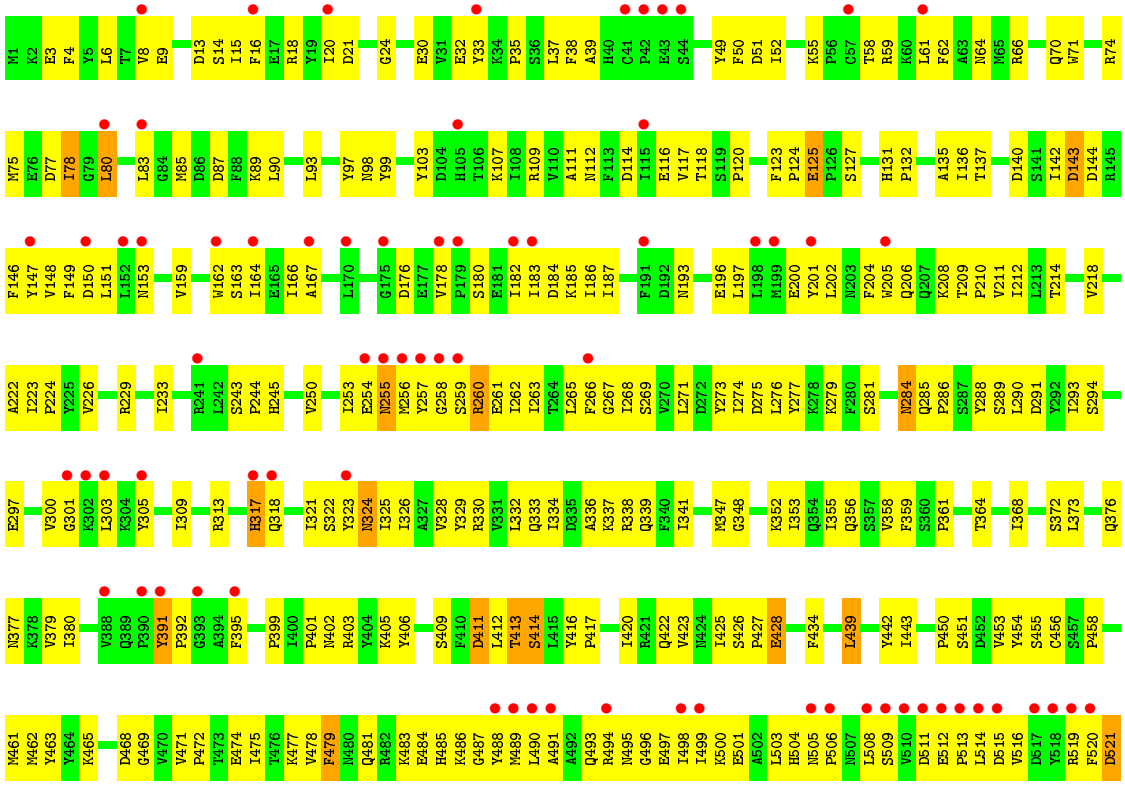
Chain C:

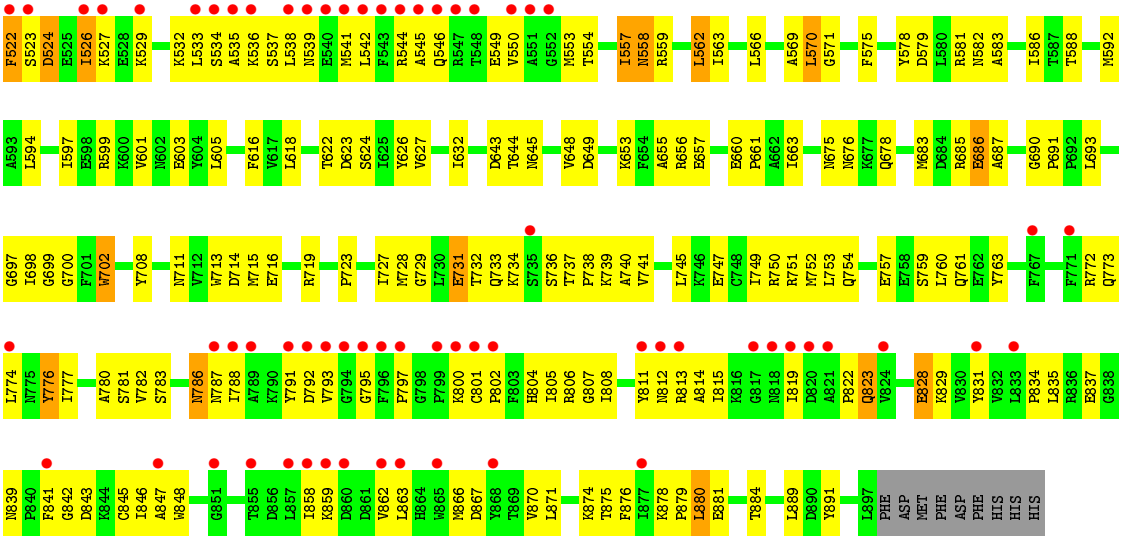




- Molecule 1: DNA polymerase

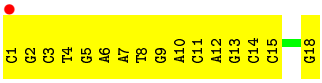
Chain D:





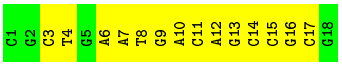
• Molecule 2: DNA (5'-D(*CP*GP*CP*(CTG)P*GP*AP*AP*TP*GP*AP*CP*AP*GP*CP*C P*GP*CP*G)-3')

Chain E:



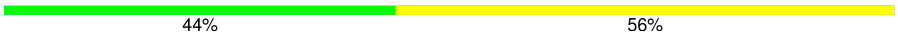
• Molecule 2: DNA (5'-D(*CP*GP*CP*(CTG)P*GP*AP*AP*TP*GP*AP*CP*AP*GP*CP*C P*GP*CP*G)-3')

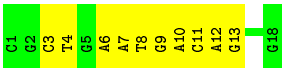
Chain G:



• Molecule 2: DNA (5'-D(*CP*GP*CP*(CTG)P*GP*AP*AP*TP*GP*AP*CP*AP*GP*CP*C P*GP*CP*G)-3')

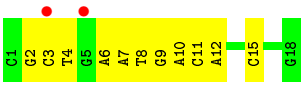
Chain I:





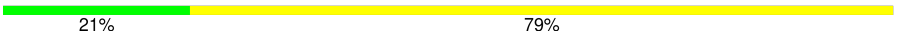
• Molecule 2: DNA (5'-D(*CP*GP*CP*(CTG)P*GP*AP*AP*TP*GP*AP*CP*AP*GP*CP*C P*GP*CP*G)-3')

Chain K:



• Molecule 3: DNA (5'-D(*GP*CP*GP*GP*CP*TP*GP*TP*CP*AP*TP*TP*CP*A)-3')

Chain F:

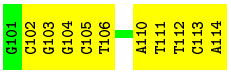


• Molecule 3: DNA (5'-D(*GP*CP*GP*GP*CP*TP*GP*TP*CP*AP*TP*TP*CP*A)-3')

Chain H:

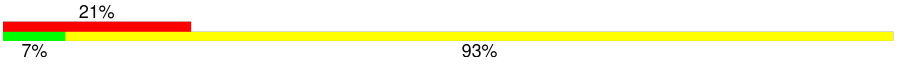
• Molecule 3: DNA (5'-D(*GP*CP*GP*GP*CP*TP*GP*TP*CP*AP*TP*TP*CP*A)-3')

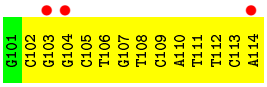
Chain J:



• Molecule 3: DNA (5'-D(*GP*CP*GP*GP*CP*TP*GP*TP*CP*AP*TP*TP*CP*A)-3')

Chain L:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	133.53Å 123.44Å 164.29Å 90.00° 96.84° 90.00°	Depositor
Resolution (Å)	50.00 – 2.65 45.00 – 2.65	Depositor EDS
% Data completeness (in resolution range)	91.5 (50.00-2.65) 96.4 (45.00-2.65)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.87 (at 2.65Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.224 , 0.276 0.227 , 0.276	Depositor DCC
R_{free} test set	13763 reflections (10.49%)	DCC
Wilson B-factor (Å^2)	48.7	Xtriage
Anisotropy	0.140	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 62.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 290748 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	32166	wwPDB-VP
Average B, all atoms (Å^2)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.66% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CTG, SO4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.41	0/7523	0.62	0/10175
1	B	0.40	0/7475	0.59	0/10121
1	C	0.42	0/7511	0.62	0/10154
1	D	0.33	0/7275	0.56	0/9887
2	E	0.35	0/389	0.72	0/596
2	G	0.47	0/389	0.74	0/596
2	I	0.57	0/389	0.83	0/596
2	K	0.27	0/389	0.65	0/596
3	F	0.27	0/312	0.72	0/478
3	H	0.36	0/312	0.73	0/478
3	J	0.50	0/312	0.80	0/478
3	L	0.26	0/312	0.65	0/478
All	All	0.39	0/32588	0.61	0/44633

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7342	0	7193	401	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	7294	0	7096	374	0
1	C	7332	0	7212	295	0
1	D	7097	0	6752	404	0
2	E	369	0	204	29	0
2	G	369	0	204	31	0
2	I	369	0	204	20	0
2	K	369	0	204	19	0
3	F	280	0	154	25	0
3	H	280	0	154	22	0
3	J	280	0	154	19	0
3	L	280	0	154	14	0
4	C	5	0	0	0	0
5	A	111	0	0	14	0
5	B	129	0	0	11	0
5	C	178	0	0	15	0
5	D	33	0	0	3	0
5	E	5	0	0	0	0
5	F	4	0	0	3	0
5	G	11	0	0	0	0
5	H	4	0	0	1	0
5	I	13	0	0	0	0
5	J	7	0	0	0	0
5	K	3	0	0	1	0
5	L	2	0	0	0	0
All	All	32166	0	29685	1633	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 27.

