Full wwPDB X-ray Structure Validation Report (i)

Aug 30, 2023 – 02:24 AM EDT

PDB ID	:	3M3Y
Title	:	RNA polymerase II elongation complex C
Authors	:	Wang, D.; Zhu, G.; Huang, X.; Lippard, S.J.
Deposited on	:	2010-03-10
Resolution	:	3.18 Å(reported)

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

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

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

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

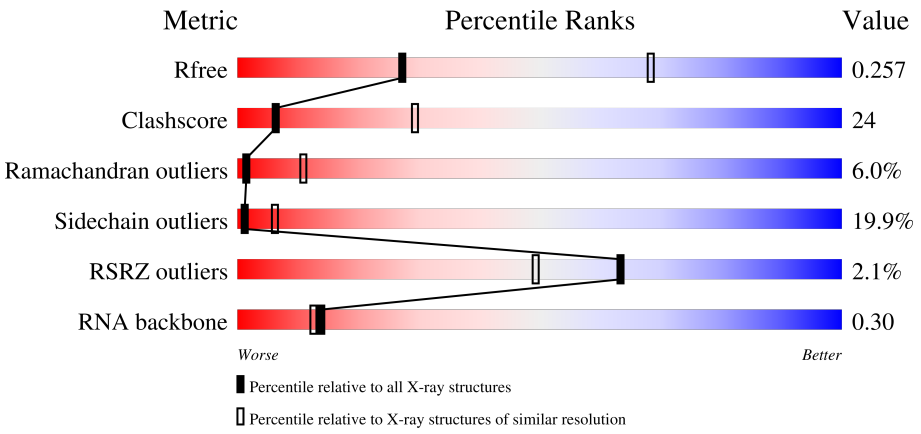
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.18 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1467 (3.20-3.16)
Clashscore	141614	1599 (3.20-3.16)
Ramachandran outliers	138981	1574 (3.20-3.16)
Sidechain outliers	138945	1573 (3.20-3.16)
RSRZ outliers	127900	1423 (3.20-3.16)
RNA backbone	3102	1054 (3.50-2.86)

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

Mol	Chain	Length	Quality of chain
1	A	1733	.% 41% 30% 9% • 20%
2	B	1224	2% 46% 33% 9% • 10%
3	C	318	40% 32% 12% 16%
4	E	215	2% 57% 34% 8%

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Mol	Chain	Length	Quality of chain
5	F	155	29% 20% 5% 46%
6	H	146	3% 45% 32% 13% 9%
7	I	122	56% 29% 13%
8	J	70	37% 37% 16% 7%
9	K	120	% 68% 25% 5%
10	L	70	7% 34% 19% 13% 34%
11	R	11	9% 27% 27% 45%
12	T	28	36% 18% 50% 32%
13	N	14	21% 100%

2 Entry composition (i)

There are 16 unique types of molecules in this entry. The entry contains 29241 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-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1395	10969	6917	1923	2068	61	0	0	0

- Molecule 2 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	1106	8792	5568	1538	1631	55	0	0	0

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	266	2095	1317	348	417	13	0	0	0

- Molecule 4 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	E	214	1752	1111	309	321	11	0	0	0

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	F	84	679	434	115	127	3	0	0	0

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	H	133	1068	673	180	211	4	0	0	0

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
7	I	119	971	596	179	186	10	0	0	0

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
8	J	65	532	339	93	94	6	0	0	0

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
9	K	114	919	590	156	171	2	0	0	0

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	L	46	363	224	72	63	4	0	0	0

- Molecule 11 is a RNA chain called RNA (5'-R(*AP*UP*GP*GP*AP*GP*AP*GP*GP*AP *C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
11	R	11	240	108	50	72	10	0	0	0

- Molecule 12 is a DNA chain called DNA (28-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
12	T	28	550	265	92	166	27	0	0	0

- Molecule 13 is a DNA chain called DNA (5'-D(*GP*TP*GP*GP*TP*TP*AP*TP*GP*GP *GP*TP*AP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
13	N	14	293	140	55	85	13	0	0	0

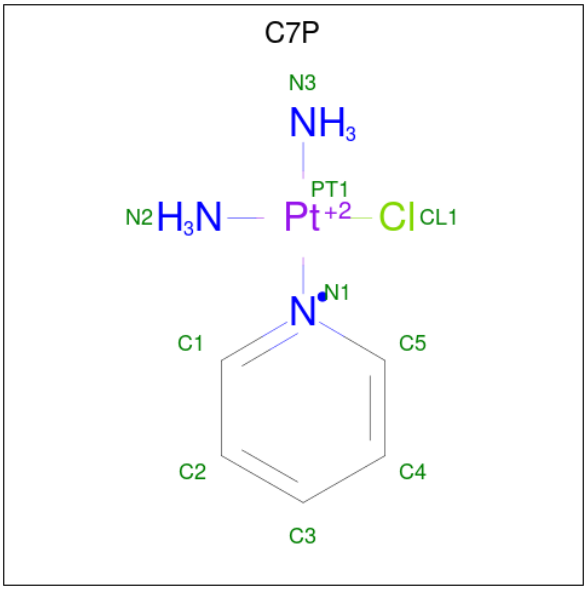
- Molecule 14 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	A	2	Total Zn 2 2	0	0
14	B	1	Total Zn 1 1	0	0
14	C	1	Total Zn 1 1	0	0
14	I	2	Total Zn 2 2	0	0
14	J	1	Total Zn 1 1	0	0
14	L	1	Total Zn 1 1	0	0

- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	A	1	Total Mg 1 1	0	0

- Molecule 16 is cis-diammine(pyridine)chloroplatinum(II) (three-letter code: C7P) (formula: $C_5H_{11}ClN_3Pt$).



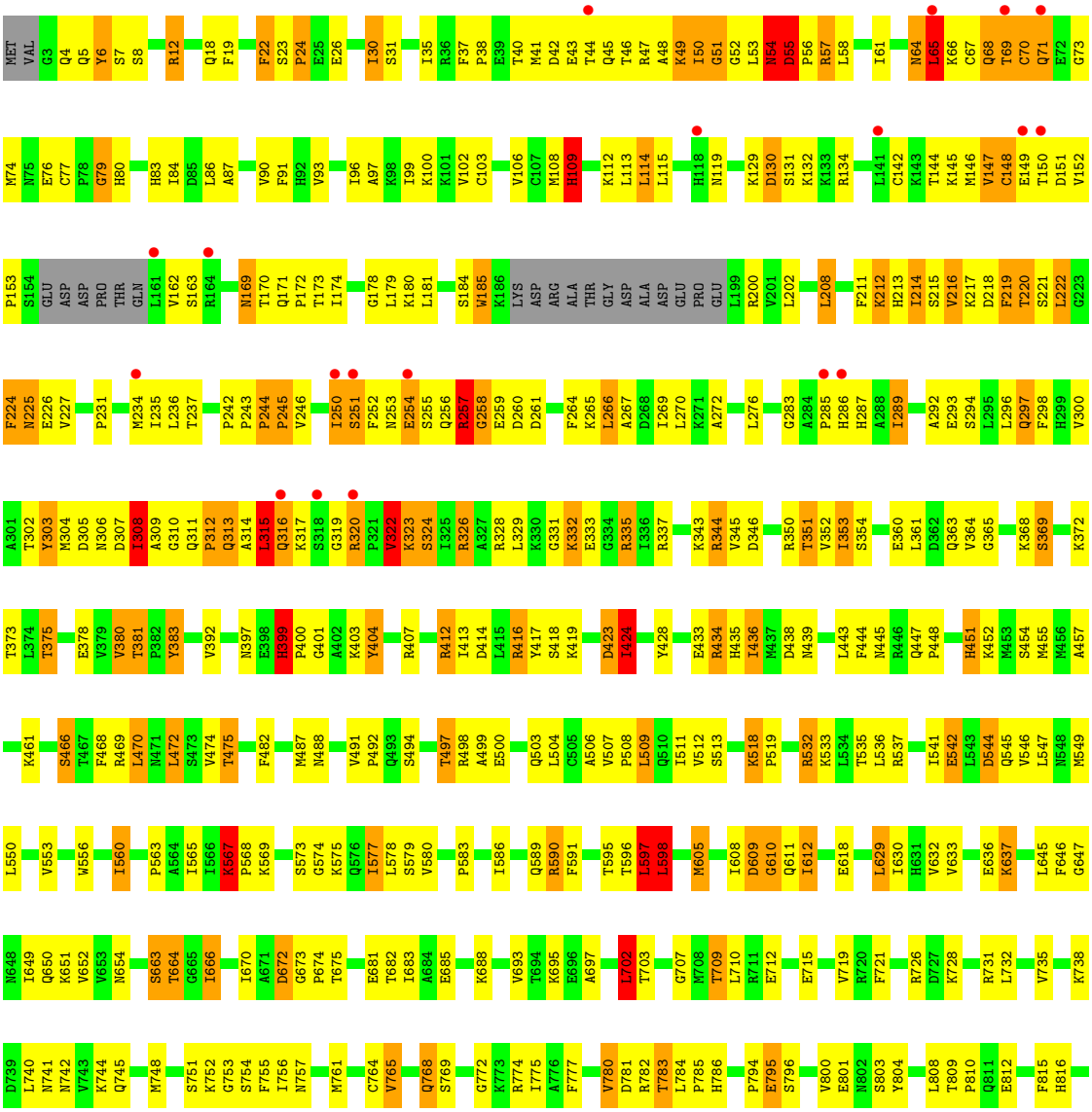
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	T	1	Total C N Pt 9 5 3 1	0	0