All (1633) 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:B:85:MET:HE2	1:B:87:ASP:H	1.09	1.15
3:L:104:DG:H2"	3:L:105:DC:H5"	1.19	1.14
1:B:309:ILE:HA	1:B:312:LEU:HB2	1.31	1.11
3:J:104:DG:H2"	3:J:105:DC:H5"	1.22	1.11
2:K:10:DA:H2"	2:K:11:DC:H5"	1.20	1.08
1:D:514:LEU:HD21	1:D:532:LYS:HG3	1.33	1.06
1:A:833:LEU:HD21	1:A:866:MET:HB2	1.40	1.03
3:J:104:DG:C2'	3:J:105:DC:H5"	1.88	1.02
1:D:495:ASN:HD21	1:D:521:ASP:HA	1.21	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:806:ARG:HH11	1:A:844:LYS:HE3	1.26	1.00
1:B:347:MET:HE1	1:B:562:LEU:HD11	1.43	0.98
1:D:541:MET:HA	1:D:544:ARG:HD3	1.44	0.98
1:C:482:ARG:NH1	1:C:556:GLN:HE21	1.60	0.97
1:C:41:CYS:HB3	1:C:58:THR:HG22	1.43	0.97
1:C:392:PRO:O	1:C:587:THR:HG21	1.65	0.96
1:A:384:ARG:HD3	1:A:385:SER:H	1.27	0.96
1:A:153:ASN:ND2	1:A:158:ASN:HD22	1.62	0.96
1:B:171:GLN:HE21	1:B:177:GLU:HG2	1.31	0.95
1:C:855:THR:HG22	1:C:857:LEU:H	1.31	0.95
1:D:509:SER:HB3	1:D:532:LYS:O	1.66	0.95
1:A:72:ILE:O	1:A:76:GLU:HG3	1.66	0.95
1:A:785:ALA:HB1	1:A:788:ILE:HD11	1.48	0.95
2:E:14:DC:H2"	2:E:15:DC:H5'	1.50	0.94
3:L:104:DG:C2'	3:L:105:DC:H5"	1.98	0.94
1:B:164:ILE:H	1:B:164:ILE:HD13	1.30	0.94
2:K:10:DA:C2'	2:K:11:DC:H5"	1.97	0.93
1:D:80:LEU:H	1:D:80:LEU:HD22	1.36	0.91
1:B:642:ARG:H	1:B:646:HIS:HD2	1.07	0.91
1:C:163:SER:HB3	1:C:318:GLN:HE22	1.31	0.91
3:F:103:DG:H2"	3:F:104:DG:H5'	1.51	0.90
1:D:511:ASP:HA	1:D:533:LEU:HD11	1.53	0.90
2:K:8:DT:H2"	2:K:9:DG:H5'	1.52	0.90
2:I:10:DA:H2"	2:I:11:DC:H5'	1.54	0.89
1:A:153:ASN:HD22	1:A:158:ASN:HD22	0.91	0.89
1:D:811:TYR:OH	1:D:822:PRO:HG2	1.73	0.88
1:B:82:ALA:H	1:B:382:GLN:HE21	1.22	0.87
3:J:110:DA:H2"	3:J:111:DT:H5'	1.57	0.87
1:B:642:ARG:H	1:B:646:HIS:CD2	1.93	0.87
1:A:347:MET:HB2	1:A:558:ASN:HD21	1.38	0.87
1:B:303:LEU:HD12	1:B:323:TYR:HA	1.56	0.86
1:A:835:LEU:HD23	1:A:866:MET:HA	1.58	0.86
1:A:153:ASN:HD22	1:A:158:ASN:ND2	1.74	0.86
1:C:572:ASN:ND2	1:C:574:TRP:H	1.71	0.86
1:C:482:ARG:NH1	1:C:560:LYS:HB2	1.91	0.85
1:C:152:LEU:HD11	1:C:190:PRO:HB2	1.57	0.85
1:D:516:VAL:HG11	1:D:522:PHE:HE1	1.41	0.85
1:C:572:ASN:HD22	1:C:574:TRP:H	1.22	0.85
1:B:166:ILE:H	1:B:166:ILE:HD12	1.38	0.85
2:K:10:DA:H2"	2:K:11:DC:C5'	2.06	0.85
1:C:303:LEU:HG	1:C:326:ILE:HD12	1.57	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:660:GLU:HB2	1:C:661:PRO:HD3	1.59	0.84
1:D:532:LYS:HA	1:D:532:LYS:HE2	1.57	0.84
1:A:451:SER:HB2	5:A:921:HOH:O	1.77	0.84
1:D:686:GLU:HG3	1:D:715:MET:CE	2.08	0.84
1:D:542:LEU:HD11	1:D:546:GLN:NE2	1.92	0.83
1:A:384:ARG:HD3	1:A:385:SER:N	1.94	0.83
3:F:110:DA:H2"	3:F:111:DT:H5'	1.58	0.83
1:D:514:LEU:H	1:D:544:ARG:HH22	1.22	0.83
1:D:163:SER:HB3	1:D:318:GLN:HE22	1.43	0.83
1:A:788:ILE:HD12	1:A:826:GLU:HB2	1.61	0.83
1:B:825:VAL:HB	1:B:828:GLU:HG3	1.60	0.83
3:J:112:DT:H2"	3:J:113:DC:H5"	1.59	0.82
2:E:8:DT:H2'	2:E:9:DG:C8	2.15	0.82
1:A:805:ILE:HA	1:A:808:ILE:HD12	1.61	0.82
1:B:482:ARG:NH2	1:B:560:LYS:HD2	1.95	0.82
1:D:535:ALA:HB1	1:D:539:ASN:ND2	1.94	0.82
1:A:506:PRO:HB2	1:A:535:ALA:HB2	1.61	0.81
2:G:4:CTG:H6	2:G:4:CTG:H5'	1.62	0.81
1:D:738:PRO:HB3	1:D:780:ALA:O	1.80	0.81
1:A:73:LYS:HE3	1:A:73:LYS:HA	1.61	0.81
1:D:493:GLN:HA	1:D:549:GLU:OE1	1.81	0.80
1:A:822:PRO:HD2	1:A:855:THR:HB	1.63	0.80
1:A:776:TYR:OH	1:A:853:GLU:HG3	1.82	0.80
1:C:308:PRO:HG2	1:C:311:LYS:HG2	1.64	0.80
1:A:738:PRO:HB3	1:A:779:ILE:O	1.81	0.80
3:J:105:DC:H2'	3:J:106:DT:H71	1.63	0.79
3:H:113:DC:H2"	3:H:114:DA:H5"	1.64	0.79
1:D:686:GLU:HG3	1:D:715:MET:HE1	1.65	0.79
1:A:112:ASN:HB2	5:A:928:HOH:O	1.82	0.79
1:A:660:GLU:HB2	1:A:661:PRO:HD3	1.65	0.79
1:A:34:LYS:HG3	1:A:62:PHE:O	1.82	0.79
1:A:825:VAL:HG23	1:A:828:GLU:HG3	1.63	0.78
1:B:119:SER:HB2	1:B:124:PRO:HG3	1.64	0.78
1:A:783:SER:HA	3:F:111:DT:OP1	1.83	0.78
1:D:336:ALA:HA	1:D:339:GLN:HE21	1.48	0.78
1:D:255:ASN:ND2	1:D:256:MET:H	1.82	0.77
1:A:224:PRO:HA	1:A:263:ILE:HD12	1.63	0.77
1:C:542:LEU:O	1:C:546:GLN:HG3	1.83	0.77
1:A:482:ARG:HE	1:A:556:GLN:NE2	1.82	0.77
1:D:495:ASN:ND2	1:D:521:ASP:HA	1.98	0.77
1:A:734:LYS:HG2	1:A:736:SER:OG	1.85	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:818:ASN:HD21	1:B:857:LEU:CD1	1.98	0.77
1:B:82:ALA:H	1:B:382:GLN:NE2	1.83	0.77
1:D:286:PRO:O	1:D:829:LYS:HD2	1.84	0.76
2:E:10:DA:H2"	2:E:11:DC:C5'	2.15	0.76
1:C:167:ALA:HA	1:C:176:ASP:HB2	1.67	0.76
1:C:711:ASN:HD21	1:C:754:GLN:HE21	1.30	0.76
1:B:159:VAL:HG21	1:B:317:HIS:CD2	2.20	0.76
1:D:303:LEU:HG	1:D:326:ILE:HD12	1.67	0.76
1:A:642:ARG:H	1:A:646:HIS:HD2	1.33	0.76
1:D:493:GLN:HA	1:D:549:GLU:CD	2.05	0.76
1:A:736:SER:HA	1:A:782:VAL:HB	1.67	0.76
1:C:482:ARG:HH12	1:C:556:GLN:HE21	1.30	0.76
1:D:109:ARG:HB3	1:D:211:VAL:HG23	1.67	0.76
2:G:8:DT:H2'	2:G:9:DG:C8	2.21	0.76
1:B:109:ARG:HH21	1:B:208:LYS:HG2	1.51	0.75
1:C:797:PRO:HG3	1:C:806:ARG:NH1	2.02	0.75
1:A:712:VAL:HG22	1:A:724:LYS:O	1.86	0.75
1:D:180:SER:O	1:D:183:ILE:HG22	1.85	0.75
1:D:260:ARG:HG2	1:D:261:GLU:N	2.01	0.75
2:G:4:CTG:O6	2:G:4:CTG:H2'	1.86	0.75
1:D:66:ARG:O	1:D:70:GLN:HG2	1.87	0.75
1:D:8:VAL:HG11	1:D:93:LEU:HD11	1.66	0.75
1:B:117:VAL:HG22	1:B:133:ILE:HA	1.68	0.75
1:C:73:LYS:NZ	1:C:73:LYS:HB3	2.02	0.75
1:D:426:SER:HB2	1:D:472:PRO:HD3	1.68	0.75
1:A:241:ARG:HH11	1:A:241:ARG:HG3	1.52	0.74
3:J:112:DT:H2"	3:J:113:DC:C5'	2.16	0.74
1:B:896:SER:HB2	1:B:899:ASP:OD1	1.87	0.74
1:B:229:ARG:O	1:B:233:ILE:HD13	1.86	0.74
1:D:391:TYR:HB2	1:D:392:PRO:HD2	1.69	0.74
1:A:194:GLU:OE1	1:A:229:ARG:HD2	1.88	0.74
1:C:231:LYS:HG3	1:C:236:GLU:HA	1.69	0.74
1:C:241:ARG:HG2	1:C:246:ARG:NE	2.03	0.74
1:D:514:LEU:CD2	1:D:532:LYS:HG3	2.13	0.74
1:B:164:ILE:N	1:B:164:ILE:HD13	2.02	0.74
3:J:104:DG:H2"	3:J:105:DC:C5'	2.10	0.73
2:E:6:DA:H2"	2:E:7:DA:H5'	1.70	0.73
1:C:236:GLU:HG2	1:C:240:LYS:HD2	1.71	0.73
3:L:113:DC:H2"	3:L:114:DA:O4'	1.87	0.73
2:E:10:DA:H2"	2:E:11:DC:H5"	1.69	0.73
1:D:223:ILE:HB	1:D:224:PRO:HD3	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:642:ARG:H	1:A:646:HIS:CD2	2.07	0.73
1:A:555:ALA:HB1	1:A:559:ARG:HH12	1.53	0.73
1:B:403:ARG:HH11	1:B:403:ARG:HB3	1.53	0.73
1:C:159:VAL:HG21	1:C:317:HIS:CD2	2.24	0.73
1:D:736:SER:HA	1:D:782:VAL:HB	1.69	0.72
1:B:771:PHE:CE2	1:B:872:LEU:HB2	2.24	0.72
1:A:110:VAL:HG22	1:A:212:ILE:HB	1.71	0.72
2:I:6:DA:H2"	2:I:7:DA:H5'	1.71	0.72
1:D:118:THR:OG1	1:D:313:ARG:HG3	1.89	0.72
3:J:104:DG:C3'	3:J:105:DC:H5"	2.19	0.72
1:B:728:MET:HG3	3:H:113:DC:H5'	1.72	0.72
1:B:164:ILE:H	1:B:164:ILE:CD1	2.02	0.72
1:A:33:TYR:HB3	1:A:65:MET:HE2	1.71	0.72
3:F:110:DA:H2"	3:F:111:DT:C5'	2.19	0.72
1:C:116:GLU:HB2	1:C:135:ALA:HB3	1.70	0.71
1:D:738:PRO:HG2	1:D:741:VAL:HB	1.72	0.71
1:B:491:ALA:HA	1:B:494:ARG:HG2	1.71	0.71
1:A:231:LYS:HG3	1:A:236:GLU:HA	1.70	0.71
2:G:11:DC:H2"	2:G:12:DA:H5'	1.71	0.71
3:H:110:DA:H2"	3:H:111:DT:H5'	1.72	0.71
1:A:778:SER:O	1:A:779:ILE:HD13	1.89	0.71
1:D:364:THR:O	1:D:368:ILE:HG13	1.90	0.71
1:A:642:ARG:NH1	1:A:642:ARG:HB2	2.06	0.71
1:C:38:PHE:CE2	1:C:59:ARG:HG3	2.25	0.71
1:D:490:LEU:HD23	5:D:939:HOH:O	1.90	0.71
1:D:137:THR:HB	1:D:328:VAL:HG21	1.72	0.71
1:B:606:ASN:HD21	1:B:614:GLU:H	1.37	0.70
1:D:660:GLU:HB2	1:D:661:PRO:HD3	1.72	0.70
1:B:505:ASN:N	1:B:506:PRO:HD3	2.05	0.70
1:B:303:LEU:HG	1:B:326:ILE:HG13	1.73	0.70
1:D:109:ARG:HD2	1:D:209:THR:O	1.92	0.70
1:B:815:ILE:O	1:B:818:ASN:HB2	1.91	0.70
1:A:308:PRO:HG2	1:A:311:LYS:HG2	1.74	0.70
1:A:806:ARG:HH11	1:A:844:LYS:CE	2.03	0.70
1:C:104:ASP:OD2	1:C:106:THR:HB	1.92	0.70
2:G:6:DA:H2"	2:G:7:DA:C5'	2.22	0.70
1:A:449:ARG:HH12	1:A:452:ASP:HB3	1.57	0.70
1:D:291:ASP:OD1	1:D:301:GLY:HA3	1.92	0.70
2:E:13:DG:H2"	2:E:14:DC:C5'	2.22	0.69
1:D:111:ALA:HB3	1:D:210:PRO:HB3	1.72	0.69
3:F:104:DG:H5"	5:F:256:HOH:O	1.91	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:10:DA:H2"	2:I:11:DC:C5'	2.23	0.69
1:D:109:ARG:CZ	1:D:142:ILE:HD12	2.22	0.69
1:D:841:PHE:CZ	1:D:862:VAL:HG22	2.28	0.69
3:F:113:DC:H5	5:F:475:HOH:O	1.76	0.69
1:A:412:LEU:HG	1:A:683:MET:HG2	1.73	0.69
2:K:11:DC:H2"	2:K:12:DA:H5'	1.75	0.69
1:B:403:ARG:HH11	1:B:403:ARG:CB	2.06	0.69
1:D:80:LEU:H	1:D:80:LEU:CD2	2.06	0.69
2:G:10:DA:H2"	2:G:11:DC:O5'	1.90	0.69
1:B:133:ILE:HD12	1:B:198:LEU:HD21	1.75	0.69
1:A:236:GLU:HG2	1:A:240:LYS:HE2	1.74	0.68
1:C:427:PRO:HD3	5:C:959:HOH:O	1.93	0.68
1:A:422:GLN:NE2	1:A:680:LEU:H	1.90	0.68
1:A:780:ALA:HB3	1:A:831:TYR:HD1	1.58	0.68
1:C:302:LYS:HB3	5:C:1077:HOH:O	1.92	0.68
1:B:750:ARG:HH11	1:B:754:GLN:NE2	1.90	0.68
1:A:376:GLN:HE21	1:A:378:LYS:HD2	1.58	0.68
1:B:732:THR:HG23	1:B:733:GLN:NE2	2.08	0.68
1:D:542:LEU:HD11	1:D:546:GLN:HE21	1.57	0.68
1:C:62:PHE:CE2	1:C:68:ALA:HA	2.28	0.68
1:C:202:LEU:O	1:C:206:GLN:HG2	1.93	0.68
1:A:708:TYR:CZ	1:A:728:MET:HG3	2.28	0.68
1:D:579:ASP:HB3	1:D:582:ASN:HB2	1.74	0.68
1:C:403:ARG:NH2	1:C:889:LEU:HD23	2.08	0.68
1:A:41:CYS:HB2	1:A:42:PRO:HD2	1.74	0.68
1:C:41:CYS:HB3	1:C:58:THR:CG2	2.22	0.68
2:K:15:DC:H2'	5:K:269:HOH:O	1.93	0.68
1:D:336:ALA:HA	1:D:339:GLN:NE2	2.08	0.68
1:B:85:MET:CE	1:B:87:ASP:H	1.99	0.68
1:D:731:GLU:HA	1:D:734:LYS:CG	2.24	0.68
1:D:51:ASP:HB2	5:D:910:HOH:O	1.94	0.68
1:A:514:LEU:H	1:A:541:MET:CE	2.07	0.68
1:B:745:LEU:O	1:B:749:ILE:HG13	1.94	0.67
1:C:711:ASN:ND2	1:C:754:GLN:HE21	1.91	0.67
2:I:4:CTG:O6	2:I:4:CTG:H2'	1.93	0.67
1:D:288:TYR:HA	1:D:293:ILE:HD11	1.75	0.67
1:A:511:ASP:OD2	1:A:533:LEU:HA	1.95	0.67
1:C:218:VAL:HG22	1:C:223:ILE:HG13	1.75	0.67
1:A:392:PRO:O	1:A:587:THR:HG21	1.95	0.67
1:A:514:LEU:HG	1:A:526:ILE:HG23	1.76	0.67
1:C:686:GLU:HG3	1:C:715:MET:CE	2.25	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:534:SER:O	1:D:538:LEU:HD13	1.93	0.67
1:B:145:ARG:HD3	1:B:185:LYS:O	1.94	0.67
3:J:110:DA:H1'	3:J:111:DT:H5"	1.78	0.66
1:D:284:ASN:HD22	1:D:285:GLN:N	1.93	0.66
1:D:373:LEU:HD12	1:D:380:ILE:HG22	1.76	0.66
1:A:824:VAL:O	1:A:825:VAL:HG13	1.95	0.66
1:B:506:PRO:HB3	1:B:536:LYS:HG2	1.78	0.66
1:C:482:ARG:HH12	1:C:556:GLN:NE2	1.93	0.66
1:D:546:GLN:O	1:D:550:VAL:HG23	1.95	0.66
2:E:6:DA:H2"	2:E:7:DA:C5'	2.24	0.66
1:A:362:ILE:HD11	1:A:572:ASN:HD22	1.60	0.66
1:D:116:GLU:HB2	1:D:135:ALA:HB3	1.77	0.66
1:D:858:ILE:O	1:D:862:VAL:HG23	1.94	0.66
1:B:223:ILE:HB	1:B:224:PRO:HD3	1.76	0.66
1:D:148:VAL:HG21	1:D:325:ILE:HD11	1.77	0.66
3:F:110:DA:H1'	3:F:111:DT:H5"	1.78	0.66
1:B:512:GLU:O	1:B:514:LEU:HD22	1.96	0.66
1:C:482:ARG:CZ	1:C:556:GLN:HE21	2.08	0.66
1:D:686:GLU:HG3	1:D:715:MET:HE3	1.78	0.66
1:A:568:GLY:HA3	2:E:3:DC:O2	1.95	0.66
1:B:894:LYS:HB2	1:B:894:LYS:NZ	2.10	0.66
1:C:818:ASN:HD22	1:C:821:ALA:HB2	1.61	0.66
1:D:514:LEU:HD21	1:D:532:LYS:CG	2.18	0.65
1:A:693:LEU:HD12	1:A:694:GLY:N	2.11	0.65
3:F:104:DG:H2"	3:F:105:DC:O5'	1.96	0.65
1:D:546:GLN:HG2	1:D:549:GLU:OE1	1.96	0.65
3:H:110:DA:H2"	3:H:111:DT:C5'	2.25	0.65
1:B:732:THR:HG23	1:B:733:GLN:HE21	1.59	0.65
1:B:482:ARG:CZ	1:B:560:LYS:HD2	2.25	0.65
1:C:524:ASP:HA	1:C:527:LYS:HE2	1.77	0.65
1:C:9:GLU:OE2	1:C:266:PHE:HA	1.96	0.65
1:A:514:LEU:HD11	1:A:529:LYS:NZ	2.11	0.65
1:C:194:GLU:HB3	5:C:969:HOH:O	1.94	0.65
1:B:386:HIS:HB2	1:B:573:VAL:CG2	2.27	0.65
1:C:439:LEU:HD12	1:C:443:ILE:HD11	1.77	0.65
1:B:875:THR:O	1:B:879:PRO:HG3	1.97	0.65
1:C:301:GLY:O	1:C:330:ARG:NH1	2.30	0.65
1:D:505:ASN:N	1:D:506:PRO:HD3	2.11	0.65
1:C:19:TYR:CE1	1:C:27:ARG:HB2	2.32	0.65
1:A:785:ALA:CB	1:A:788:ILE:HD11	2.26	0.65
1:B:85:MET:HE2	1:B:87:ASP:N	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:ASN:ND2	1:A:257:TYR:HD1	1.94	0.65
1:A:482:ARG:HE	1:A:556:GLN:HE22	1.45	0.65
1:C:216:TRP:O	1:C:217:ASN:HB2	1.97	0.65
1:D:515:ASP:O	1:D:516:VAL:HG23	1.97	0.64
2:G:16:DG:H2"	2:G:17:DC:C5'	2.27	0.64
2:K:2:DG:H3'	2:K:3:DC:C5'	2.26	0.64
1:D:535:ALA:HB1	1:D:539:ASN:HD21	1.61	0.64
2:G:6:DA:H2"	2:G:7:DA:H5'	1.79	0.64
1:D:38:PHE:HB2	1:D:83:LEU:HB2	1.77	0.64
1:C:298:LEU:O	1:C:299:ASN:HB2	1.98	0.64
1:D:326:ILE:O	1:D:330:ARG:HG2	1.96	0.64
1:C:881:GLU:HA	1:C:884:THR:OG1	1.98	0.64
1:B:790:LYS:HE3	1:B:791:TYR:CE1	2.32	0.64
1:B:534:SER:OG	1:B:537:SER:HB2	1.98	0.64
2:E:13:DG:H2"	2:E:14:DC:H5'	1.78	0.64
1:B:702:TRP:CD1	1:B:708:TYR:HB3	2.33	0.64
1:A:347:MET:HG2	1:A:358:VAL:HG23	1.79	0.64
1:A:395:PHE:HB2	1:A:591:GLN:HG2	1.78	0.64
1:A:643:ASP:HA	1:A:693:LEU:HD23	1.79	0.64
1:C:822:PRO:HD2	1:C:855:THR:OG1	1.98	0.64
1:A:708:TYR:CE2	1:A:728:MET:HG3	2.33	0.64
1:D:87:ASP:CG	1:D:90:LEU:HD13	2.18	0.64
2:E:11:DC:H2"	2:E:12:DA:H5'	1.79	0.64
1:C:27:ARG:HE	1:C:27:ARG:HA	1.62	0.64
3:H:112:DT:H6	3:H:112:DT:H5'	1.63	0.64
1:A:734:LYS:HB3	1:A:737:THR:OG1	1.98	0.63
1:D:182:ILE:O	1:D:186:ILE:HG13	1.98	0.63
1:D:491:ALA:O	1:D:495:ASN:ND2	2.31	0.63
1:B:386:HIS:HB2	1:B:573:VAL:HG22	1.79	0.63
1:D:837:GLU:OE1	1:D:837:GLU:HA	1.98	0.63
1:B:512:GLU:N	1:B:513:PRO:HD3	2.14	0.63
1:A:489:MET:HE3	1:A:553:MET:SD	2.38	0.63
1:A:119:SER:HB2	1:A:131:HIS:CD2	2.32	0.63
1:A:60:LYS:HE3	5:A:966:HOH:O	1.98	0.63
3:J:110:DA:H2"	3:J:111:DT:C5'	2.27	0.63
1:C:303:LEU:CG	1:C:326:ILE:HD12	2.28	0.63
1:A:602:ASN:HD21	1:A:617:VAL:H	1.46	0.63
1:B:486:LYS:HA	1:B:556:GLN:NE2	2.14	0.63
1:A:554:THR:O	1:A:558:ASN:HB2	1.99	0.63
1:D:114:ASP:HB3	1:D:328:VAL:HG22	1.79	0.63
1:A:362:ILE:CD1	1:A:572:ASN:HD22	2.10	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:503:LEU:O	1:D:503:LEU:HD23	1.99	0.63
1:A:203:ASN:O	1:A:207:GLN:HG2	1.98	0.63
1:A:556:GLN:OE1	1:A:557:ILE:HG13	1.99	0.63
1:A:693:LEU:HD12	1:A:694:GLY:H	1.63	0.63
1:B:440:HIS:HB3	5:B:1007:HOH:O	1.98	0.63
1:A:221:PHE:O	1:A:224:PRO:HD2	1.99	0.62
1:A:641:PHE:HA	1:A:646:HIS:CD2	2.33	0.62
1:C:686:GLU:OE1	1:C:716:GLU:HG2	1.99	0.62
1:D:478:VAL:HG13	1:D:559:ARG:HG3	1.80	0.62
1:A:68:ALA:O	1:A:72:ILE:HG13	1.98	0.62
1:B:494:ARG:HG3	1:B:495:ASN:N	2.14	0.62
1:D:255:ASN:HD22	1:D:256:MET:H	1.45	0.62
1:A:744:ALA:HB2	1:A:767:PHE:CE2	2.34	0.62
1:B:522:PHE:HD1	1:B:522:PHE:H	1.46	0.62
1:B:893:LYS:C	1:B:894:LYS:HG3	2.18	0.62
1:B:403:ARG:NH1	1:B:887:ALA:O	2.33	0.62
1:D:422:GLN:HG3	1:D:678:GLN:O	2.00	0.62
1:D:144:ASP:O	1:D:185:LYS:HD3	2.00	0.62
1:D:61:LEU:HD23	1:D:62:PHE:N	2.15	0.62
1:A:362:ILE:HG12	1:A:572:ASN:ND2	2.15	0.62
1:D:805:ILE:HA	1:D:808:ILE:HD12	1.81	0.62
1:B:727:ILE:HB	1:B:733:GLN:NE2	2.14	0.62
1:A:785:ALA:HB1	1:A:788:ILE:CD1	2.28	0.62
1:B:166:ILE:H	1:B:166:ILE:CD1	2.12	0.62
1:B:728:MET:HE3	3:H:113:DC:OP1	2.00	0.62
1:B:752:MET:HG2	1:B:760:LEU:HD22	1.80	0.62
1:A:854:ILE:CD1	1:A:862:VAL:HG21	2.30	0.61
1:D:361:PRO:HD2	2:K:3:DC:O5'	2.00	0.61
1:C:597:ILE:HD11	1:C:663:ILE:HG23	1.80	0.61
1:A:707:ARG:NH2	1:A:731:GLU:OE1	2.34	0.61
1:A:514:LEU:H	1:A:541:MET:HE2	1.66	0.61
1:C:148:VAL:HG21	1:C:325:ILE:HD11	1.82	0.61
3:F:108:DT:H2"	3:F:109:DC:O5'	2.01	0.61
1:B:166:ILE:N	1:B:166:ILE:HD12	2.13	0.61
2:E:7:DA:H2'	2:E:8:DT:H72	1.82	0.61
1:A:642:ARG:HH11	1:A:642:ARG:HB2	1.65	0.61
1:C:46:ALA:O	1:C:47:THR:HG23	2.00	0.61
1:D:511:ASP:HA	1:D:533:LEU:CD1	2.30	0.61
1:D:412:LEU:HB2	1:D:623:ASP:HB2	1.83	0.61
1:A:855:THR:HG23	1:A:858:ILE:HG12	1.83	0.61
1:B:818:ASN:HD21	1:B:857:LEU:HD12	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:18:DG:OP1	2:E:18:DG:H3'	2.01	0.61
1:A:631:LYS:NZ	1:A:631:LYS:H	1.97	0.61
1:C:231:LYS:HG3	1:C:236:GLU:CA	2.31	0.61
1:D:554:THR:O	1:D:558:ASN:HB2	2.01	0.61
1:B:749:ILE:O	1:B:753:LEU:HG	2.01	0.60
1:C:471:VAL:HB	1:C:472:PRO:HD3	1.83	0.60
1:B:498:ILE:HD12	1:B:498:ILE:N	2.16	0.60
1:B:109:ARG:NH2	1:B:208:LYS:HG2	2.16	0.60
1:D:731:GLU:HA	1:D:734:LYS:HG2	1.82	0.60
1:D:804:HIS:O	1:D:808:ILE:HG13	2.02	0.60
1:C:130:LYS:HG3	1:C:131:HIS:CE1	2.37	0.60
1:B:668:ARG:O	1:B:672:GLU:HG3	2.01	0.60
1:A:685:ARG:NH2	1:A:714:ASP:OD2	2.34	0.60
1:B:821:ALA:HB1	1:B:822:PRO:HD2	1.82	0.60
3:F:113:DC:H2"	3:F:114:DA:H5"	1.83	0.60
1:D:328:VAL:O	1:D:332:LEU:HD13	2.01	0.60
1:B:777:ILE:CD1	1:B:853:GLU:HG2	2.32	0.60
1:B:182:ILE:O	1:B:186:ILE:HG13	2.02	0.60
1:C:149:PHE:O	1:C:197:LEU:HD11	2.00	0.60
1:D:757:GLU:O	1:D:761:GLN:HG3	2.01	0.60
1:A:478:VAL:HG13	1:A:559:ARG:HD2	1.84	0.60
1:C:180:SER:O	1:C:183:ILE:HG22	2.02	0.60
1:A:153:ASN:HB3	1:A:158:ASN:ND2	2.16	0.60
2:E:10:DA:C2'	2:E:11:DC:H5"	2.32	0.60
1:D:788:ILE:O	1:D:792:ASP:HB2	2.02	0.60
1:D:645:ASN:ND2	1:D:719:ARG:HH11	1.98	0.60
1:A:844:LYS:HD2	1:A:844:LYS:H	1.66	0.60
1:B:163:SER:HB3	1:B:166:ILE:HD13	1.83	0.60
1:B:233:ILE:HD12	1:B:233:ILE:N	2.17	0.60
1:C:223:ILE:HB	1:C:224:PRO:HD3	1.84	0.60
1:B:179:PRO:HG2	1:B:329:TYR:CD2	2.36	0.60
1:C:455:SER:OG	1:C:676:ASN:HA	2.02	0.60
1:D:150:ASP:OD1	1:D:321:ILE:HD11	2.02	0.60
1:C:182:ILE:O	1:C:186:ILE:HG13	2.02	0.60
1:B:706:LYS:HD3	3:H:113:DC:H1'	1.83	0.59
1:D:442:TYR:HB3	1:D:592:MET:CE	2.31	0.59
1:B:808:ILE:HD13	1:B:824:VAL:HG11	1.82	0.59
1:B:858:ILE:O	1:B:862:VAL:HG23	2.01	0.59
1:D:218:VAL:HA	1:D:222:ALA:HB3	1.84	0.59
1:C:284:ASN:HD22	1:C:285:GLN:N	2.01	0.59
1:C:109:ARG:HD2	1:C:209:THR:O	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:10:DA:H1'	2:I:11:DC:H5"	1.84	0.59
1:B:403:ARG:HH22	1:B:889:LEU:HD21	1.66	0.59
1:A:255:ASN:HD22	1:A:257:TYR:HD1	1.49	0.59
1:C:130:LYS:HG3	1:C:131:HIS:ND1	2.17	0.59
1:B:508:LEU:HG	1:B:509:SER:H	1.67	0.59
1:A:771:PHE:HA	1:A:774:LEU:HD12	1.83	0.59
1:D:504:HIS:C	1:D:506:PRO:HD3	2.22	0.59
1:B:777:ILE:HD11	1:B:853:GLU:HG2	1.84	0.59
3:F:105:DC:H2"	3:F:106:DT:O5'	2.02	0.59
1:D:218:VAL:HG22	1:D:223:ILE:HG13	1.83	0.59
2:I:8:DT:H2'	2:I:9:DG:C8	2.36	0.59
1:A:97:TYR:O	1:A:352:LYS:HE2	2.02	0.59
2:E:10:DA:H2"	2:E:11:DC:H5'	1.84	0.59
1:A:641:PHE:HA	1:A:646:HIS:HD2	1.67	0.59
1:B:599:ARG:HH11	1:B:599:ARG:HG2	1.67	0.59
1:C:482:ARG:NH1	1:C:556:GLN:NE2	2.41	0.59
2:E:2:DG:H3'	2:E:3:DC:C5'	2.32	0.59
3:J:102:DC:H2"	3:J:103:DG:OP2	2.01	0.59
1:D:305:TYR:OH	1:D:309:ILE:HG12	2.02	0.59
1:C:461:MET:SD	1:C:581:ARG:HD2	2.43	0.59
1:D:71:TRP:O	1:D:75:MET:HG2	2.03	0.59
1:D:197:LEU:O	1:D:197:LEU:HD23	2.03	0.59
1:A:17:GLU:OE1	1:A:97:TYR:OH	2.20	0.59
1:D:797:PRO:HG3	1:D:806:ARG:HH11	1.68	0.59
1:C:38:PHE:CZ	1:C:59:ARG:HG3	2.38	0.58
1:D:862:VAL:O	1:D:866:MET:HB3	2.03	0.58
1:C:285:GLN:HE21	1:C:286:PRO:CD	2.15	0.58
1:D:807:GLY:HA2	1:D:845:CYS:O	2.03	0.58
1:C:658:ARG:NH1	5:C:978:HOH:O	2.35	0.58
1:B:786:ASN:O	1:B:826:GLU:OE1	2.22	0.58
1:C:818:ASN:ND2	1:C:857:LEU:HD11	2.19	0.58
1:D:495:ASN:HD21	1:D:521:ASP:CA	2.08	0.58
1:D:80:LEU:N	1:D:80:LEU:HD22	2.14	0.58
3:J:113:DC:H5'	3:J:113:DC:H6	1.68	0.58
3:H:105:DC:H2'	3:H:106:DT:H71	1.83	0.58
1:A:876:PHE:O	1:A:879:PRO:HG2	2.03	0.58
1:D:509:SER:CB	1:D:532:LYS:O	2.48	0.58
1:C:572:ASN:HD22	1:C:574:TRP:N	1.98	0.58
2:I:7:DA:C2'	2:I:8:DT:H72	2.33	0.58
1:C:587:THR:HG22	1:C:588:THR:N	2.18	0.58
1:D:297:GLU:OE2	1:D:337:LYS:HE3	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:LYS:HE2	1:A:173:GLN:HB3	1.85	0.58
2:I:6:DA:H2"	2:I:7:DA:C5'	2.33	0.58
1:B:894:LYS:HB2	1:B:894:LYS:HZ3	1.67	0.58
2:E:4:CTG:H2"	2:E:5:DG:OP2	2.04	0.58
1:D:442:TYR:HB3	1:D:592:MET:HE3	1.85	0.58
1:C:154:SER:C	1:C:156:TYR:H	2.05	0.58
1:D:605:LEU:HD22	1:D:632:ILE:HD11	1.86	0.58
1:A:470:VAL:O	1:A:474:GLU:HG2	2.04	0.58
1:D:529:LYS:HB3	1:D:532:LYS:HD2	1.86	0.57
1:C:818:ASN:ND2	1:C:821:ALA:HB2	2.18	0.57
1:D:159:VAL:HB	1:D:317:HIS:CD2	2.39	0.57
1:D:700:GLY:N	1:D:753:LEU:HD22	2.19	0.57
1:D:884:THR:HG21	1:D:891:TYR:HD1	1.69	0.57
1:B:231:LYS:CG	1:B:236:GLU:HA	2.34	0.57
1:C:85:MET:HA	1:C:380:ILE:HD11	1.85	0.57
1:A:285:GLN:HE21	1:A:285:GLN:HA	1.68	0.57
1:C:297:GLU:OE1	1:C:338:ARG:NH1	2.37	0.57
1:B:772:ARG:HG2	1:B:772:ARG:HH11	1.68	0.57
1:D:458:PRO:HB2	1:D:588:THR:HG22	1.85	0.57
1:D:416:TYR:HB2	1:D:417:PRO:HD3	1.86	0.57
1:A:485:HIS:C	1:A:487:GLY:H	2.06	0.57
1:A:129:ALA:HA	1:A:225:TYR:CE1	2.40	0.57
1:C:658:ARG:HH11	1:C:658:ARG:HG3	1.70	0.57
1:A:873:GLU:OE2	1:A:877:ILE:HD12	2.04	0.57
1:C:477:LYS:HG2	1:C:481:GLN:NE2	2.20	0.57
1:D:653:LYS:HE3	1:D:657:GLU:OE1	2.05	0.57
1:C:503:LEU:HD21	1:C:538:LEU:HB2	1.86	0.57
1:A:819:ILE:HG13	1:A:823:GLN:OE1	2.05	0.57
1:B:752:MET:HE3	1:B:889:LEU:HD12	1.86	0.57
1:C:83:LEU:N	1:C:83:LEU:HD22	2.19	0.57
1:B:751:ARG:HH11	1:B:759:SER:HB3	1.69	0.57
1:B:60:LYS:HE3	1:B:62:PHE:CE2	2.40	0.57
1:A:112:ASN:HD21	1:A:331:VAL:CG1	2.18	0.57
1:D:253:ILE:HD11	1:D:262:ILE:HD13	1.87	0.57
1:A:338:ARG:HB3	1:A:340:PHE:CE1	2.39	0.57
1:D:751:ARG:NH1	1:D:763:TYR:HB2	2.20	0.57
1:A:51:ASP:HB2	5:A:915:HOH:O	2.05	0.57
1:A:732:THR:CG2	1:A:745:LEU:HB3	2.35	0.57
1:B:120:PRO:HG2	1:B:156:TYR:CE2	2.40	0.57
1:C:835:LEU:HD11	1:C:846:ILE:HB	1.85	0.57
1:A:506:PRO:HB2	1:A:535:ALA:CB	2.33	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:ILE:HB	1:A:224:PRO:HD3	1.86	0.57
1:D:747:GLU:O	1:D:751:ARG:HG3	2.05	0.57
1:B:309:ILE:CA	1:B:312:LEU:HB2	2.20	0.57
1:A:806:ARG:HD3	1:A:844:LYS:HE3	1.87	0.57
1:A:777:ILE:HD11	1:A:848:TRP:HZ2	1.70	0.57
1:B:811:TYR:OH	1:B:822:PRO:HG2	2.04	0.57
1:A:542:LEU:O	1:A:546:GLN:HG2	2.05	0.57
1:A:213:LEU:HD13	1:A:223:ILE:HD11	1.85	0.57
1:A:227:TYR:CD2	1:A:263:ILE:HD13	2.40	0.57
1:A:598:GLU:HG3	1:A:617:VAL:HG11	1.85	0.57
2:E:7:DA:C2'	2:E:8:DT:H72	2.35	0.56
1:A:362:ILE:CG1	1:A:572:ASN:HD22	2.19	0.56
1:D:83:LEU:HB3	1:D:379:VAL:HG12	1.86	0.56
1:A:808:ILE:O	1:A:811:TYR:HB3	2.04	0.56
3:H:113:DC:C2'	3:H:114:DA:H5"	2.35	0.56
1:A:231:LYS:HG3	1:A:236:GLU:CA	2.35	0.56
1:D:186:ILE:HG22	1:D:187:ILE:N	2.20	0.56
1:A:139:TYR:CD2	1:A:332:LEU:HD21	2.40	0.56
1:A:839:ASN:HD22	1:A:841:PHE:HB2	1.70	0.56
1:C:855:THR:HG22	1:C:857:LEU:N	2.13	0.56
1:C:162:TRP:HB3	1:C:188:TYR:CE1	2.41	0.56
2:I:8:DT:H6	2:I:8:DT:H5"	1.70	0.56
2:G:16:DG:H2"	2:G:17:DC:H5"	1.87	0.56
1:C:81:GLU:HG2	1:C:83:LEU:HD22	1.87	0.56
1:A:631:LYS:HZ2	1:A:631:LYS:H	1.52	0.56
1:D:162:TRP:CD1	1:D:321:ILE:HB	2.40	0.56
1:A:499:ILE:HB	1:A:542:LEU:HD13	1.87	0.56
1:B:421:ARG:HG2	1:B:421:ARG:HH11	1.70	0.56
1:D:786:ASN:O	1:D:787:ASN:HB2	2.05	0.56
1:A:732:THR:HG22	1:A:745:LEU:HB3	1.86	0.56
1:C:130:LYS:HE3	1:C:131:HIS:HE1	1.71	0.56
1:C:285:GLN:HE21	1:C:286:PRO:HD2	1.70	0.56
1:C:768:GLU:HG2	1:C:872:LEU:HD21	1.88	0.56
1:D:713:TRP:CZ3	1:D:723:PRO:HD3	2.40	0.56
1:D:202:LEU:O	1:D:205:TRP:HB3	2.06	0.56
1:D:795:GLY:O	1:D:813:ARG:NH1	2.38	0.56
1:C:55:LYS:N	1:C:55:LYS:HD2	2.18	0.56
1:D:39:ALA:O	1:D:58:THR:HG22	2.05	0.56
1:D:303:LEU:CG	1:D:326:ILE:HD12	2.34	0.56
1:B:486:LYS:HA	1:B:556:GLN:HE22	1.70	0.56
1:B:271:LEU:HB3	1:B:276:LEU:HD11	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:818:ASN:HD21	1:B:857:LEU:HD13	1.70	0.56
1:A:555:ALA:HB1	1:A:559:ARG:NH1	2.20	0.56
1:B:498:ILE:H	1:B:498:ILE:HD12	1.69	0.56
1:D:3:GLU:HB2	1:D:20:ILE:O	2.06	0.56
1:D:597:ILE:O	1:D:601:VAL:HG23	2.03	0.56
1:D:348:GLY:O	1:D:352:LYS:N	2.38	0.56
1:A:811:TYR:HE1	1:A:858:ILE:HD11	1.69	0.56
1:C:238:THR:O	1:C:241:ARG:HB2	2.06	0.56
1:A:643:ASP:HB2	5:A:923:HOH:O	2.05	0.56
1:C:524:ASP:HA	1:C:527:LYS:CE	2.35	0.56
1:B:458:PRO:HG3	1:B:592:MET:SD	2.46	0.56
1:B:523:SER:O	1:B:526:ILE:HG12	2.06	0.56
1:D:402:ASN:OD1	1:D:403:ARG:N	2.32	0.56
1:A:408:MET:CE	1:A:655:ALA:HB2	2.36	0.56
1:B:446:VAL:HG22	1:B:446:VAL:O	2.06	0.56
1:D:686:GLU:HA	1:D:686:GLU:OE1	2.05	0.56
1:D:412:LEU:HD12	1:D:623:ASP:HA	1.87	0.56
1:B:494:ARG:NH1	1:B:495:ASN:HB2	2.21	0.56
1:B:808:ILE:HG22	1:B:812:ASN:ND2	2.20	0.56
1:A:643:ASP:CA	1:A:693:LEU:HD23	2.36	0.55
1:A:154:SER:HB2	1:A:155:PRO:HD2	1.88	0.55
1:C:143:ASP:OD2	1:C:208:LYS:NZ	2.39	0.55
1:A:34:LYS:HD2	1:A:63:ALA:O	2.07	0.55
1:D:471:VAL:HB	1:D:472:PRO:HD3	1.88	0.55
1:D:359:PHE:O	1:D:361:PRO:HD3	2.07	0.55
1:D:644:THR:O	1:D:648:VAL:HG23	2.07	0.55
1:A:49:TYR:CE1	1:A:59:ARG:HD3	2.40	0.55
1:C:254:GLU:HA	1:C:259:SER:HA	1.87	0.55
1:B:767:PHE:HE1	1:B:774:LEU:HD11	1.72	0.55
1:A:656:ARG:HA	1:A:660:GLU:HG3	1.87	0.55
1:A:241:ARG:NH1	5:A:985:HOH:O	2.38	0.55
1:A:555:ALA:O	1:A:559:ARG:HG2	2.06	0.55
2:G:15:DC:H6	2:G:15:DC:H5'	1.70	0.55
1:B:406:TYR:HB3	1:B:629:ALA:HB3	1.89	0.55
1:A:397:LYS:O	1:A:399:PRO:HD3	2.06	0.55
1:A:503:LEU:HD23	1:A:503:LEU:N	2.20	0.55
1:C:6:LEU:HB2	1:C:18:ARG:O	2.06	0.55
1:B:745:LEU:HD22	1:B:883:PHE:HE2	1.71	0.55
1:C:118:THR:HG23	1:C:310:SER:O	2.07	0.55
1:C:351:ALA:O	1:C:352:LYS:HB2	2.04	0.55
3:J:113:DC:H5'	3:J:113:DC:C6	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:486:LYS:O	1:D:490:LEU:HD13	2.06	0.55
3:H:104:DG:H1'	3:H:105:DC:H5"	1.89	0.55
1:A:338:ARG:HB3	1:A:340:PHE:CD1	2.42	0.55
1:D:212:ILE:HD13	1:D:269:SER:HB2	1.87	0.55
1:D:512:GLU:CB	1:D:513:PRO:HA	2.37	0.55
1:D:411:ASP:HB2	1:D:686:GLU:OE2	2.05	0.55
3:F:109:DC:H2"	3:F:110:DA:C5'	2.37	0.55
1:A:212:ILE:HD13	1:A:269:SER:HB2	1.88	0.55
1:B:494:ARG:HH11	1:B:494:ARG:HG3	1.71	0.55
1:D:489:MET:SD	1:D:553:MET:HA	2.46	0.55
1:C:600:LYS:HD2	5:C:921:HOH:O	2.06	0.55
1:A:433:THR:HG22	1:A:461:MET:HE1	1.89	0.55
1:B:748:CYS:O	1:B:752:MET:HG3	2.06	0.55
1:C:686:GLU:OE1	1:C:716:GLU:CG	2.55	0.55
1:C:686:GLU:HG3	1:C:715:MET:HE1	1.89	0.55
1:A:810:THR:HG21	1:A:845:CYS:O	2.06	0.55
1:B:541:MET:O	1:B:544:ARG:HB2	2.06	0.55
2:K:6:DA:H2"	2:K:7:DA:O5'	2.07	0.55
1:B:825:VAL:CB	1:B:828:GLU:HG3	2.34	0.55
1:B:485:HIS:HA	1:B:488:TYR:CD2	2.42	0.55
1:B:846:ILE:HD11	1:B:858:ILE:HD12	1.88	0.55
1:A:433:THR:HG22	1:A:461:MET:CE	2.37	0.55
1:A:517:ASP:OD1	1:A:519:ARG:HD3	2.07	0.55
1:A:809:LEU:C	1:A:811:TYR:H	2.10	0.55
1:B:878:LYS:C	1:B:878:LYS:HD3	2.27	0.55
1:A:162:TRP:HB3	1:A:188:TYR:CE1	2.41	0.55
1:B:361:PRO:HD2	2:G:3:DC:H5"	1.89	0.55
1:A:775:ASN:HB3	1:A:778:SER:OG	2.07	0.55
1:B:405:LYS:HA	1:B:698:ILE:O	2.07	0.55
1:B:732:THR:CG2	1:B:733:GLN:HE21	2.20	0.55
1:D:752:MET:HG2	1:D:760:LEU:HD12	1.89	0.55
1:C:495:ASN:HB3	1:C:522:PHE:CE2	2.42	0.55
1:A:668:ARG:O	1:A:672:GLU:HG3	2.06	0.55
1:C:73:LYS:HB3	1:C:73:LYS:HZ3	1.72	0.54
2:I:7:DA:H2"	2:I:8:DT:OP2	2.07	0.54
1:B:117:VAL:HG21	1:B:225:TYR:CE2	2.43	0.54
1:A:730:LEU:HD22	1:A:883:PHE:CE1	2.42	0.54
1:A:116:GLU:HB2	1:A:135:ALA:HB3	1.89	0.54
3:L:105:DC:H2'	3:L:106:DT:H72	1.90	0.54
1:B:222:ALA:O	1:B:226:VAL:HG23	2.07	0.54
1:B:604:TYR:O	1:B:607:GLU:HB3	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:105:DC:H2'	3:J:106:DT:C7	2.35	0.54
2:G:14:DC:H2"	2:G:15:DC:H5"	1.89	0.54
1:A:411:ASP:OD1	1:A:686:GLU:HG3	2.07	0.54
1:D:284:ASN:C	1:D:284:ASN:HD22	2.11	0.54
1:B:255:ASN:HD21	1:B:257:TYR:HD1	1.54	0.54
2:I:12:DA:H8	2:I:12:DA:H5"	1.73	0.54
1:D:541:MET:CA	1:D:544:ARG:HD3	2.30	0.54
1:A:703:THR:HG21	1:A:707:ARG:HH11	1.72	0.54
1:D:6:LEU:HB2	1:D:18:ARG:O	2.07	0.54
1:B:351:ALA:O	1:B:352:LYS:HB2	2.07	0.54
1:C:111:ALA:CB	1:C:210:PRO:HB3	2.38	0.54
3:H:104:DG:C2'	3:H:105:DC:H5"	2.38	0.54
1:B:148:VAL:HG21	1:B:325:ILE:HD11	1.90	0.54
1:C:393:GLY:O	1:C:587:THR:HG23	2.06	0.54
1:D:109:ARG:HD3	1:D:208:LYS:O	2.07	0.54
1:A:449:ARG:NH1	1:A:452:ASP:HB3	2.20	0.54
1:A:499:ILE:HD11	1:A:522:PHE:CZ	2.43	0.54
1:B:268:ILE:HG22	1:B:269:SER:N	2.23	0.54
1:D:541:MET:O	1:D:544:ARG:N	2.38	0.54
3:L:113:DC:H2'	3:L:114:DA:C8	2.42	0.54
2:G:16:DG:H2"	2:G:17:DC:H5'	1.90	0.54
3:H:104:DG:H2"	3:H:105:DC:C5'	2.38	0.54
1:C:112:ASN:HB2	5:C:1035:HOH:O	2.07	0.54
1:A:109:ARG:HD2	1:A:209:THR:O	2.08	0.54
1:A:850:SER:O	1:A:852:THR:HG23	2.08	0.54
1:C:162:TRP:HB3	1:C:188:TYR:CZ	2.43	0.54
1:B:421:ARG:HD2	1:B:476:THR:OG1	2.08	0.54
1:D:347:MET:SD	1:D:562:LEU:HD21	2.47	0.54
1:B:685:ARG:HG2	1:B:685:ARG:HH11	1.72	0.54
1:B:322:SER:O	1:B:326:ILE:HG12	2.08	0.54
1:B:330:ARG:O	1:B:334:ILE:HG13	2.08	0.54
1:C:660:GLU:CB	1:C:661:PRO:HD3	2.35	0.54
1:B:218:VAL:HA	1:B:222:ALA:HB3	1.90	0.54
1:C:657:GLU:C	1:C:658:ARG:HD2	2.29	0.54
1:B:422:GLN:HG3	1:B:678:GLN:O	2.08	0.54
1:D:9:GLU:CG	1:D:267:GLY:H	2.21	0.54
1:A:778:SER:C	1:A:779:ILE:HD13	2.28	0.53
1:C:150:ASP:OD1	1:C:151:LEU:N	2.41	0.53
1:B:152:LEU:HD11	1:B:190:PRO:HB2	1.90	0.53
1:B:9:GLU:HG2	1:B:266:PHE:HD2	1.73	0.53
1:A:642:ARG:HH11	1:A:642:ARG:CB	2.21	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:731:GLU:HA	1:D:734:LYS:HG3	1.90	0.53
1:A:362:ILE:HG12	1:A:572:ASN:HD22	1.74	0.53
1:C:506:PRO:HB3	1:C:535:ALA:HB2	1.90	0.53
1:B:317:HIS:O	1:B:320:TYR:HB3	2.08	0.53
2:E:13:DG:H1	3:F:105:DC:H42	1.55	0.53
1:D:760:LEU:HD23	1:D:760:LEU:C	2.29	0.53
1:B:597:ILE:O	1:B:601:VAL:HG23	2.08	0.53
1:A:800:LYS:O	1:A:802:PRO:HD3	2.09	0.53
1:A:353:ILE:HB	5:A:973:HOH:O	2.08	0.53
1:C:169:LYS:O	1:C:175:GLY:HA3	2.08	0.53
1:C:440:HIS:CE1	1:C:444:ASN:HD22	2.26	0.53
1:C:411:ASP:HB2	1:C:686:GLU:OE2	2.07	0.53
1:B:472:PRO:O	1:B:475:ILE:HG22	2.08	0.53
2:E:13:DG:H2"	2:E:14:DC:H5"	1.89	0.53
1:D:546:GLN:O	1:D:549:GLU:HG2	2.09	0.53
1:A:774:LEU:HB3	5:A:1004:HOH:O	2.08	0.53
1:A:867:ASP:O	1:A:871:LEU:HB2	2.08	0.53
1:A:449:ARG:HH12	1:A:452:ASP:CB	2.21	0.53
1:D:423:VAL:HB	1:D:425:ILE:HG13	1.91	0.53
1:D:209:THR:HG21	1:D:244:PRO:HB3	1.91	0.53
1:A:530:ILE:HA	1:A:533:LEU:HD12	1.90	0.53
1:A:496:GLY:HA2	1:A:542:LEU:HD11	1.91	0.53
1:C:516:VAL:HG11	1:C:526:ILE:HD13	1.90	0.53
1:D:485:HIS:HA	1:D:488:TYR:HB2	1.91	0.53
1:B:170:LEU:N	1:B:170:LEU:HD12	2.23	0.53
1:C:392:PRO:C	1:C:587:THR:HG21	2.28	0.53
1:B:504:HIS:C	1:B:506:PRO:HD3	2.28	0.53
1:B:60:LYS:HE3	1:B:62:PHE:CZ	2.43	0.53
1:C:254:GLU:HG3	1:C:258:GLY:O	2.09	0.53
1:C:579:ASP:HB3	1:C:582:ASN:HB2	1.90	0.53
3:L:108:DT:H2"	3:L:109:DC:O5'	2.09	0.53
1:D:812:ASN:O	1:D:815:ILE:HG12	2.08	0.53
1:B:285:GLN:HG3	1:B:292:TYR:HE2	1.74	0.53
1:D:74:ARG:HA	1:D:77:ASP:OD2	2.09	0.53
1:D:114:ASP:HB3	1:D:328:VAL:CG2	2.39	0.53
1:D:656:ARG:HA	1:D:660:GLU:HG2	1.91	0.53
1:B:599:ARG:O	1:B:603:GLU:HG3	2.09	0.53
1:C:283:THR:HG23	5:C:961:HOH:O	2.08	0.53
1:A:481:GLN:O	1:A:484:GLU:HB3	2.09	0.53
1:A:833:LEU:CD2	1:A:866:MET:HB2	2.27	0.53
1:B:191:PHE:CZ	1:B:200:GLU:HG2	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:738:PRO:HG2	1:D:741:VAL:CB	2.38	0.52
1:D:426:SER:OG	1:D:427:PRO:HD2	2.09	0.52
1:C:605:LEU:HA	1:C:608:VAL:HG22	1.92	0.52
1:B:529:LYS:O	1:B:533:LEU:HD22	2.08	0.52
1:A:806:ARG:CD	1:A:844:LYS:HE3	2.39	0.52
1:A:779:ILE:HG21	1:A:871:LEU:HG	1.90	0.52
1:C:83:LEU:HB3	1:C:379:VAL:HG12	1.90	0.52
1:D:38:PHE:CZ	1:D:59:ARG:HG3	2.44	0.52
1:C:297:GLU:O	1:C:337:LYS:HE2	2.09	0.52
1:A:304:LYS:HA	1:A:304:LYS:HE3	1.91	0.52
2:G:6:DA:H2"	2:G:7:DA:H5"	1.91	0.52
1:A:129:ALA:HA	1:A:225:TYR:CZ	2.45	0.52
3:H:104:DG:H2"	3:H:105:DC:H5"	1.91	0.52
1:B:475:ILE:HD13	1:B:475:ILE:O	2.09	0.52
1:B:654:PHE:O	1:B:658:ARG:HB2	2.10	0.52
1:D:516:VAL:HG11	1:D:522:PHE:CE1	2.33	0.52
3:F:108:DT:H4'	5:F:137:HOH:O	2.08	0.52
1:D:286:PRO:HG2	1:D:739:LYS:NZ	2.24	0.52
2:I:7:DA:H2'	2:I:8:DT:H72	1.91	0.52
1:B:727:ILE:HG21	1:B:732:THR:HG21	1.92	0.52
1:A:49:TYR:O	1:A:57:CYS:N	2.40	0.52
1:C:514:LEU:HB3	1:C:541:MET:CE	2.39	0.52
1:B:685:ARG:NH2	1:B:714:ASP:OD1	2.41	0.52
1:D:745:LEU:O	1:D:749:ILE:HG13	2.10	0.52
1:A:159:VAL:HG21	1:A:317:HIS:CD2	2.44	0.52
1:D:734:LYS:HB2	1:D:737:THR:OG1	2.09	0.52
1:C:785:ALA:HB1	1:C:788:ILE:HD11	1.91	0.52
1:D:123:PHE:CD1	1:D:124:PRO:HD2	2.44	0.52
1:B:253:ILE:HD12	1:B:254:GLU:H	1.75	0.52
3:H:101:DG:H2"	3:H:102:DC:OP2	2.08	0.52
1:B:197:LEU:HD23	1:B:198:LEU:N	2.25	0.52
1:D:757:GLU:HB2	1:D:889:LEU:HD22	1.91	0.52
1:D:52:ILE:HB	1:D:428:GLU:HG2	1.92	0.52
1:D:277:TYR:O	1:D:281:SER:HB2	2.09	0.52
1:D:536:LYS:O	1:D:536:LYS:HD3	2.09	0.52
1:B:320:TYR:O	1:B:323:TYR:HB3	2.09	0.52
1:D:469:GLY:C	1:D:472:PRO:HD2	2.30	0.52
1:B:599:ARG:HG2	1:B:599:ARG:NH1	2.24	0.52
1:D:750:ARG:HG3	1:D:754:GLN:NE2	2.24	0.52
1:A:294:SER:O	1:A:298:LEU:HD12	2.09	0.52
1:A:112:ASN:HD21	1:A:331:VAL:HG11	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:204:PHE:CE1	1:D:208:LYS:HG3	2.45	0.52
1:A:52:ILE:HG13	1:A:53:TYR:CD1	2.45	0.52
1:D:254:GLU:HG3	1:D:259:SER:HB2	1.92	0.52
1:C:477:LYS:HG2	1:C:481:GLN:HE21	1.74	0.52
1:B:799:PRO:O	1:B:800:LYS:HB2	2.10	0.52
1:D:519:ARG:HH11	1:D:519:ARG:HG3	1.75	0.52
1:B:884:THR:HB	1:B:889:LEU:O	2.10	0.51
1:B:486:LYS:O	1:B:490:LEU:HB2	2.10	0.51
1:D:496:GLY:HA2	1:D:545:ALA:CB	2.41	0.51
1:D:218:VAL:HG23	1:D:222:ALA:HB3	1.92	0.51
1:B:300:VAL:O	1:B:300:VAL:HG13	2.11	0.51
1:C:233:ILE:O	1:C:233:ILE:HG22	2.10	0.51
1:D:255:ASN:ND2	1:D:256:MET:N	2.55	0.51
1:C:241:ARG:HA	1:C:246:ARG:HD3	1.92	0.51
1:B:9:GLU:HG3	5:B:928:HOH:O	2.10	0.51
1:D:112:ASN:ND2	1:D:214:THR:HG23	2.26	0.51
1:D:125:GLU:HG3	1:D:127:SER:H	1.75	0.51
1:A:214:THR:OG1	1:A:215:GLY:N	2.42	0.51
1:D:451:SER:HB3	1:D:456:CYS:SG	2.50	0.51
1:B:303:LEU:HD12	1:B:323:TYR:CA	2.35	0.51
1:A:362:ILE:HB	2:E:3:DC:OP1	2.10	0.51
1:B:247:LYS:HE3	1:B:266:PHE:CZ	2.45	0.51
1:C:283:THR:HG21	5:C:1042:HOH:O	2.10	0.51
1:C:176:ASP:O	1:C:303:LEU:HD21	2.10	0.51
1:D:411:ASP:O	1:D:683:MET:HA	2.10	0.51
1:B:706:LYS:HE2	3:H:113:DC:O2	2.11	0.51
1:D:557:ILE:HG22	1:D:558:ASN:N	2.25	0.51
1:D:399:PRO:O	1:D:401:PRO:HD3	2.10	0.51
1:D:461:MET:CE	1:D:581:ARG:HD2	2.40	0.51
1:D:461:MET:HE3	1:D:581:ARG:HD2	1.92	0.51
1:C:362:ILE:HG23	1:C:575:PHE:HD1	1.75	0.51
1:C:176:ASP:O	1:C:177:GLU:HB2	2.10	0.51
1:D:884:THR:HG21	1:D:891:TYR:CD1	2.45	0.51
1:A:645:ASN:HB2	5:A:972:HOH:O	2.11	0.51
1:B:347:MET:HE1	1:B:562:LEU:CD1	2.30	0.51
1:B:180:SER:O	1:B:183:ILE:HG22	2.11	0.51
1:D:18:ARG:NH2	1:D:211:VAL:HA	2.26	0.51
1:D:260:ARG:HG2	1:D:261:GLU:H	1.74	0.51
3:L:108:DT:H2"	3:L:109:DC:C5'	2.41	0.51
1:A:743:LYS:O	1:A:746:LYS:HB3	2.11	0.51
1:A:771:PHE:O	1:A:774:LEU:HB2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:52:ILE:HD12	1:D:428:GLU:HG3	1.93	0.51
1:D:835:LEU:HB3	1:D:839:ASN:ND2	2.25	0.51
1:D:616:PHE:HB3	1:D:627:VAL:HG13	1.93	0.51
1:D:111:ALA:CB	1:D:210:PRO:HB3	2.38	0.51
1:A:241:ARG:HG3	1:A:241:ARG:NH1	2.23	0.51
1:A:35:PRO:HG3	1:A:65:MET:HA	1.93	0.51
1:D:500:LYS:O	1:D:503:LEU:HB3	2.11	0.51
1:A:544:ARG:HG3	1:A:544:ARG:NH1	2.26	0.51
1:D:406:TYR:CE2	1:D:691:PRO:HD2	2.46	0.51
1:B:312:LEU:O	1:B:312:LEU:HD13	2.11	0.51
2:I:6:DA:H1'	2:I:7:DA:H5"	1.93	0.51
1:A:819:ILE:HG12	1:A:819:ILE:O	2.11	0.51
1:B:557:ILE:HG22	5:B:945:HOH:O	2.09	0.51
1:C:382:GLN:HG2	1:C:383:GLY:N	2.26	0.51
1:D:738:PRO:HG2	1:D:741:VAL:CG2	2.41	0.50
1:C:121:ASP:HA	1:C:819:ILE:HG12	1.91	0.50
1:B:884:THR:O	1:B:888:LYS:N	2.44	0.50
2:G:16:DG:C2'	2:G:17:DC:H5"	2.41	0.50
1:A:514:LEU:HG	1:A:526:ILE:HD12	1.93	0.50
1:B:485:HIS:CD2	1:B:555:ALA:HB1	2.46	0.50
1:B:785:ALA:HB2	1:B:808:ILE:HD11	1.93	0.50
1:B:421:ARG:HB3	1:B:680:LEU:HD12	1.92	0.50
1:D:834:PRO:HG3	1:D:871:LEU:HB2	1.93	0.50
1:B:102:LYS:HD3	1:B:103:TYR:N	2.26	0.50
1:A:536:LYS:HD3	1:A:536:LYS:C	2.31	0.50
1:B:202:LEU:O	1:B:206:GLN:HG2	2.11	0.50
1:A:833:LEU:HD23	1:A:834:PRO:O	2.12	0.50
1:B:179:PRO:HB2	1:B:182:ILE:HG12	1.93	0.50
1:C:381:PRO:HG3	5:C:1070:HOH:O	2.10	0.50
1:D:222:ALA:O	1:D:226:VAL:HG23	2.12	0.50
1:B:231:LYS:HG2	1:B:236:GLU:HA	1.93	0.50
1:D:416:TYR:O	1:D:420:ILE:HG13	2.12	0.50
1:A:725:LEU:HD11	1:A:750:ARG:HB2	1.93	0.50
1:B:25:ARG:HG2	1:B:25:ARG:HH11	1.75	0.50
1:B:377:ASN:N	1:B:377:ASN:HD22	2.09	0.50
1:D:275:ASP:O	1:D:279:LYS:HB2	2.12	0.50
1:D:146:PHE:CE1	1:D:182:ILE:HB	2.47	0.50
1:C:254:GLU:HG3	1:C:259:SER:HB2	1.92	0.50
1:B:435:LYS:H	1:B:435:LYS:HD3	1.76	0.50
1:C:825:VAL:HB	1:C:828:GLU:CD	2.32	0.50
1:D:97:TYR:O	1:D:99:TYR:N	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:170:LEU:H	1:B:170:LEU:HD12	1.77	0.50
1:D:483:LYS:HB3	1:D:483:LYS:NZ	2.27	0.50
1:A:863:LEU:HA	1:A:866:MET:HE2	1.94	0.50
2:G:3:DC:H2"	2:G:4:CTG:OP2	2.12	0.50
1:B:494:ARG:HG3	1:B:495:ASN:H	1.76	0.50
1:B:614:GLU:HB3	1:B:616:PHE:CE1	2.46	0.50
1:A:63:ALA:HB3	1:A:67:ASP:OD1	2.11	0.50
1:A:213:LEU:CD1	1:A:223:ILE:HD11	2.42	0.50
1:B:194:GLU:O	1:B:197:LEU:N	2.45	0.50
1:C:530:ILE:O	1:C:533:LEU:HB2	2.12	0.50
1:D:454:TYR:HB2	1:D:462:MET:HG2	1.93	0.50
1:B:197:LEU:HD23	1:B:197:LEU:C	2.32	0.49
1:B:403:ARG:HH22	1:B:889:LEU:CD2	2.25	0.49
1:A:780:ALA:HB3	1:A:831:TYR:CD1	2.41	0.49
1:C:394:ALA:HB1	1:C:622:THR:HA	1.94	0.49
1:B:129:ALA:HA	1:B:225:TYR:CE1	2.48	0.49
1:C:403:ARG:NH2	1:C:889:LEU:CD2	2.74	0.49
1:C:514:LEU:HB3	1:C:541:MET:HE3	1.94	0.49
2:G:6:DA:H1'	2:G:7:DA:H5"	1.94	0.49
1:D:20:ILE:HD13	1:D:107:LYS:CB	2.42	0.49
1:D:9:GLU:HG3	1:D:267:GLY:H	1.77	0.49
1:D:355:ILE:O	1:D:358:VAL:HG13	2.12	0.49
1:A:380:ILE:HD12	1:A:576:ARG:CZ	2.43	0.49
1:A:73:LYS:CA	1:A:73:LYS:HE3	2.38	0.49
1:A:34:LYS:HG2	1:A:61:LEU:HD21	1.94	0.49
1:D:330:ARG:O	1:D:334:ILE:HG13	2.13	0.49
1:C:38:PHE:HB2	1:C:83:LEU:HB2	1.93	0.49
1:C:412:LEU:HD13	1:C:415:LEU:HD13	1.94	0.49
1:C:221:PHE:O	1:C:224:PRO:HD2	2.12	0.49
1:B:444:ASN:HA	1:B:599:ARG:HE	1.77	0.49
1:C:78:ILE:CD1	1:C:80:LEU:HD23	2.42	0.49
1:C:145:ARG:HD3	1:C:185:LYS:O	2.12	0.49
1:D:313:ARG:O	1:D:317:HIS:ND1	2.36	0.49
1:B:808:ILE:HG22	1:B:812:ASN:HD21	1.77	0.49
1:D:700:GLY:HA2	1:D:753:LEU:HD22	1.95	0.49
1:B:421:ARG:HB3	1:B:680:LEU:CD1	2.41	0.49
1:C:668:ARG:HG2	1:C:668:ARG:NH1	2.28	0.49
1:A:253:ILE:C	1:A:253:ILE:HD12	2.33	0.49
1:D:487:GLY:HA2	1:D:490:LEU:HB2	1.94	0.49
1:A:376:GLN:HE21	1:A:378:LYS:CD	2.24	0.49
1:D:776:TYR:HE1	1:D:848:TRP:CZ2	2.31	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:102:DC:H2"	3:L:103:DG:OP2	2.13	0.49
1:B:428:GLU:OE1	1:B:470:VAL:HG23	2.12	0.49
2:K:10:DA:C3'	2:K:11:DC:H5"	2.41	0.49
2:E:14:DC:H2"	2:E:15:DC:C5'	2.33	0.49
1:B:498:ILE:HG22	1:B:498:ILE:O	2.11	0.49
1:A:804:HIS:O	1:A:808:ILE:HG13	2.13	0.49
3:F:108:DT:H1'	3:F:109:DC:H5'	1.94	0.49
1:D:149:PHE:HB3	1:D:197:LEU:HD21	1.95	0.49
1:B:699:GLY:O	1:B:753:LEU:HD22	2.12	0.49
1:B:221:PHE:C	1:B:224:PRO:HD2	2.33	0.49
1:C:621:ASP:OD1	3:J:114:DA:H5'	2.13	0.49
1:B:395:PHE:HB2	1:B:591:GLN:HG2	1.94	0.49
1:A:410:PHE:HZ	1:A:659:MET:HE1	1.77	0.49
1:D:89:LYS:O	1:D:93:LEU:HD13	2.12	0.49
1:C:239:ALA:C	1:C:241:ARG:H	2.17	0.49
1:B:405:LYS:N	5:B:918:HOH:O	2.44	0.49
3:H:109:DC:H2"	3:H:110:DA:H5'	1.95	0.49
3:H:110:DA:H1'	3:H:111:DT:H5"	1.93	0.49
1:C:285:GLN:HA	1:C:285:GLN:NE2	2.28	0.49
1:C:285:GLN:HA	1:C:285:GLN:HE21	1.78	0.49
1:A:49:TYR:CE1	1:A:59:ARG:HB2	2.47	0.49
1:A:75:MET:HE3	1:A:80:LEU:O	2.13	0.49
1:D:117:VAL:HG13	1:D:132:PRO:O	2.13	0.49
1:B:13:ASP:CG	1:B:66:ARG:HE	2.15	0.49
1:A:446:VAL:O	1:A:446:VAL:HG23	2.13	0.49
1:B:582:ASN:O	1:B:586:ILE:HG13	2.13	0.49
1:D:645:ASN:HD21	1:D:719:ARG:HH11	1.61	0.48
1:A:544:ARG:HH11	1:A:544:ARG:HG3	1.77	0.48
1:B:475:ILE:C	1:B:475:ILE:HD13	2.33	0.48
1:A:408:MET:HE1	1:A:655:ALA:HB2	1.95	0.48
1:B:496:GLY:O	1:B:542:LEU:HD11	2.13	0.48
1:B:499:ILE:O	1:B:542:LEU:HD22	2.12	0.48
1:A:298:LEU:N	1:A:298:LEU:HD12	2.28	0.48
1:C:361:PRO:HD2	2:I:3:DC:H5"	1.95	0.48
1:B:85:MET:HA	1:B:380:ILE:HD11	1.95	0.48
2:G:6:DA:C2'	2:G:7:DA:H5"	2.43	0.48
1:C:516:VAL:HG21	1:C:522:PHE:HE1	1.78	0.48
1:B:530:ILE:HA	1:B:533:LEU:HB2	1.95	0.48
1:B:150:ASP:OD1	1:B:321:ILE:HD11	2.13	0.48
1:D:439:LEU:HD12	1:D:443:ILE:HD11	1.95	0.48
1:A:5:TYR:HE1	1:A:101:ILE:HD13	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:ASP:OD1	1:A:90:LEU:HG	2.13	0.48
2:G:12:DA:H2"	2:G:13:DG:O5'	2.13	0.48
1:D:805:ILE:HD13	1:D:808:ILE:HD12	1.96	0.48
1:C:154:SER:O	1:C:156:TYR:N	2.46	0.48
1:A:276:LEU:HG	1:A:340:PHE:HB3	1.95	0.48
1:A:738:PRO:O	1:A:742:GLN:HB2	2.14	0.48
1:D:146:PHE:CD1	1:D:146:PHE:N	2.82	0.48
1:D:594:LEU:O	1:D:597:ILE:HG22	2.12	0.48
1:B:435:LYS:N	1:B:435:LYS:CD	2.76	0.48
1:B:863:LEU:HA	1:B:866:MET:CE	2.43	0.48
1:C:646:HIS:HB3	5:C:1043:HOH:O	2.13	0.48
1:C:342:ASN:HB2	5:C:919:HOH:O	2.12	0.48
2:I:10:DA:C2'	2:I:11:DC:C5'	2.90	0.48
1:B:482:ARG:HH22	1:B:560:LYS:HD2	1.76	0.48
1:B:698:ILE:HD13	1:B:889:LEU:HD11	1.94	0.48
1:D:841:PHE:CE2	1:D:862:VAL:HG22	2.48	0.48
1:B:231:LYS:HG3	1:B:236:GLU:HA	1.95	0.48
1:D:4:PHE:CE2	1:D:103:TYR:HB2	2.48	0.48
1:C:189:MET:O	1:C:191:PHE:CE1	2.67	0.48
1:B:234:PHE:CD1	1:B:234:PHE:N	2.81	0.48
1:A:313:ARG:NH1	5:A:979:HOH:O	2.34	0.48
2:E:13:DG:H1	3:F:105:DC:N4	2.12	0.48
1:A:642:ARG:N	1:A:646:HIS:HD2	2.06	0.48
1:D:605:LEU:CD2	1:D:632:ILE:HD11	2.43	0.48
1:B:472:PRO:HA	1:B:475:ILE:HG22	1.94	0.48
1:C:516:VAL:HG21	1:C:522:PHE:CE1	2.48	0.48
2:I:12:DA:H2"	2:I:13:DG:C5'	2.44	0.48
1:C:10:GLN:HG3	1:C:65:MET:CE	2.43	0.48
1:C:791:TYR:CD2	1:C:801:CYS:HA	2.49	0.48
1:C:81:GLU:HB2	1:C:384:ARG:NH2	2.29	0.48
1:D:409:SER:HB3	1:D:626:TYR:CD2	2.48	0.48
3:F:110:DA:C2'	3:F:111:DT:C5'	2.91	0.48
1:B:497:GLU:CG	1:B:498:ILE:HD12	2.44	0.48
1:D:806:ARG:HD2	1:D:843:ASP:OD1	2.14	0.48
1:D:597:ILE:HD11	1:D:663:ILE:HG23	1.95	0.48
1:A:49:TYR:HB2	1:A:57:CYS:O	2.13	0.48
1:B:285:GLN:HG3	1:B:292:TYR:CE2	2.49	0.48
1:C:668:ARG:HG2	1:C:668:ARG:HH11	1.79	0.48
1:A:605:LEU:HA	1:A:608:VAL:HG22	1.96	0.48
1:D:526:ILE:HG13	1:D:526:ILE:O	2.13	0.48
1:C:231:LYS:O	1:C:231:LYS:HG2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:104:ASP:OD1	1:C:107:LYS:HE2	2.14	0.48
1:C:285:GLN:HE21	1:C:285:GLN:CA	2.25	0.48
1:B:772:ARG:NH2	1:B:868:TYR:HB2	2.29	0.48
1:B:9:GLU:CG	1:B:266:PHE:HD2	2.27	0.48
1:A:373:LEU:HD12	1:A:380:ILE:HG22	1.95	0.48
1:D:491:ALA:HB1	1:D:521:ASP:N	2.29	0.47
1:A:771:PHE:CD1	1:A:774:LEU:HD12	2.48	0.47
1:B:831:TYR:O	1:B:847:ALA:HA	2.13	0.47
2:G:11:DC:H2"	2:G:12:DA:C5'	2.42	0.47
1:C:209:THR:HA	1:C:210:PRO:HD3	1.59	0.47
1:D:254:GLU:HG3	1:D:258:GLY:O	2.14	0.47
1:A:43:GLU:HA	1:A:56:PRO:HG3	1.95	0.47
1:B:647:TRP:O	1:B:650:PHE:HB3	2.14	0.47
1:C:188:TYR:CD2	1:C:190:PRO:HD3	2.49	0.47
1:B:831:TYR:CD2	1:B:850:SER:HA	2.49	0.47
1:D:880:LEU:HD22	1:D:884:THR:HG23	1.96	0.47
1:D:9:GLU:OE2	1:D:266:PHE:HA	2.15	0.47
1:B:867:ASP:OD1	1:B:870:VAL:HB	2.14	0.47
1:B:177:GLU:O	1:B:177:GLU:HG3	2.13	0.47
3:F:103:DG:C2'	3:F:104:DG:H5'	2.34	0.47
1:C:73:LYS:HZ2	1:C:73:LYS:HB3	1.79	0.47
1:D:859:LYS:O	1:D:863:LEU:HD13	2.14	0.47
1:C:137:THR:HB	1:C:328:VAL:HG21	1.95	0.47
1:B:218:VAL:O	1:B:223:ILE:HG13	2.14	0.47
1:B:512:GLU:N	1:B:513:PRO:CD	2.76	0.47
1:A:274:ILE:HG23	1:A:275:ASP:N	2.29	0.47
1:B:384:ARG:HH11	1:B:384:ARG:HG3	1.79	0.47
1:D:514:LEU:HD12	1:D:514:LEU:N	2.29	0.47
1:D:85:MET:HA	1:D:380:ILE:HD11	1.96	0.47
1:B:791:TYR:CD2	1:B:801:CYS:HA	2.50	0.47
1:B:863:LEU:HA	1:B:866:MET:HE2	1.96	0.47
1:D:811:TYR:HH	1:D:822:PRO:HG2	1.79	0.47
1:A:779:ILE:HG21	1:A:871:LEU:CD2	2.45	0.47
1:B:811:TYR:O	1:B:815:ILE:HG12	2.15	0.47
1:B:132:PRO:HA	1:B:194:GLU:OE1	2.14	0.47
1:A:15:ILE:HG12	1:A:65:MET:CE	2.44	0.47
1:B:494:ARG:NH1	1:B:494:ARG:HG3	2.29	0.47
1:D:361:PRO:HD2	2:K:3:DC:P	2.54	0.47
1:A:428:GLU:OE1	1:A:470:VAL:HG23	2.15	0.47
1:A:364:THR:O	1:A:368:ILE:HG13	2.15	0.47
1:B:183:ILE:HG23	1:B:184:ASP:OD1	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:7:DA:H2'	2:G:8:DT:H72	1.97	0.47
1:B:109:ARG:NH1	1:B:142:ILE:HD12	2.29	0.47
1:C:240:LYS:O	1:C:246:ARG:HA	2.15	0.47
1:A:489:MET:SD	1:A:553:MET:HG2	2.55	0.47
1:A:489:MET:HE3	1:A:553:MET:HG2	1.97	0.47
1:A:714:ASP:OD1	1:A:718:THR:N	2.48	0.47
1:B:846:ILE:CD1	1:B:858:ILE:HD12	2.45	0.47
1:B:508:LEU:HG	1:B:509:SER:N	2.28	0.47
1:A:877:ILE:O	1:A:878:LYS:C	2.51	0.47
1:D:700:GLY:CA	1:D:753:LEU:HD22	2.44	0.47
1:A:8:VAL:C	1:A:9:GLU:HG2	2.35	0.47
1:C:724:LYS:HE2	5:C:975:HOH:O	2.13	0.47
1:D:273:TYR:HA	1:D:276:LEU:HB2	1.97	0.47
1:A:594:LEU:HD11	1:A:625:ILE:HG23	1.97	0.47
1:A:471:VAL:HB	1:A:472:PRO:CD	2.44	0.47
1:A:772:ARG:O	1:A:774:LEU:N	2.48	0.47
1:A:731:GLU:HA	1:A:734:LYS:HB2	1.96	0.47
2:G:14:DC:C2'	2:G:15:DC:H5"	2.45	0.47
1:C:403:ARG:HH22	1:C:889:LEU:HD23	1.80	0.47
1:A:52:ILE:HD12	1:A:428:GLU:HB3	1.96	0.47
1:D:699:GLY:C	1:D:753:LEU:HD22	2.35	0.47
1:A:274:ILE:CG2	1:A:275:ASP:N	2.78	0.47
1:D:183:ILE:HG23	1:D:184:ASP:N	2.30	0.47
1:B:491:ALA:HB3	1:B:518:TYR:O	2.15	0.47
1:B:876:PHE:O	1:B:879:PRO:HG2	2.15	0.47
1:B:534:SER:CB	1:B:537:SER:HB2	2.45	0.47
1:D:807:GLY:C	1:D:847:ALA:H	2.17	0.47
1:A:485:HIS:C	1:A:487:GLY:N	2.67	0.47
1:D:97:TYR:O	1:D:352:LYS:NZ	2.36	0.47
1:A:415:LEU:O	1:A:419:ILE:HG13	2.15	0.47
1:D:265:LEU:CB	1:D:268:ILE:HD12	2.45	0.47
1:B:338:ARG:O	1:B:339:GLN:HB2	2.15	0.47
1:D:791:TYR:CD2	1:D:801:CYS:HA	2.50	0.47
1:A:494:ARG:NH2	1:A:521:ASP:HB3	2.29	0.47
1:D:516:VAL:HG21	1:D:522:PHE:HZ	1.80	0.47
1:A:61:LEU:HD23	1:A:61:LEU:C	2.36	0.47
1:A:736:SER:HB2	1:A:782:VAL:O	2.14	0.47
1:B:489:MET:HB3	1:B:552:GLY:HA3	1.97	0.47
1:B:421:ARG:HD3	1:B:475:ILE:HD12	1.97	0.47
1:A:433:THR:HA	1:A:460:GLY:O	2.14	0.47
1:C:440:HIS:CE1	1:C:444:ASN:ND2	2.83	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:606:ASN:ND2	1:A:613:GLY:N	2.63	0.47
1:C:15:ILE:CD1	1:C:92:TYR:HB2	2.45	0.47
1:A:836:ARG:HG3	1:A:865:TRP:O	2.14	0.47
1:B:468:ASP:N	1:B:468:ASP:OD2	2.42	0.47
1:C:138:HIS:CD2	1:C:138:HIS:C	2.88	0.47
3:F:109:DC:H2"	3:F:110:DA:H5'	1.97	0.46
1:B:227:TYR:CD2	1:B:263:ILE:HD13	2.50	0.46
1:A:499:ILE:O	1:A:542:LEU:HD22	2.14	0.46
1:B:421:ARG:NH1	1:B:421:ARG:HG2	2.30	0.46
1:C:118:THR:OG1	1:C:313:ARG:HG3	2.15	0.46
1:B:408:MET:CE	1:B:685:ARG:HD3	2.45	0.46
1:C:839:ASN:HB2	1:C:840:PRO:HD2	1.97	0.46
1:B:797:PRO:HG3	1:B:806:ARG:NH1	2.29	0.46
1:C:376:GLN:O	1:C:377:ASN:HB2	2.15	0.46
1:B:376:GLN:NE2	1:B:378:LYS:NZ	2.62	0.46
1:B:739:LYS:HA	1:B:739:LYS:HE2	1.97	0.46
2:E:4:CTG:H2'	2:E:4:CTG:O6	2.13	0.46
1:A:559:ARG:HG2	1:A:559:ARG:HH11	1.80	0.46
1:C:83:LEU:HB3	1:C:379:VAL:CG1	2.44	0.46
1:A:514:LEU:HG	1:A:526:ILE:CG2	2.43	0.46
1:D:503:LEU:HA	1:D:506:PRO:HG3	1.98	0.46
1:D:143:ASP:O	1:D:144:ASP:HB3	2.16	0.46
1:B:856:ASP:HA	1:B:859:LYS:HB2	1.97	0.46
1:A:661:PRO:O	1:A:665:ARG:HG3	2.16	0.46
1:D:336:ALA:CA	1:D:339:GLN:HE21	2.23	0.46
1:C:455:SER:HA	1:C:675:ASN:O	2.16	0.46
1:C:284:ASN:HD21	1:C:829:LYS:NZ	2.14	0.46
1:B:597:ILE:HD13	1:B:667:PHE:CZ	2.50	0.46
1:B:502:ALA:HB3	1:B:539:ASN:OD1	2.15	0.46
1:B:809:LEU:O	1:B:813:ARG:HB2	2.15	0.46
1:C:558:ASN:HA	1:C:558:ASN:HD22	1.58	0.46
1:D:353:ILE:HB	5:D:937:HOH:O	2.15	0.46
1:A:132:PRO:HD2	5:A:1001:HOH:O	2.15	0.46
1:C:152:LEU:CD1	1:C:190:PRO:HB2	2.36	0.46
1:D:255:ASN:O	1:D:256:MET:C	2.52	0.46
1:A:362:ILE:HG22	1:A:363:LYS:N	2.30	0.46
1:B:878:LYS:HB3	1:B:879:PRO:CD	2.45	0.46
1:D:253:ILE:HD11	1:D:262:ILE:CD1	2.45	0.46
1:A:472:PRO:HA	1:A:475:ILE:HG13	1.96	0.46
1:A:4:PHE:O	1:A:19:TYR:HB2	2.14	0.46
1:D:685:ARG:C	1:D:685:ARG:HD2	2.36	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:206:GLN:HA	1:D:206:GLN:NE2	2.31	0.46
3:J:112:DT:H2"	3:J:113:DC:H5'	1.97	0.46
1:C:61:LEU:HD23	1:C:62:PHE:N	2.30	0.46
1:C:284:ASN:C	1:C:284:ASN:HD22	2.19	0.46
1:A:546:GLN:HG3	1:A:547:ARG:N	2.31	0.46
1:D:453:VAL:HG23	1:D:454:TYR:CD2	2.50	0.46
1:B:468:ASP:HB3	5:B:1000:HOH:O	2.14	0.46
1:A:354:GLN:O	1:A:357:SER:HB2	2.15	0.46
1:D:498:ILE:HA	1:D:501:GLU:HB3	1.96	0.46
1:A:106:THR:HG22	1:A:106:THR:O	2.15	0.46
1:A:612:GLU:OE1	1:A:612:GLU:HA	2.15	0.46
1:B:164:ILE:HB	1:B:183:ILE:HD11	1.97	0.46
1:B:750:ARG:HH11	1:B:754:GLN:HE22	1.60	0.46
1:B:478:VAL:HG13	1:B:559:ARG:HG3	1.98	0.46
1:B:485:HIS:O	1:B:489:MET:HG3	2.16	0.46
1:C:154:SER:C	1:C:156:TYR:N	2.68	0.46
1:B:395:PHE:HB2	1:B:591:GLN:HE21	1.81	0.46
1:D:13:ASP:HB3	1:D:64:ASN:HB2	1.97	0.46
1:C:598:GLU:HG3	1:C:617:VAL:HG11	1.97	0.46
1:C:52:ILE:HB	1:C:428:GLU:HG2	1.97	0.46
1:A:467:ARG:HG3	1:A:467:ARG:HH11	1.81	0.46
3:J:110:DA:C2'	3:J:111:DT:C5'	2.94	0.46
1:A:747:GLU:OE2	1:A:747:GLU:HA	2.16	0.46
1:B:273:TYR:HA	1:B:276:LEU:HB2	1.97	0.46
1:B:406:TYR:CD2	1:B:633:ILE:HG13	2.51	0.46
1:B:395:PHE:CB	1:B:591:GLN:HG2	2.45	0.46
1:A:636:VAL:HG21	1:A:650:PHE:CZ	2.50	0.46
1:A:21:ASP:OD2	1:A:21:ASP:C	2.54	0.46
1:C:163:SER:HB3	1:C:318:GLN:NE2	2.15	0.46
1:D:209:THR:HA	1:D:210:PRO:HD3	1.81	0.46
1:D:83:LEU:HB3	1:D:379:VAL:CG1	2.46	0.46
1:D:83:LEU:HD22	1:D:83:LEU:H	1.81	0.46
1:D:167:ALA:HA	1:D:176:ASP:HB2	1.97	0.46
1:C:354:GLN:HB3	1:C:356:GLN:OE1	2.16	0.46
1:C:436:VAL:HG13	1:C:436:VAL:O	2.16	0.46
1:A:811:TYR:O	1:A:815:ILE:HG12	2.16	0.46
1:D:303:LEU:HD12	1:D:323:TYR:HA	1.97	0.46
1:D:697:GLY:HA3	1:D:753:LEU:O	2.16	0.46
1:B:678:GLN:HG2	1:B:680:LEU:HG	1.98	0.46
1:A:294:SER:HA	1:A:334:ILE:HD11	1.98	0.46
1:D:496:GLY:HA2	1:D:545:ALA:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:370:PHE:CD2	1:C:370:PHE:C	2.88	0.46
1:A:219:GLU:HG2	1:A:219:GLU:O	2.16	0.46
1:B:149:PHE:CD1	1:B:149:PHE:N	2.84	0.46
2:K:8:DT:C2'	2:K:9:DG:H5'	2.36	0.46
1:D:481:GLN:CB	1:D:559:ARG:HD3	2.45	0.46
1:A:685:ARG:NH1	1:A:688:ILE:HG13	2.30	0.46
1:B:776:TYR:CE1	1:B:777:ILE:HG13	2.50	0.46
1:B:179:PRO:HG2	1:B:329:TYR:CE2	2.51	0.46
1:D:881:GLU:HA	1:D:884:THR:OG1	2.15	0.46
1:A:499:ILE:HD11	1:A:522:PHE:HZ	1.80	0.46
1:D:132:PRO:HB3	1:D:229:ARG:NH2	2.31	0.46
1:C:305:TYR:OH	1:C:309:ILE:CG1	2.63	0.46
1:C:173:GLN:HB2	1:C:173:GLN:HE21	1.58	0.46
1:A:855:THR:C	1:A:857:LEU:H	2.19	0.45
1:B:555:ALA:O	1:B:559:ARG:HD3	2.16	0.45
1:A:162:TRP:CD1	1:A:321:ILE:HB	2.51	0.45
1:B:617:VAL:HB	5:B:973:HOH:O	2.16	0.45
2:K:9:DG:H2"	2:K:10:DA:C8	2.51	0.45
1:B:233:ILE:CD1	1:B:233:ILE:N	2.78	0.45
1:A:310:SER:C	1:A:311:LYS:HD3	2.36	0.45
1:B:435:LYS:CD	1:B:435:LYS:H	2.29	0.45
1:B:739:LYS:HE2	1:B:742:GLN:HE22	1.82	0.45
1:A:534:SER:O	1:A:538:LEU:HG	2.15	0.45
1:D:413:THR:O	1:D:414:SER:C	2.53	0.45
1:B:545:ALA:O	1:B:549:GLU:HB2	2.17	0.45
1:A:761:GLN:OE1	1:A:893:LYS:CG	2.64	0.45
1:D:516:VAL:HG21	1:D:522:PHE:CZ	2.52	0.45
1:D:163:SER:HB3	1:D:318:GLN:NE2	2.21	0.45
2:G:12:DA:H1'	2:G:13:DG:H5'	1.99	0.45
1:B:634:ASP:O	1:B:636:VAL:N	2.49	0.45
2:K:7:DA:H2"	2:K:8:DT:C6	2.52	0.45
1:A:776:TYR:CE1	1:A:863:LEU:HD11	2.51	0.45
1:C:38:PHE:HB2	1:C:379:VAL:HG11	1.98	0.45
1:A:514:LEU:HD11	1:A:529:LYS:CE	2.46	0.45
1:A:744:ALA:O	1:A:747:GLU:N	2.50	0.45
1:D:420:ILE:HG12	1:D:586:ILE:HD11	1.98	0.45
1:A:491:ALA:HA	1:A:494:ARG:HE	1.81	0.45
1:A:795:GLY:C	1:A:809:LEU:HD13	2.36	0.45
2:E:12:DA:H2"	2:E:13:DG:O5'	2.17	0.45
1:A:779:ILE:HG21	1:A:871:LEU:CG	2.47	0.45
1:B:506:PRO:HB3	1:B:536:LYS:CG	2.44	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:514:LEU:HD11	1:A:529:LYS:HZ1	1.79	0.45
1:A:489:MET:HE3	1:A:553:MET:CG	2.47	0.45
1:A:602:ASN:ND2	1:A:616:PHE:H	2.15	0.45
1:D:793:VAL:C	1:D:795:GLY:H	2.20	0.45
1:C:453:VAL:HG23	1:C:454:TYR:CG	2.52	0.45
1:A:447:ALA:O	1:A:448:GLU:C	2.55	0.45
1:A:795:GLY:O	1:A:809:LEU:HD13	2.16	0.45
1:C:9:GLU:HG3	1:C:267:GLY:H	1.81	0.45
1:C:9:GLU:HG3	1:C:267:GLY:N	2.32	0.45
1:B:386:HIS:O	1:B:573:VAL:HG21	2.17	0.45
1:B:685:ARG:CG	1:B:685:ARG:HH11	2.29	0.45
1:C:92:TYR:C	1:C:92:TYR:CD1	2.90	0.45
1:D:405:LYS:O	1:D:690:GLY:HA2	2.17	0.45
1:D:329:TYR:O	1:D:333:GLN:HG3	2.17	0.45
2:K:4:CTG:H2'	2:K:4:CTG:O6	2.17	0.45
1:B:541:MET:HG3	1:B:544:ARG:HD3	1.99	0.45
1:D:750:ARG:HH11	1:D:750:ARG:HG2	1.81	0.45
1:B:516:VAL:HG12	1:B:517:ASP:N	2.32	0.45
1:A:314:GLU:HG2	1:A:315:SER:N	2.31	0.45
2:E:5:DG:H2"	2:E:6:DA:O5'	2.16	0.45
1:A:731:GLU:N	1:A:731:GLU:OE1	2.48	0.45
1:B:508:LEU:CG	1:B:509:SER:H	2.30	0.45
1:D:842:GLY:O	1:D:843:ASP:HB2	2.16	0.45
1:A:730:LEU:HD22	1:A:883:PHE:HE1	1.82	0.45
1:D:750:ARG:HG2	1:D:750:ARG:NH1	2.32	0.45
1:C:451:SER:HB3	1:C:456:CYS:SG	2.57	0.45
1:C:898:PHE:N	1:C:898:PHE:CD2	2.83	0.45
1:B:51:ASP:OD1	1:B:51:ASP:C	2.54	0.45
1:C:134:ASP:O	1:C:135:ALA:HB2	2.17	0.45
1:C:20:ILE:HD13	1:C:107:LYS:CB	2.47	0.45
1:B:700:GLY:HA2	1:B:753:LEU:HD22	1.99	0.45
1:B:145:ARG:HB2	1:B:147:TYR:CE1	2.51	0.45
1:B:408:MET:HE1	1:B:685:ARG:HD3	1.98	0.45
1:B:529:LYS:O	1:B:533:LEU:HB2	2.17	0.45
1:C:362:ILE:HD12	1:C:575:PHE:HB2	1.99	0.45
1:C:305:TYR:OH	1:C:309:ILE:HG12	2.16	0.45
1:C:700:GLY:HA2	1:C:753:LEU:HD22	1.99	0.45
3:L:111:DT:H4'	3:L:111:DT:OP1	2.16	0.45
1:A:197:LEU:HD23	1:A:197:LEU:C	2.37	0.45
2:I:7:DA:H2"	2:I:8:DT:C7	2.47	0.45
1:C:197:LEU:O	1:C:197:LEU:HD23	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:698:ILE:HG13	1:D:753:LEU:HD23	1.99	0.45
1:D:813:ARG:HH11	1:D:813:ARG:HG3	1.81	0.45
1:C:89:LYS:HE3	1:C:354:GLN:NE2	2.32	0.45
1:A:761:GLN:OE1	1:A:893:LYS:HG2	2.17	0.45
1:D:140:ASP:OD1	1:D:142:ILE:HB	2.16	0.44
1:D:490:LEU:O	1:D:494:ARG:NE	2.50	0.44
1:D:655:ALA:O	1:D:660:GLU:HG2	2.16	0.44
1:C:686:GLU:HG3	1:C:715:MET:HE3	1.97	0.44
1:D:751:ARG:HD3	1:D:759:SER:OG	2.16	0.44
1:D:713:TRP:HZ3	1:D:723:PRO:HD3	1.82	0.44
1:C:254:GLU:OE2	1:C:259:SER:HB2	2.18	0.44
1:B:413:THR:O	1:B:414:SER:C	2.54	0.44
1:A:167:ALA:HB1	1:A:178:VAL:HG21	1.99	0.44
1:C:277:TYR:O	1:C:281:SER:CB	2.65	0.44
1:B:116:GLU:HA	1:B:116:GLU:OE1	2.16	0.44
1:A:279:LYS:HG2	1:A:279:LYS:O	2.16	0.44
1:A:854:ILE:HD11	1:A:858:ILE:HG13	1.99	0.44
1:A:854:ILE:HG23	1:A:859:LYS:HB2	1.99	0.44
1:A:347:MET:HG2	1:A:358:VAL:CG2	2.45	0.44
1:A:778:SER:HB2	5:A:1004:HOH:O	2.16	0.44
1:C:83:LEU:H	1:C:83:LEU:HD22	1.82	0.44
1:D:814:ALA:HB1	1:D:841:PHE:HE1	1.83	0.44
1:D:475:ILE:HD13	1:D:566:LEU:HD22	1.98	0.44
1:A:83:LEU:HD12	1:A:83:LEU:N	2.31	0.44
1:A:846:ILE:O	1:A:846:ILE:HG23	2.18	0.44
1:A:832:VAL:O	1:A:833:LEU:HB2	2.16	0.44
1:A:740:ALA:HB3	1:A:778:SER:O	2.17	0.44
1:D:118:THR:HG1	1:D:313:ARG:HG3	1.82	0.44
1:B:606:ASN:OD1	1:B:616:PHE:HE1	2.00	0.44
1:B:126:PRO:HG2	5:B:986:HOH:O	2.17	0.44
1:C:111:ALA:HB3	1:C:210:PRO:HB3	1.98	0.44
1:A:878:LYS:N	1:A:879:PRO:HD2	2.33	0.44
1:C:854:ILE:CD1	1:C:862:VAL:HG21	2.47	0.44
1:A:299:ASN:O	1:A:300:VAL:HB	2.16	0.44
1:D:149:PHE:CE2	1:D:201:TYR:HA	2.52	0.44
1:D:135:ALA:O	1:D:136:ILE:HG13	2.17	0.44
1:C:285:GLN:NE2	1:C:286:PRO:HD2	2.33	0.44
1:C:537:SER:O	1:C:541:MET:HG3	2.15	0.44
1:D:265:LEU:HB3	1:D:268:ILE:HD12	2.00	0.44
1:A:775:ASN:N	5:A:1004:HOH:O	2.50	0.44
1:A:240:LYS:O	1:A:246:ARG:HA	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:530:ILE:HA	1:A:533:LEU:CD1	2.47	0.44
1:D:439:LEU:HD13	1:D:443:ILE:HG13	1.99	0.44
1:A:594:LEU:HD11	1:A:625:ILE:CG2	2.47	0.44
1:D:465:LYS:NZ	1:D:675:ASN:ND2	2.65	0.44
1:C:708:TYR:CZ	1:C:728:MET:HG3	2.53	0.44
1:B:252:VAL:HG23	1:B:252:VAL:O	2.17	0.44
1:C:439:LEU:HD12	1:C:443:ILE:CD1	2.45	0.44
1:C:594:LEU:O	1:C:597:ILE:HG22	2.17	0.44
1:A:285:GLN:NE2	1:A:285:GLN:HA	2.32	0.44
1:B:499:ILE:HD13	1:B:530:ILE:HD12	1.99	0.44
1:B:25:ARG:NH1	1:B:25:ARG:HG2	2.33	0.44
1:C:305:TYR:CZ	1:C:309:ILE:HG12	2.53	0.44
1:A:772:ARG:HG3	1:A:868:TYR:CD2	2.52	0.44
1:A:231:LYS:HB3	1:A:231:LYS:NZ	2.32	0.44
1:B:894:LYS:CB	1:B:894:LYS:NZ	2.77	0.44
1:B:154:SER:HB2	1:B:155:PRO:HD2	1.98	0.44
1:D:434:PHE:CE2	1:D:450:PRO:HB3	2.53	0.44
1:B:50:PHE:O	1:B:378:LYS:HA	2.18	0.44
1:C:171:GLN:C	1:C:173:GLN:H	2.20	0.44
1:B:305:TYR:OH	1:B:309:ILE:HG22	2.18	0.44
1:D:578:TYR:CD1	1:D:579:ASP:N	2.86	0.44
1:C:495:ASN:O	1:C:498:ILE:HB	2.17	0.44
1:B:282:PHE:HB2	5:B:940:HOH:O	2.16	0.44
2:E:6:DA:H1'	2:E:7:DA:H5"	1.99	0.44
1:A:411:ASP:O	1:A:683:MET:HA	2.18	0.44
1:B:154:SER:C	1:B:156:TYR:H	2.21	0.44
1:B:867:ASP:CG	1:B:870:VAL:HB	2.39	0.44
1:B:625:ILE:HG12	1:B:683:MET:HE1	1.99	0.44
1:C:13:ASP:HB3	1:C:64:ASN:HB2	1.99	0.44
1:C:642:ARG:HH21	1:C:642:ARG:HG3	1.82	0.44
1:A:835:LEU:N	1:A:844:LYS:O	2.34	0.43
1:A:37:LEU:HD11	1:A:72:ILE:HD11	2.00	0.43
3:F:105:DC:H2"	3:F:106:DT:C5'	2.47	0.43
1:D:686:GLU:OE1	1:D:716:GLU:HG2	2.18	0.43
1:D:166:ILE:HD12	1:D:318:GLN:NE2	2.33	0.43
1:B:404:TYR:HA	5:B:918:HOH:O	2.18	0.43
1:B:730:LEU:HD13	1:B:883:PHE:CE1	2.53	0.43
1:B:761:GLN:OE1	1:B:893:LYS:HE3	2.18	0.43
1:B:444:ASN:HA	1:B:599:ARG:NE	2.33	0.43
1:D:698:ILE:HG12	1:D:752:MET:O	2.18	0.43
1:A:499:ILE:HG22	1:A:499:ILE:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:464:TYR:HB3	1:A:467:ARG:HG2	2.00	0.43
1:D:479:PHE:CD1	1:D:563:ILE:HD13	2.53	0.43
1:D:50:PHE:HA	1:D:55:LYS:O	2.17	0.43
1:C:404:TYR:HA	5:C:992:HOH:O	2.18	0.43
1:A:751:ARG:NE	1:A:763:TYR:HB2	2.32	0.43
3:L:104:DG:C3'	3:L:105:DC:H5"	2.49	0.43
1:C:167:ALA:CA	1:C:176:ASP:HB2	2.43	0.43
1:D:686:GLU:HB3	1:D:687:ALA:H	1.66	0.43
1:D:322:SER:O	1:D:326:ILE:HG13	2.17	0.43
1:A:831:TYR:O	1:A:847:ALA:HA	2.18	0.43
1:C:514:LEU:HD21	1:C:526:ILE:HG23	2.00	0.43
1:B:634:ASP:C	1:B:636:VAL:N	2.71	0.43
1:D:570:LEU:HD23	1:D:575:PHE:CE2	2.53	0.43
1:D:781:SER:O	1:D:831:TYR:HA	2.19	0.43
1:C:274:ILE:HG23	1:C:275:ASP:N	2.33	0.43
1:C:633:ILE:HD13	1:C:633:ILE:HA	1.91	0.43
1:B:362:ILE:HG12	2:G:3:DC:OP1	2.18	0.43
1:C:83:LEU:H	1:C:83:LEU:CD2	2.31	0.43
1:B:271:LEU:HD11	1:B:356:GLN:HA	2.00	0.43
1:C:523:SER:OG	1:C:526:ILE:HG13	2.18	0.43
1:B:255:ASN:ND2	1:B:257:TYR:HD1	2.16	0.43
1:B:742:GLN:HB2	1:B:742:GLN:HE21	1.62	0.43
1:A:105:HIS:ND1	1:A:106:THR:N	2.65	0.43
1:A:862:VAL:HG12	1:A:863:LEU:HD12	2.00	0.43
1:A:776:TYR:HB2	1:A:866:MET:HE1	1.99	0.43
1:B:216:TRP:O	1:B:217:ASN:HB2	2.18	0.43
1:D:751:ARG:CZ	1:D:763:TYR:HB2	2.48	0.43
1:B:286:PRO:HG2	1:B:292:TYR:CZ	2.54	0.43
1:C:53:TYR:CE1	1:C:428:GLU:HA	2.53	0.43
1:D:376:GLN:O	1:D:377:ASN:HB2	2.18	0.43
1:B:686:GLU:HG3	1:B:715:MET:SD	2.58	0.43
1:D:599:ARG:O	1:D:603:GLU:HG3	2.18	0.43
1:D:878:LYS:N	1:D:879:PRO:HD2	2.33	0.43
1:C:425:ILE:O	1:C:426:SER:HB2	2.18	0.43
1:B:558:ASN:HD22	1:B:558:ASN:HA	1.51	0.43
3:H:107:DG:H4'	5:H:358:HOH:O	2.19	0.43
1:A:809:LEU:C	1:A:811:TYR:N	2.70	0.43
1:A:410:PHE:CD1	1:A:410:PHE:N	2.86	0.43
1:D:255:ASN:HD22	1:D:256:MET:N	2.14	0.43
1:C:20:ILE:HD13	1:C:107:LYS:HB2	2.00	0.43
1:B:750:ARG:HG2	1:B:754:GLN:NE2	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:206:GLN:NE2	1:C:206:GLN:HA	2.33	0.43
2:E:1:DC:H2'	2:E:2:DG:C5	2.54	0.43
1:A:744:ALA:O	1:A:745:LEU:C	2.56	0.43
1:D:20:ILE:CG2	1:D:24:GLY:HA2	2.48	0.43
1:B:170:LEU:CD1	1:B:170:LEU:H	2.32	0.43
1:B:470:VAL:O	1:B:474:GLU:HG2	2.18	0.43
1:C:277:TYR:O	1:C:281:SER:HB3	2.19	0.43
1:A:792:ASP:N	1:A:792:ASP:OD2	2.47	0.43
1:B:454:TYR:HB3	1:B:463:TYR:O	2.18	0.43
1:B:433:THR:HA	1:B:460:GLY:O	2.18	0.43
1:B:87:ASP:OD1	1:B:90:LEU:HD22	2.19	0.43
1:B:706:LYS:HD3	3:H:113:DC:C1'	2.49	0.43
5:B:1014:HOH:O	2:G:6:DA:H5'	2.19	0.43
1:D:180:SER:HA	1:D:183:ILE:HB	2.01	0.43
1:C:559:ARG:HA	1:C:559:ARG:HD3	1.90	0.43
1:C:481:GLN:HB3	1:C:559:ARG:HH11	1.83	0.43
1:A:836:ARG:HG3	1:A:836:ARG:HH11	1.82	0.43
1:A:821:ALA:O	1:A:822:PRO:C	2.57	0.43
1:A:854:ILE:HD13	1:A:859:LYS:HA	2.01	0.43
2:E:4:CTG:O5'	2:E:4:CTG:H6	2.19	0.43
1:B:811:TYR:HB2	1:B:847:ALA:O	2.18	0.43
1:D:391:TYR:H	1:D:391:TYR:HD1	1.66	0.43
1:A:544:ARG:HB3	1:A:547:ARG:NH2	2.32	0.43
1:A:304:LYS:O	1:A:319:ARG:HD3	2.18	0.43
1:D:519:ARG:NH1	1:D:519:ARG:HG3	2.33	0.43
1:C:362:ILE:HG23	1:C:575:PHE:CD1	2.54	0.43
1:C:145:ARG:HB2	1:C:147:TYR:CE1	2.54	0.43
1:A:613:GLY:O	1:A:614:GLU:C	2.56	0.43
1:B:441:ASP:HB3	1:B:447:ALA:HB2	2.00	0.43
1:D:37:LEU:HD12	1:D:71:TRP:CE3	2.54	0.43
1:A:734:LYS:C	1:A:736:SER:N	2.71	0.43
1:A:129:ALA:HB1	1:A:229:ARG:HG2	2.01	0.43
1:C:235:GLY:O	1:C:236:GLU:C	2.57	0.43
1:B:491:ALA:HA	1:B:494:ARG:CG	2.45	0.43
1:A:203:ASN:HD22	1:A:203:ASN:HA	1.57	0.43
1:B:497:GLU:HG2	1:B:498:ILE:HD12	1.99	0.43
1:D:395:PHE:HD2	1:D:594:LEU:HD23	1.84	0.43
2:I:12:DA:H2"	2:I:13:DG:H5'	2.00	0.43
1:C:540:GLU:O	1:C:544:ARG:HG3	2.19	0.43
1:A:579:ASP:HB3	1:A:582:ASN:HB2	2.01	0.43
1:B:312:LEU:HD12	1:B:320:TYR:HB2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:109:DC:H1'	3:F:110:DA:H5"	2.01	0.43
1:A:31:VAL:HG12	1:A:33:TYR:N	2.34	0.43
1:B:727:ILE:HG21	1:B:732:THR:CG2	2.48	0.43
1:D:187:ILE:O	1:D:187:ILE:HG22	2.19	0.43
1:D:206:GLN:HE21	1:D:206:GLN:HA	1.84	0.43
1:B:625:ILE:HG12	1:B:683:MET:CE	2.49	0.43
1:D:569:ALA:O	1:D:571:GLY:N	2.52	0.43
1:C:3:GLU:O	1:C:99:TYR:OH	2.36	0.43
1:D:324:ASN:HD22	1:D:324:ASN:C	2.19	0.43
1:A:854:ILE:CG1	1:A:858:ILE:HG13	2.49	0.43
1:A:854:ILE:HG23	1:A:859:LYS:CB	2.49	0.43
1:C:163:SER:CB	1:C:166:ILE:HD12	2.49	0.43
1:D:411:ASP:CG	1:D:624:SER:HB3	2.39	0.43
1:C:83:LEU:CD2	1:C:83:LEU:N	2.82	0.43
1:C:62:PHE:CD2	1:C:68:ALA:HA	2.54	0.43
1:D:731:GLU:CA	1:D:734:LYS:HG2	2.48	0.43
1:C:465:LYS:NZ	1:C:675:ASN:ND2	2.66	0.43
1:C:111:ALA:HB2	1:C:210:PRO:HB3	2.00	0.43
1:A:298:LEU:HD11	1:A:334:ILE:HG12	1.99	0.43
1:C:775:ASN:OD1	1:C:777:ILE:N	2.50	0.43
1:A:510:VAL:O	1:A:510:VAL:HG23	2.18	0.43
1:B:728:MET:HA	1:B:728:MET:HE3	2.01	0.42
2:G:11:DC:H2"	2:G:12:DA:C8	2.54	0.42
1:A:706:LYS:HE3	3:F:113:DC:H1'	2.01	0.42
1:C:182:ILE:HG21	1:C:329:TYR:CD1	2.54	0.42
1:C:506:PRO:CG	1:C:535:ALA:HB2	2.49	0.42
1:B:499:ILE:HB	1:B:542:LEU:HD13	2.01	0.42
1:B:658:ARG:HH11	1:B:658:ARG:HG3	1.84	0.42
1:A:137:THR:HB	1:A:328:VAL:HG21	2.00	0.42
1:A:653:LYS:HD3	1:A:657:GLU:OE1	2.18	0.42
1:B:195:LYS:O	1:B:199:MET:HB2	2.18	0.42
1:D:15:ILE:HD12	1:D:33:TYR:HB2	2.01	0.42
1:D:426:SER:HB2	1:D:472:PRO:CD	2.45	0.42
1:B:494:ARG:HH12	1:B:495:ASN:HB2	1.83	0.42
1:B:751:ARG:NE	1:B:763:TYR:HB2	2.34	0.42
1:A:874:LYS:HG3	1:A:875:THR:HG23	2.01	0.42
1:A:776:TYR:CD1	1:A:863:LEU:HD11	2.54	0.42
1:B:123:PHE:HA	1:B:124:PRO:HD3	1.77	0.42
1:D:330:ARG:HA	1:D:330:ARG:HD3	1.85	0.42
1:C:267:GLY:HA2	5:C:1018:HOH:O	2.18	0.42
2:K:3:DC:H2"	2:K:4:CTG:H72	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:546:GLN:HE21	1:A:546:GLN:HB2	1.61	0.42
1:A:139:TYR:CE2	1:A:332:LEU:HD21	2.54	0.42
1:A:491:ALA:C	1:A:493:GLN:H	2.21	0.42
1:B:517:ASP:OD1	1:B:519:ARG:HB2	2.20	0.42
1:D:78:ILE:O	1:D:78:ILE:HG13	2.19	0.42
1:A:260:ARG:HH11	1:A:260:ARG:HG2	1.85	0.42
1:A:392:PRO:C	1:A:587:THR:HG21	2.40	0.42
1:A:745:LEU:HD12	1:A:745:LEU:HA	1.83	0.42
1:D:297:GLU:OE1	1:D:338:ARG:NH1	2.52	0.42
1:A:428:GLU:OE2	1:A:428:GLU:N	2.43	0.42
1:D:685:ARG:NH1	1:D:714:ASP:OD2	2.49	0.42
1:D:685:ARG:NH2	1:D:714:ASP:OD2	2.50	0.42
1:D:167:ALA:O	1:D:178:VAL:HB	2.20	0.42
1:A:752:MET:HG2	1:A:889:LEU:HD13	2.02	0.42
1:C:725:LEU:HD11	1:C:750:ARG:HB2	1.99	0.42
1:D:708:TYR:CZ	1:D:728:MET:HG3	2.54	0.42
1:D:819:ILE:HG13	1:D:819:ILE:O	2.19	0.42
1:A:508:LEU:HD22	1:A:508:LEU:N	2.33	0.42
1:B:326:ILE:O	1:B:330:ARG:HG2	2.19	0.42
1:C:298:LEU:O	1:C:299:ASN:CB	2.66	0.42
1:D:512:GLU:CB	1:D:537:SER:HB2	2.50	0.42
1:A:796:PHE:CE1	1:A:813:ARG:HD3	2.55	0.42
1:C:438:PRO:HD2	1:C:441:ASP:OD2	2.19	0.42
1:C:369:ILE:HG12	1:C:474:GLU:HG2	2.02	0.42
1:D:823:GLN:HB3	1:D:823:GLN:HE21	1.60	0.42
1:A:844:LYS:N	1:A:844:LYS:HD2	2.31	0.42
1:C:163:SER:OG	1:C:166:ILE:HG13	2.19	0.42
1:B:119:SER:CB	1:B:124:PRO:HG3	2.42	0.42
1:D:284:ASN:C	1:D:284:ASN:ND2	2.73	0.42
1:D:361:PRO:HD2	2:K:3:DC:OP1	2.19	0.42
1:C:186:ILE:HG22	1:C:187:ILE:N	2.35	0.42
1:A:408:MET:HE3	1:A:655:ALA:HB2	2.02	0.42
2:I:12:DA:H2'	2:I:13:DG:C8	2.54	0.42
1:D:740:ALA:HB1	1:D:774:LEU:HD13	2.02	0.42
1:C:465:LYS:NZ	1:C:675:ASN:HD21	2.17	0.42
1:D:700:GLY:HA2	1:D:753:LEU:CD2	2.49	0.42
1:A:776:TYR:CZ	1:A:777:ILE:HG13	2.54	0.42
1:A:41:CYS:HB3	1:A:58:THR:HG22	2.01	0.42
1:A:514:LEU:CG	1:A:529:LYS:HE3	2.49	0.42
1:C:597:ILE:O	1:C:601:VAL:HG23	2.19	0.42
1:D:880:LEU:HD22	1:D:884:THR:CG2	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:285:GLN:NE2	1:B:286:PRO:HD2	2.35	0.42
1:B:834:PRO:O	1:B:866:MET:HA	2.19	0.42
1:A:3:GLU:HB2	1:A:20:ILE:O	2.20	0.42
1:C:457:SER:O	1:C:459:ASN:N	2.52	0.42
1:A:234:PHE:N	1:A:234:PHE:CD1	2.87	0.42
1:C:528:GLU:HA	1:C:528:GLU:OE2	2.19	0.42
1:C:811:TYR:CE2	1:C:815:ILE:HD13	2.55	0.42
1:C:411:ASP:O	1:C:683:MET:HA	2.20	0.42
1:B:273:TYR:OH	1:B:340:PHE:HB2	2.20	0.42
1:B:9:GLU:HG2	1:B:266:PHE:CD2	2.53	0.42
1:D:434:PHE:HE1	1:D:461:MET:O	2.03	0.42
1:D:461:MET:HB3	1:D:463:TYR:CE1	2.54	0.42
1:A:606:ASN:HD21	1:A:613:GLY:N	2.17	0.42
1:D:475:ILE:HD13	1:D:566:LEU:CD2	2.50	0.42
1:D:566:LEU:HD12	1:D:566:LEU:O	2.20	0.42
1:C:458:PRO:CG	1:C:592:MET:SD	3.08	0.42
1:A:309:ILE:HD12	1:A:312:LEU:HD23	2.01	0.42
2:K:11:DC:H2"	2:K:12:DA:C5'	2.48	0.42
3:J:110:DA:H1'	3:J:111:DT:C5'	2.49	0.42
1:A:779:ILE:HG21	1:A:871:LEU:HD21	2.02	0.42
1:A:221:PHE:C	1:A:224:PRO:HD2	2.39	0.42
1:D:303:LEU:CD1	1:D:326:ILE:HD12	2.49	0.42
1:A:422:GLN:HE21	1:A:422:GLN:HB2	1.70	0.42
1:C:218:VAL:HA	1:C:222:ALA:HB3	2.01	0.42
1:B:224:PRO:HA	1:B:263:ILE:HD12	2.01	0.42
1:B:126:PRO:HB2	1:B:224:PRO:HB2	2.02	0.42
1:A:489:MET:SD	1:A:553:MET:N	2.92	0.42
1:B:489:MET:SD	1:B:490:LEU:N	2.93	0.42
1:C:283:THR:O	1:C:283:THR:HG23	2.20	0.42
1:D:250:VAL:HG22	1:D:263:ILE:HD12	2.02	0.42
1:A:434:PHE:HD1	1:A:435:LYS:O	2.03	0.42
1:A:191:PHE:CZ	1:A:200:GLU:HG2	2.55	0.42
1:D:800:LYS:O	1:D:802:PRO:HD3	2.20	0.42
1:C:482:ARG:O	1:C:486:LYS:HB2	2.19	0.41
1:B:82:ALA:N	1:B:382:GLN:HE21	2.02	0.41
1:A:347:MET:HE3	1:A:347:MET:HA	2.02	0.41
1:A:659:MET:O	1:A:660:GLU:C	2.59	0.41
1:A:556:GLN:HG3	1:A:557:ILE:H	1.85	0.41
1:D:782:VAL:HG12	1:D:783:SER:N	2.33	0.41
1:B:147:TYR:CD1	1:B:147:TYR:N	2.89	0.41
3:H:112:DT:C6	3:H:112:DT:H5'	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:804:HIS:NE2	3:L:110:DA:OP1	2.49	0.41
1:C:197:LEU:C	1:C:197:LEU:HD23	2.40	0.41
1:D:132:PRO:HA	1:D:229:ARG:CZ	2.50	0.41
1:A:789:ALA:HA	1:A:792:ASP:OD1	2.20	0.41
1:C:251:LYS:HB3	1:C:262:ILE:HG13	2.01	0.41
1:A:202:LEU:O	1:A:206:GLN:HG2	2.20	0.41
1:B:501:GLU:HG3	1:B:501:GLU:O	2.19	0.41
1:D:271:LEU:HD21	1:D:356:GLN:HA	2.01	0.41
1:C:96:THR:HG22	1:C:96:THR:O	2.20	0.41
1:D:687:ALA:HB2	1:D:715:MET:SD	2.60	0.41
1:D:208:LYS:O	1:D:209:THR:C	2.58	0.41
1:B:132:PRO:HB3	1:B:194:GLU:OE2	2.20	0.41
1:D:583:ALA:O	1:D:586:ILE:HB	2.21	0.41
1:C:258:GLY:N	5:C:987:HOH:O	2.53	0.41
1:D:523:SER:HB2	1:D:527:LYS:HA	2.02	0.41
1:C:14:SER:HB2	1:C:32:GLU:OE1	2.20	0.41
1:D:49:TYR:CD1	1:D:49:TYR:N	2.88	0.41
1:B:201:TYR:O	1:B:204:PHE:HB3	2.20	0.41
1:B:326:ILE:HG23	1:B:330:ARG:CZ	2.51	0.41
1:D:741:VAL:HG11	1:D:875:THR:O	2.20	0.41
2:G:13:DG:H1'	2:G:14:DC:H5'	2.02	0.41
3:H:105:DC:H2"	3:H:106:DT:O5'	2.21	0.41
1:B:202:LEU:HD21	1:B:238:THR:O	2.19	0.41
1:D:273:TYR:CE2	1:D:341:ILE:HG13	2.56	0.41
1:C:493:GLN:HB2	1:C:549:GLU:OE2	2.20	0.41
1:B:335:ASP:OD2	1:B:341:ILE:HG12	2.20	0.41
1:B:726:LYS:NZ	5:B:970:HOH:O	2.54	0.41
1:A:776:TYR:OH	1:A:854:ILE:HG22	2.20	0.41
1:A:37:LEU:C	1:A:38:PHE:CD1	2.94	0.41
3:F:109:DC:H2"	3:F:110:DA:H5"	2.01	0.41
1:B:771:PHE:HE2	1:B:872:LEU:HB2	1.80	0.41
1:D:760:LEU:CD2	1:D:760:LEU:C	2.88	0.41
1:B:170:LEU:O	1:B:173:GLN:HB2	2.21	0.41
1:D:193:ASN:ND2	1:D:196:GLU:H	2.18	0.41
1:D:243:SER:C	1:D:245:HIS:H	2.24	0.41
1:A:626:TYR:N	1:A:626:TYR:CD1	2.89	0.41
1:B:373:LEU:HD12	1:B:380:ILE:HG22	2.03	0.41
1:C:660:GLU:HB2	1:C:661:PRO:CD	2.41	0.41
1:D:201:TYR:O	1:D:204:PHE:HB3	2.20	0.41
1:B:405:LYS:O	1:B:690:GLY:HA2	2.20	0.41
1:D:373:LEU:CD1	1:D:380:ILE:HG22	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:489:MET:HG3	1:A:552:GLY:HA3	2.03	0.41
1:D:757:GLU:CB	1:D:889:LEU:HD22	2.51	0.41
1:D:442:TYR:HB3	1:D:592:MET:HE2	2.03	0.41
1:D:876:PHE:O	1:D:880:LEU:HB2	2.21	0.41
1:B:544:ARG:HH21	1:B:544:ARG:HG2	1.85	0.41
1:A:294:SER:O	1:A:298:LEU:CD1	2.69	0.41
1:B:75:MET:HA	1:B:78:ILE:HG22	2.03	0.41
1:B:836:ARG:HG3	1:B:865:TRP:O	2.20	0.41
1:B:153:ASN:OD1	1:B:158:ASN:HB3	2.20	0.41
1:D:727:ILE:HB	1:D:733:GLN:OE1	2.19	0.41
1:A:402:ASN:OD1	1:A:403:ARG:N	2.54	0.41
1:C:811:TYR:OH	1:C:822:PRO:HG2	2.21	0.41
1:B:207:GLN:O	1:B:208:LYS:HG3	2.21	0.41
1:D:391:TYR:CD1	1:D:391:TYR:N	2.89	0.41
1:D:289:SER:O	1:D:290:LEU:C	2.58	0.41
1:B:216:TRP:H	1:B:218:VAL:HG23	1.86	0.41
1:D:499:ILE:HG13	1:D:545:ALA:HB3	2.01	0.41
1:B:557:ILE:HD13	1:B:557:ILE:HA	1.87	0.41
1:A:50:PHE:CD2	1:A:56:PRO:HA	2.55	0.41
1:D:151:LEU:HD11	1:D:153:ASN:O	2.21	0.41
1:B:279:LYS:HE3	1:B:280:PHE:CE2	2.55	0.41
2:G:8:DT:C2'	2:G:9:DG:C8	2.98	0.41
1:D:471:VAL:N	1:D:472:PRO:CD	2.84	0.41
1:C:150:ASP:OD2	1:C:317:HIS:CE1	2.73	0.41
1:C:61:LEU:HD23	1:C:62:PHE:O	2.20	0.41
1:D:83:LEU:N	1:D:83:LEU:HD22	2.35	0.41
1:C:658:ARG:HG3	1:C:658:ARG:NH1	2.34	0.41
1:B:426:SER:HB2	1:B:472:PRO:HD2	2.03	0.41
1:B:268:ILE:CG2	1:B:269:SER:N	2.82	0.41
3:L:107:DG:H2"	3:L:108:DT:O5'	2.20	0.41
1:D:274:ILE:CG2	1:D:275:ASP:N	2.84	0.41
1:D:453:VAL:HG23	1:D:454:TYR:CG	2.56	0.41
1:C:428:GLU:HG3	1:C:428:GLU:H	1.66	0.41
3:L:111:DT:H2'	3:L:112:DT:C7	2.51	0.41
1:C:369:ILE:HG21	1:C:577:TYR:CZ	2.55	0.41
1:B:873:GLU:HA	1:B:877:ILE:HB	2.03	0.41
1:C:72:ILE:O	1:C:76:GLU:HG3	2.21	0.41
1:C:434:PHE:CE2	1:C:450:PRO:HB3	2.56	0.41
1:B:260:ARG:HG2	1:B:260:ARG:HH11	1.86	0.41
3:J:105:DC:H2"	3:J:106:DT:C6	2.56	0.41
1:A:777:ILE:CG2	1:A:777:ILE:O	2.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:75:MET:O	1:D:80:LEU:HB2	2.21	0.41
1:D:163:SER:OG	1:D:166:ILE:HG13	2.21	0.41
2:G:3:DC:H6	2:G:3:DC:H2'	1.59	0.41
1:D:147:TYR:CE2	1:D:187:ILE:HD12	2.56	0.41
1:C:284:ASN:HD21	1:C:829:LYS:HZ3	1.69	0.41
3:H:104:DG:C1'	3:H:105:DC:H5"	2.51	0.41
1:D:9:GLU:HG3	1:D:267:GLY:N	2.35	0.41
1:D:454:TYR:CB	1:D:462:MET:HG2	2.50	0.41
1:D:727:ILE:HG21	1:D:732:THR:OG1	2.20	0.41
1:A:458:PRO:HG3	1:A:592:MET:SD	2.60	0.41
1:C:353:ILE:HD12	1:C:357:SER:CB	2.51	0.41
1:D:618:LEU:HD11	1:D:702:TRP:CZ3	2.56	0.41
1:C:483:LYS:HB2	1:C:483:LYS:NZ	2.36	0.41
1:B:313:ARG:HD2	1:B:320:TYR:CE2	2.56	0.41
1:A:806:ARG:HG3	1:A:843:ASP:OD1	2.21	0.41
1:D:164:ILE:HD11	1:D:183:ILE:O	2.21	0.41
3:L:113:DC:H2'	3:L:114:DA:H8	1.84	0.41
1:D:578:TYR:C	1:D:578:TYR:CD1	2.93	0.41
1:A:150:ASP:OD1	1:A:317:HIS:CE1	2.74	0.41
1:B:253:ILE:HD12	1:B:254:GLU:N	2.35	0.41
1:B:377:ASN:N	1:B:377:ASN:ND2	2.69	0.41
1:C:189:MET:O	1:C:191:PHE:CD1	2.74	0.41
1:C:454:TYR:HB2	1:C:462:MET:HG2	2.03	0.41
1:C:854:ILE:HG23	1:C:859:LYS:HB2	2.02	0.41
1:A:457:SER:HA	1:A:458:PRO:HD3	1.93	0.41
1:C:113:PHE:CE1	1:C:213:LEU:HD11	2.55	0.41
1:C:488:TYR:CD2	1:C:519:ARG:HD2	2.56	0.41
1:A:735:SER:HG	3:F:112:DT:P	2.40	0.41
1:D:16:PHE:CE2	1:D:30:GLU:HG3	2.55	0.41
1:B:104:ASP:C	1:B:104:ASP:OD2	2.59	0.41
1:D:846:ILE:O	1:D:846:ILE:HG23	2.21	0.41
1:A:903:PHE:C	1:A:903:PHE:CD1	2.94	0.41
1:D:120:PRO:HD2	1:D:131:HIS:CD2	2.56	0.41
1:A:273:TYR:CE1	1:A:335:ASP:HB2	2.56	0.41
1:A:82:ALA:O	1:A:382:GLN:HB2	2.21	0.41
1:A:389:GLN:HA	1:A:390:PRO:HD3	1.84	0.41
1:C:125:GLU:HA	1:C:125:GLU:OE1	2.21	0.41
1:B:403:ARG:NH2	1:B:889:LEU:HD21	2.35	0.41
1:D:494:ARG:O	1:D:497:GLU:HB3	2.21	0.41
3:F:113:DC:C2'	3:F:114:DA:H5"	2.51	0.41
2:K:2:DG:H3'	2:K:3:DC:H5'	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:839:ASN:ND2	1:A:841:PHE:HB2	2.35	0.41
2:I:12:DA:C8	2:I:12:DA:H5"	2.52	0.41
1:D:499:ILE:HG13	1:D:545:ALA:CB	2.50	0.41
1:D:294:SER:HB3	1:D:300:VAL:O	2.21	0.41
1:A:512:GLU:HA	1:A:513:PRO:HD3	1.98	0.41
1:B:660:GLU:HB2	1:B:661:PRO:HD3	2.02	0.41
1:D:772:ARG:O	1:D:773:GLN:NE2	2.54	0.41
1:B:20:ILE:CG2	1:B:24:GLY:HA2	2.50	0.41
1:D:233:ILE:O	1:D:233:ILE:HG22	2.21	0.41
1:A:863:LEU:HG	1:A:866:MET:HE3	2.03	0.40
1:D:286:PRO:C	1:D:829:LYS:HD2	2.42	0.40
1:C:206:GLN:HE21	1:C:206:GLN:HA	1.86	0.40
1:B:894:LYS:HZ2	1:B:894:LYS:C	2.23	0.40
1:D:186:ILE:CG2	1:D:187:ILE:N	2.83	0.40
1:B:155:PRO:HG2	1:B:156:TYR:CE1	2.56	0.40
1:B:685:ARG:CG	1:B:685:ARG:NH1	2.83	0.40
1:D:273:TYR:HE2	1:D:341:ILE:HG13	1.86	0.40
1:A:757:GLU:HB2	1:A:889:LEU:HD22	2.03	0.40
1:A:413:THR:O	1:A:414:SER:C	2.59	0.40
1:D:455:SER:OG	1:D:676:ASN:HA	2.21	0.40
1:D:867:ASP:HB3	1:D:870:VAL:HB	2.03	0.40
1:A:281:SER:HA	5:A:943:HOH:O	2.21	0.40
1:C:635:LYS:HD2	1:C:635:LYS:HA	1.82	0.40
1:D:541:MET:HA	1:D:544:ARG:CD	2.33	0.40
2:E:7:DA:C2'	2:E:8:DT:C7	2.99	0.40
2:G:15:DC:H2"	2:G:16:DG:O5'	2.22	0.40
1:A:807:GLY:HA2	1:A:810:THR:HG22	2.03	0.40
1:D:643:ASP:HA	1:D:693:LEU:HD23	2.04	0.40
1:C:87:ASP:OD2	1:C:90:LEU:HD13	2.20	0.40
1:A:45:GLN:O	1:A:47:THR:HG23	2.21	0.40
1:B:731:GLU:HA	1:B:734:LYS:HG2	2.02	0.40
1:B:326:ILE:HG23	1:B:330:ARG:NH1	2.36	0.40
1:D:62:PHE:HE2	1:D:71:TRP:HB2	1.86	0.40
1:D:74:ARG:O	1:D:75:MET:C	2.60	0.40
1:D:218:VAL:CG2	1:D:223:ILE:HG13	2.51	0.40
1:A:516:VAL:HB	1:A:526:ILE:HG13	2.03	0.40
1:A:257:TYR:CD2	1:A:786:ASN:HB3	2.57	0.40
1:D:143:ASP:O	1:D:144:ASP:CB	2.69	0.40
1:B:777:ILE:O	1:B:777:ILE:HG22	2.21	0.40
1:D:757:GLU:CG	1:D:889:LEU:HD22	2.52	0.40
1:C:658:ARG:N	1:C:658:ARG:CD	2.83	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:658:ARG:N	1:C:658:ARG:HD2	2.35	0.40
1:C:18:ARG:NH2	1:C:211:VAL:HA	2.37	0.40
1:A:829:LYS:O	1:A:850:SER:HB3	2.21	0.40
1:B:634:ASP:C	1:B:636:VAL:H	2.25	0.40
1:A:372:SER:OG	1:A:477:LYS:NZ	2.38	0.40
1:B:737:THR:HA	1:B:738:PRO:HD3	1.96	0.40
1:D:828:GLU:HB3	1:D:829:LYS:H	1.79	0.40
1:D:289:SER:O	1:D:293:ILE:HG12	2.22	0.40
1:B:273:TYR:HA	1:B:276:LEU:HD12	2.03	0.40
1:D:512:GLU:CB	1:D:513:PRO:CA	2.99	0.40
1:A:653:LYS:HD2	1:A:653:LYS:C	2.42	0.40
1:C:750:ARG:NH1	1:C:750:ARG:HG2	2.37	0.40
1:A:201:TYR:O	1:A:204:PHE:HB3	2.21	0.40
1:A:703:THR:HG21	1:A:707:ARG:NH1	2.36	0.40
1:B:811:TYR:CE2	1:B:815:ILE:HD13	2.56	0.40
2:G:11:DC:H2"	2:G:12:DA:H8	1.87	0.40
1:A:409:SER:O	1:A:686:GLU:HB2	2.21	0.40
1:B:221:PHE:O	1:B:224:PRO:HD2	2.21	0.40
1:D:481:GLN:HB3	1:D:559:ARG:HH11	1.85	0.40
1:B:755:GLU:HB3	1:B:759:SER:OG	2.22	0.40
1:D:711:ASN:HD21	1:D:723:PRO:HB2	1.87	0.40
1:D:597:ILE:HA	1:D:597:ILE:HD12	1.70	0.40
1:A:807:GLY:O	1:A:810:THR:HG22	2.21	0.40
1:B:863:LEU:HD12	1:B:866:MET:HE3	2.04	0.40
1:A:117:VAL:HG22	1:A:133:ILE:HA	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	901/906 (99%)	781 (87%)	105 (12%)	15 (2%)	11 25

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	901/906 (99%)	816 (91%)	79 (9%)	6 (1%)	26 51
1	C	898/906 (99%)	818 (91%)	68 (8%)	12 (1%)	15 33
1	D	895/906 (99%)	769 (86%)	115 (13%)	11 (1%)	16 35
All	All	3595/3624 (99%)	3184 (89%)	367 (10%)	44 (1%)	16 35

All (44) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	524	ASP
1	A	300	VAL
1	A	773	GLN
1	A	825	VAL
1	A	856	ASP
1	C	161	GLU
1	C	300	VAL
1	D	21	ASP
1	D	35	PRO
1	D	729	GLY
1	A	105	HIS
1	B	256	MET
1	B	635	LYS
1	C	172	GLU
1	C	352	LYS
1	C	458	PRO
1	C	622	THR
1	D	80	LEU
1	D	98	ASN
1	A	283	THR
1	A	614	GLU
1	A	738	PRO
1	A	849	PRO
1	B	622	THR
1	C	179	PRO
1	C	506	PRO
1	D	570	LEU
1	D	622	THR
1	A	414	SER
1	A	622	THR
1	A	869	THR
1	C	576	ARG
1	D	414	SER

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Mol	Chain	Res	Type
1	B	179	PRO
1	C	155	PRO
1	A	846	ILE
1	A	729	GLY
1	B	300	VAL
1	B	513	PRO
1	C	470	VAL
1	C	513	PRO
1	D	78	ILE
1	D	526	ILE
1	A	822	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	792/803 (99%)	742 (94%)	50 (6%)	22 44
1	B	780/803 (97%)	738 (95%)	42 (5%)	27 52
1	C	794/803 (99%)	755 (95%)	39 (5%)	31 58
1	D	743/803 (92%)	702 (94%)	41 (6%)	27 51
All	All	3109/3212 (97%)	2937 (94%)	172 (6%)	27 51

All (172) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	LYS
1	A	59	ARG
1	A	64	ASN
1	A	70	GLN
1	A	73	LYS
1	A	98	ASN
1	A	105	HIS
1	A	203	ASN
1	A	213	LEU
1	A	229	ARG

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Mol	Chain	Res	Type
1	A	242	LEU
1	A	253	ILE
1	A	273	TYR
1	A	298	LEU
1	A	304	LYS
1	A	314	GLU
1	A	318	GLN
1	A	319	ARG
1	A	372	SER
1	A	403	ARG
1	A	411	ASP
1	A	451	SER
1	A	466	ASP
1	A	467	ARG
1	A	475	ILE
1	A	479	PHE
1	A	503	LEU
1	A	544	ARG
1	A	546	GLN
1	A	556	GLN
1	A	587	THR
1	A	618	LEU
1	A	631	LYS
1	A	653	LYS
1	A	658	ARG
1	A	728	MET
1	A	731	GLU
1	A	743	LYS
1	A	745	LEU
1	A	758	GLU
1	A	772	ARG
1	A	825	VAL
1	A	826	GLU
1	A	844	LYS
1	A	848	TRP
1	A	849	PRO
1	A	860	ASP
1	A	861	ASP
1	A	888	LYS
1	A	903	PHE
1	B	43	GLU
1	B	45	GLN

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Mol	Chain	Res	Type
1	B	61	LEU
1	B	66	ARG
1	B	90	LEU
1	B	93	LEU
1	B	113	PHE
1	B	116	GLU
1	B	164	ILE
1	B	234	PHE
1	B	312	LEU
1	B	316	ASN
1	B	378	LYS
1	B	379	VAL
1	B	384	ARG
1	B	403	ARG
1	B	411	ASP
1	B	421	ARG
1	B	435	LYS
1	B	468	ASP
1	B	475	ILE
1	B	479	PHE
1	B	489	MET
1	B	495	ASN
1	B	511	ASP
1	B	522	PHE
1	B	558	ASN
1	B	573	VAL
1	B	643	ASP
1	B	646	HIS
1	B	658	ARG
1	B	685	ARG
1	B	702	TRP
1	B	728	MET
1	B	734	LYS
1	B	758	GLU
1	B	766	GLU
1	B	772	ARG
1	B	818	ASN
1	B	843	ASP
1	B	856	ASP
1	B	894	LYS
1	C	11	ILE
1	C	27	ARG

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Mol	Chain	Res	Type
1	C	55	LYS
1	C	58	THR
1	C	83	LEU
1	C	106	THR
1	C	200	GLU
1	C	255	ASN
1	C	257	TYR
1	C	279	LYS
1	C	284	ASN
1	C	314	GLU
1	C	356	GLN
1	C	370	PHE
1	C	399	PRO
1	C	428	GLU
1	C	439	LEU
1	C	468	ASP
1	C	474	GLU
1	C	511	ASP
1	C	525	GLU
1	C	561	LEU
1	C	562	LEU
1	C	572	ASN
1	C	587	THR
1	C	592	MET
1	C	640	LYS
1	C	645	ASN
1	C	658	ARG
1	C	667	PHE
1	C	672	GLU
1	C	702	TRP
1	C	760	LEU
1	C	762	GLU
1	C	843	ASP
1	C	856	ASP
1	C	874	LYS
1	C	880	LEU
1	C	898	PHE
1	D	14	SER
1	D	32	GLU
1	D	125	GLU
1	D	143	ASP
1	D	200	GLU

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Mol	Chain	Res	Type
1	D	255	ASN
1	D	257	TYR
1	D	260	ARG
1	D	284	ASN
1	D	317	HIS
1	D	324	ASN
1	D	372	SER
1	D	391	TYR
1	D	411	ASP
1	D	413	THR
1	D	428	GLU
1	D	439	LEU
1	D	468	ASP
1	D	474	GLU
1	D	477	LYS
1	D	479	PHE
1	D	484	GLU
1	D	508	LEU
1	D	520	PHE
1	D	521	ASP
1	D	522	PHE
1	D	524	ASP
1	D	557	ILE
1	D	558	ASN
1	D	562	LEU
1	D	649	ASP
1	D	686	GLU
1	D	702	TRP
1	D	731	GLU
1	D	776	TYR
1	D	777	ILE
1	D	786	ASN
1	D	823	GLN
1	D	828	GLU
1	D	874	LYS
1	D	880	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (94) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	GLN
1	A	64	ASN

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Mol	Chain	Res	Type
1	A	98	ASN
1	A	112	ASN
1	A	158	ASN
1	A	203	ASN
1	A	206	GLN
1	A	284	ASN
1	A	285	GLN
1	A	376	GLN
1	A	389	GLN
1	A	422	GLN
1	A	505	ASN
1	A	546	GLN
1	A	556	GLN
1	A	558	ASN
1	A	572	ASN
1	A	602	ASN
1	A	606	ASN
1	A	646	HIS
1	A	678	GLN
1	A	775	ASN
1	A	864	HIS
1	B	70	GLN
1	B	171	GLN
1	B	207	GLN
1	B	255	ASN
1	B	284	ASN
1	B	285	GLN
1	B	316	ASN
1	B	318	GLN
1	B	376	GLN
1	B	377	ASN
1	B	382	GLN
1	B	495	ASN
1	B	539	ASN
1	B	558	ASN
1	B	591	GLN
1	B	606	ASN
1	B	646	HIS
1	B	733	GLN
1	B	742	GLN
1	B	754	GLN
1	B	775	ASN

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Mol	Chain	Res	Type
1	B	812	ASN
1	B	818	ASN
1	C	45	GLN
1	C	112	ASN
1	C	128	GLN
1	C	173	GLN
1	C	206	GLN
1	C	207	GLN
1	C	255	ASN
1	C	284	ASN
1	C	285	GLN
1	C	318	GLN
1	C	444	ASN
1	C	493	GLN
1	C	539	ASN
1	C	556	GLN
1	C	558	ASN
1	C	572	ASN
1	C	675	ASN
1	C	678	GLN
1	C	711	ASN
1	C	864	HIS
1	D	10	GLN
1	D	206	GLN
1	D	207	GLN
1	D	245	HIS
1	D	255	ASN
1	D	284	ASN
1	D	285	GLN
1	D	318	GLN
1	D	339	GLN
1	D	444	ASN
1	D	480	ASN
1	D	495	ASN
1	D	505	ASN
1	D	507	ASN
1	D	539	ASN
1	D	546	GLN
1	D	558	ASN
1	D	572	ASN
1	D	645	ASN
1	D	675	ASN

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Mol	Chain	Res	Type
1	D	678	GLN
1	D	711	ASN
1	D	754	GLN
1	D	773	GLN
1	D	786	ASN
1	D	787	ASN
1	D	818	ASN
1	D	823	GLN

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	$\#\|Z\| > 2$
2	CTG	E	4	3,2	16,23,24	0.69	0	17,35,38	1.03	2 (11%)
2	CTG	G	4	3,2	16,23,24	0.72	0	17,35,38	1.00	2 (11%)
2	CTG	I	4	3,2	16,23,24	0.70	0	17,35,38	1.00	2 (11%)
2	CTG	K	4	3,2	16,23,24	0.77	1 (6%)	17,35,38	0.75	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CTG	E	4	3,2	-	0/7/45/46	0/2/2/2
2	CTG	G	4	3,2	-	0/7/45/46	0/2/2/2
2	CTG	I	4	3,2	-	0/7/45/46	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CTG	K	4	3,2	-	0/7/45/46	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	4	CTG	C1'-N1	2.05	1.48	1.45

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	4	CTG	C2'-C1'-N1	-3.09	111.41	115.64
2	G	4	CTG	C2'-C1'-N1	-2.83	111.76	115.64
2	I	4	CTG	C2'-C1'-N1	-2.74	111.88	115.64
2	I	4	CTG	N3-C2-N1	-2.59	114.23	116.82
2	E	4	CTG	N3-C2-N1	-2.43	114.39	116.82
2	K	4	CTG	N3-C2-N1	-2.31	114.52	116.82
2	G	4	CTG	N3-C2-N1	-2.05	114.78	116.82

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	4	CTG	3	0
2	G	4	CTG	3	0
2	I	4	CTG	1	0
2	K	4	CTG	2	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

1 ligand is 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	$\#\|Z\| > 2$
4	SO4	C	907	-	4,4,4	0.27	0	6,6,6	0.09	0

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
4	SO4	C	907	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	903/906 (99%)	0.31	65 (7%) 18 16	24, 53, 144, 162	1 (0%)
1	B	903/906 (99%)	0.37	68 (7%) 17 14	20, 59, 157, 172	0
1	C	900/906 (99%)	-0.01	7 (0%) 87 87	17, 47, 89, 109	0
1	D	897/906 (99%)	0.86	138 (15%) 3 2	48, 98, 134, 169	0
2	E	17/18 (94%)	0.44	1 (5%) 26 23	70, 88, 124, 132	0
2	G	17/18 (94%)	-0.20	0 100 100	45, 57, 79, 92	0
2	I	17/18 (94%)	-0.38	0 100 100	32, 38, 85, 94	0
2	K	17/18 (94%)	0.78	2 (11%) 6 4	59, 126, 147, 151	0
3	F	14/14 (100%)	0.54	0 100 100	85, 117, 130, 134	0
3	H	14/14 (100%)	0.15	0 100 100	53, 70, 83, 85	0
3	J	14/14 (100%)	-0.38	0 100 100	30, 45, 93, 99	0
3	L	14/14 (100%)	1.04	3 (21%) 1 1	120, 131, 135, 136	0
All	All	3727/3752 (99%)	0.38	284 (7%) 17 14	17, 62, 132, 172	1 (0%)

All (284) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	510	VAL	15.6
1	B	513	PRO	13.4
1	B	507	ASN	13.4
1	B	511	ASP	10.9
1	B	506	PRO	10.3
1	D	510	VAL	10.1
1	A	503	LEU	9.2
1	B	504	HIS	9.1
1	B	508	LEU	8.8
1	A	256	MET	8.6
1	D	535	ALA	8.4

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Mol	Chain	Res	Type	RSRZ
1	D	257	TYR	8.3
1	D	538	LEU	8.2
1	D	817	GLY	8.1
1	B	498	ILE	8.0
1	D	534	SER	8.0
1	A	508	LEU	7.9
1	B	512	GLU	7.8
1	D	491	ALA	7.6
1	B	303	LEU	7.3
1	B	509	SER	7.3
1	D	511	ASP	7.1
1	D	546	GLN	7.0
1	D	514	LEU	7.0
1	D	509	SER	6.9
1	D	545	ALA	6.9
1	A	817	GLY	6.9
1	B	516	VAL	6.8
1	B	528	GLU	6.7
1	D	841	PHE	6.4
1	C	303	LEU	6.4
1	A	504	HIS	6.3
1	D	303	LEU	6.3
1	D	256	MET	6.3
1	D	520	PHE	6.1
1	D	44	SER	6.0
1	B	532	LYS	6.0
1	D	539	ASN	6.0
1	B	503	LEU	6.0
1	D	526	ILE	5.9
1	A	502	ALA	5.9
1	B	530	ILE	5.9
1	D	550	VAL	5.9
1	A	498	ILE	5.7
1	B	523	SER	5.6
1	B	514	LEU	5.4
1	D	543	PHE	5.4
1	D	858	ILE	5.3
1	D	508	LEU	5.3
1	D	513	PRO	5.2
1	B	521	ASP	5.2
1	A	848	TRP	5.1
1	A	811	TYR	5.0

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Mol	Chain	Res	Type	RSRZ
1	B	533	LEU	5.0
1	D	547	ARG	4.9
1	D	529	LYS	4.9
1	D	819	ILE	4.8
1	D	862	VAL	4.8
1	D	548	THR	4.8
1	B	502	ALA	4.8
1	B	819	ILE	4.8
1	A	513	PRO	4.6
1	B	524	ASP	4.6
1	B	538	LEU	4.6
1	B	499	ILE	4.6
1	D	523	SER	4.6
1	D	793	VAL	4.6
1	D	533	LEU	4.5
1	A	514	LEU	4.5
1	D	512	GLU	4.4
1	D	794	GLY	4.4
1	D	792	ASP	4.3
1	D	80	LEU	4.2
1	D	820	ASP	4.2
1	D	254	GLU	4.2
1	D	868	TYR	4.2
1	A	257	TYR	4.2
1	D	847	ALA	4.1
1	A	522	PHE	4.1
1	A	526	ILE	4.1
1	A	532	LYS	4.1
1	B	314	GLU	4.0
1	D	388	VAL	4.0
1	A	786	ASN	4.0
1	B	310	SER	4.0
1	D	395	PHE	3.9
1	B	539	ASN	3.9
1	D	771	PHE	3.9
1	B	505	ASN	3.9
1	B	173	GLN	3.9
1	A	535	ALA	3.9
1	A	523	SER	3.9
1	B	536	LYS	3.9
1	B	166	ILE	3.8
1	B	172	GLU	3.8

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Mol	Chain	Res	Type	RSRZ
1	D	198	LEU	3.8
1	A	490	LEU	3.8
1	B	520	PHE	3.8
1	A	541	MET	3.8
1	D	541	MET	3.7
1	D	536	LYS	3.7
1	A	821	ALA	3.7
1	D	811	TYR	3.7
1	A	857	LEU	3.6
1	B	527	LYS	3.6
1	B	306	ASP	3.6
1	A	542	LEU	3.6
2	K	3	DC	3.6
1	A	831	TYR	3.5
1	D	791	TYR	3.5
1	D	540	GLU	3.5
1	B	518	TYR	3.5
1	D	393	GLY	3.5
1	B	535	ALA	3.5
1	D	175	GLY	3.5
1	A	799	PRO	3.5
1	D	799	PRO	3.4
1	D	518	TYR	3.4
1	D	774	LEU	3.4
1	A	785	ALA	3.4
1	A	512	GLU	3.4
1	B	542	LEU	3.3
1	D	517	ASP	3.3
1	D	802	PRO	3.3
1	B	500	LYS	3.2
1	B	496	GLY	3.2
1	A	789	ALA	3.2
1	B	534	SER	3.2
1	A	543	PHE	3.2
1	D	170	LEU	3.2
1	A	776	TYR	3.2
1	D	833	LEU	3.2
1	A	506	PRO	3.2
1	A	505	ASN	3.2
1	A	507	ASN	3.2
1	D	488	TYR	3.2
1	D	515	ASP	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	818	ASN	3.2
1	D	152	LEU	3.1
1	B	522	PHE	3.1
1	B	537	SER	3.1
1	D	855	THR	3.0
1	A	801	CYS	3.0
1	D	795	GLY	3.0
1	A	509	SER	3.0
1	D	83	LEU	3.0
1	D	522	PHE	3.0
1	D	863	LEU	3.0
1	A	515	ASP	3.0
1	D	801	CYS	3.0
1	D	490	LEU	3.0
1	D	20	ILE	3.0
1	D	115	ILE	3.0
1	D	544	ARG	2.9
1	B	492	ALA	2.9
1	D	8	VAL	2.9
1	B	865	TRP	2.9
1	A	491	ALA	2.9
1	D	191	PHE	2.9
1	B	526	ILE	2.9
1	D	42	PRO	2.9
1	A	495	ASN	2.9
1	D	391	TYR	2.8
1	D	41	CYS	2.8
1	D	489	MET	2.8
1	D	178	VAL	2.8
1	D	266	PHE	2.8
1	A	903	PHE	2.8
1	D	147	TYR	2.8
1	B	307	GLY	2.8
1	A	499	ILE	2.8
1	D	183	ILE	2.8
1	D	162	TRP	2.8
1	D	259	SER	2.7
1	B	171	GLN	2.7
1	D	857	LEU	2.7
1	A	536	LYS	2.7
1	B	501	GLU	2.7
1	D	61	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	498	ILE	2.7
1	A	538	LEU	2.7
1	B	311	LYS	2.7
1	D	519	ARG	2.7
3	L	114	DA	2.7
1	B	497	GLU	2.7
1	D	241	ARG	2.7
1	D	735	SER	2.7
1	B	495	ASN	2.6
1	A	516	VAL	2.6
1	A	518	TYR	2.6
1	A	820	ASP	2.6
1	D	33	TYR	2.6
1	D	767	PHE	2.6
1	D	153	ASN	2.6
1	D	859	LYS	2.6
1	D	800	LYS	2.6
1	B	179	PRO	2.6
1	D	182	ILE	2.6
1	B	529	LYS	2.6
1	A	548	THR	2.6
1	D	542	LEU	2.6
2	K	5	DG	2.6
1	D	813	ARG	2.6
1	A	815	ILE	2.6
1	D	318	GLN	2.5
1	D	301	GLY	2.5
1	D	305	TYR	2.5
1	B	540	GLU	2.5
1	C	522	PHE	2.5
1	D	796	PHE	2.5
1	B	836	ARG	2.5
1	D	302	LYS	2.5
1	D	255	ASN	2.5
1	C	152	LEU	2.5
1	D	494	ARG	2.5
1	A	497	GLU	2.5
1	A	835	LEU	2.5
1	B	515	ASP	2.5
1	D	205	TRP	2.4
1	D	824	VAL	2.4
1	D	317	HIS	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	851	GLY	2.4
1	B	799	PRO	2.4
1	D	57	CYS	2.4
1	D	527	LYS	2.4
1	D	787	ASN	2.4
1	B	803	PHE	2.4
1	D	105	HIS	2.4
1	B	861	ASP	2.4
1	A	793	VAL	2.3
1	B	817	GLY	2.3
1	D	789	ALA	2.3
1	A	540	GLU	2.3
1	D	821	ALA	2.3
1	B	178	VAL	2.3
1	D	831	TYR	2.3
1	A	539	ASN	2.3
3	L	103	DG	2.3
1	A	533	LEU	2.3
1	A	528	GLU	2.3
1	D	164	ILE	2.3
1	D	323	TYR	2.3
1	B	543	PHE	2.3
1	C	899	ASP	2.3
1	D	860	ASP	2.3
1	D	499	ILE	2.3
1	D	505	ASN	2.2
1	D	797	PRO	2.2
1	D	551	ALA	2.2
1	A	846	ILE	2.2
1	D	179	PRO	2.2
1	D	258	GLY	2.2
1	D	201	TYR	2.2
1	D	812	ASN	2.2
1	A	500	LYS	2.2
1	A	809	LEU	2.2
1	A	496	GLY	2.2
1	B	525	GLU	2.2
1	D	150	ASP	2.2
1	D	16	PHE	2.1
1	C	46	ALA	2.1
1	B	186	ILE	2.1
1	A	865	TRP	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	43	GLU	2.1
1	B	895	ALA	2.1
1	A	537	SER	2.1
1	D	167	ALA	2.1
1	A	795	GLY	2.1
1	C	900	MET	2.1
1	D	390	PRO	2.1
1	D	199	MET	2.1
1	D	865	TRP	2.1
1	A	555	ALA	2.1
1	B	183	ILE	2.1
1	A	828	GLU	2.1
1	D	552	GLY	2.0
1	A	784	SER	2.0
1	A	347	MET	2.0
1	C	166	ILE	2.0
1	D	788	ILE	2.0
3	L	104	DG	2.0
1	D	877	ILE	2.0
2	E	1	DC	2.0
1	D	506	PRO	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	CTG	G	4	22/23	0.93	0.17	-	65,69,71,71	0
2	CTG	I	4	22/23	0.96	0.17	-	44,50,54,54	0
2	CTG	K	4	22/23	0.64	0.37	-	144,145,151,152	0
2	CTG	E	4	22/23	0.86	0.22	-	102,103,106,107	0

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	SO4	C	907	5/5	0.96	0.12	-1.02	89,90,90,90	0

6.5 Other polymers

There are no such residues in this entry.