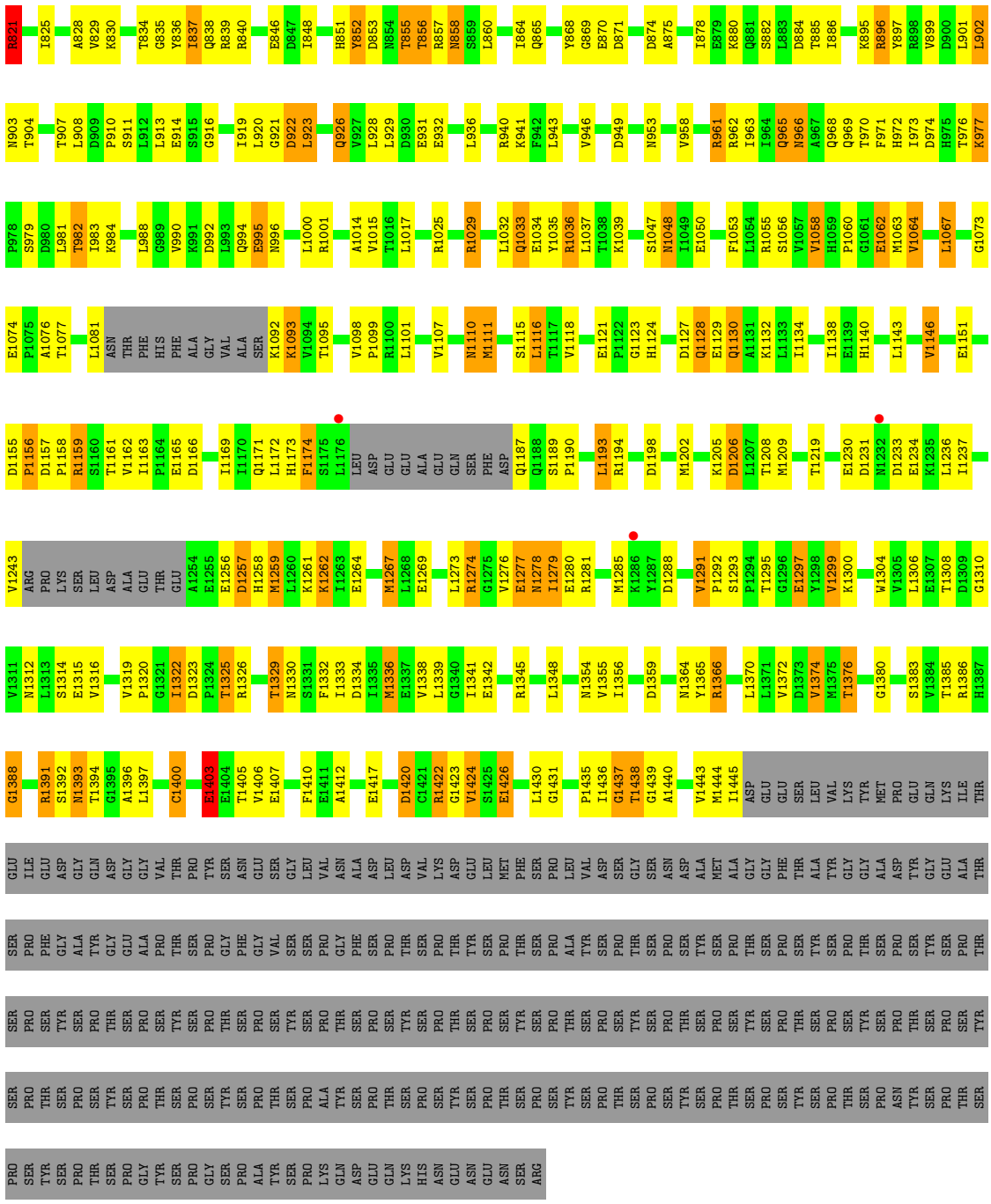
3 Residue-property plots (i)

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

- Molecule 1: DNA-directed RNA polymerase II subunit RPB1

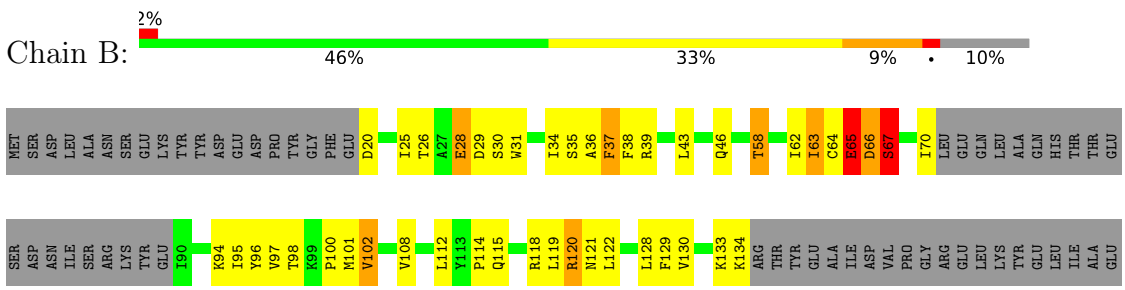
Chain A:

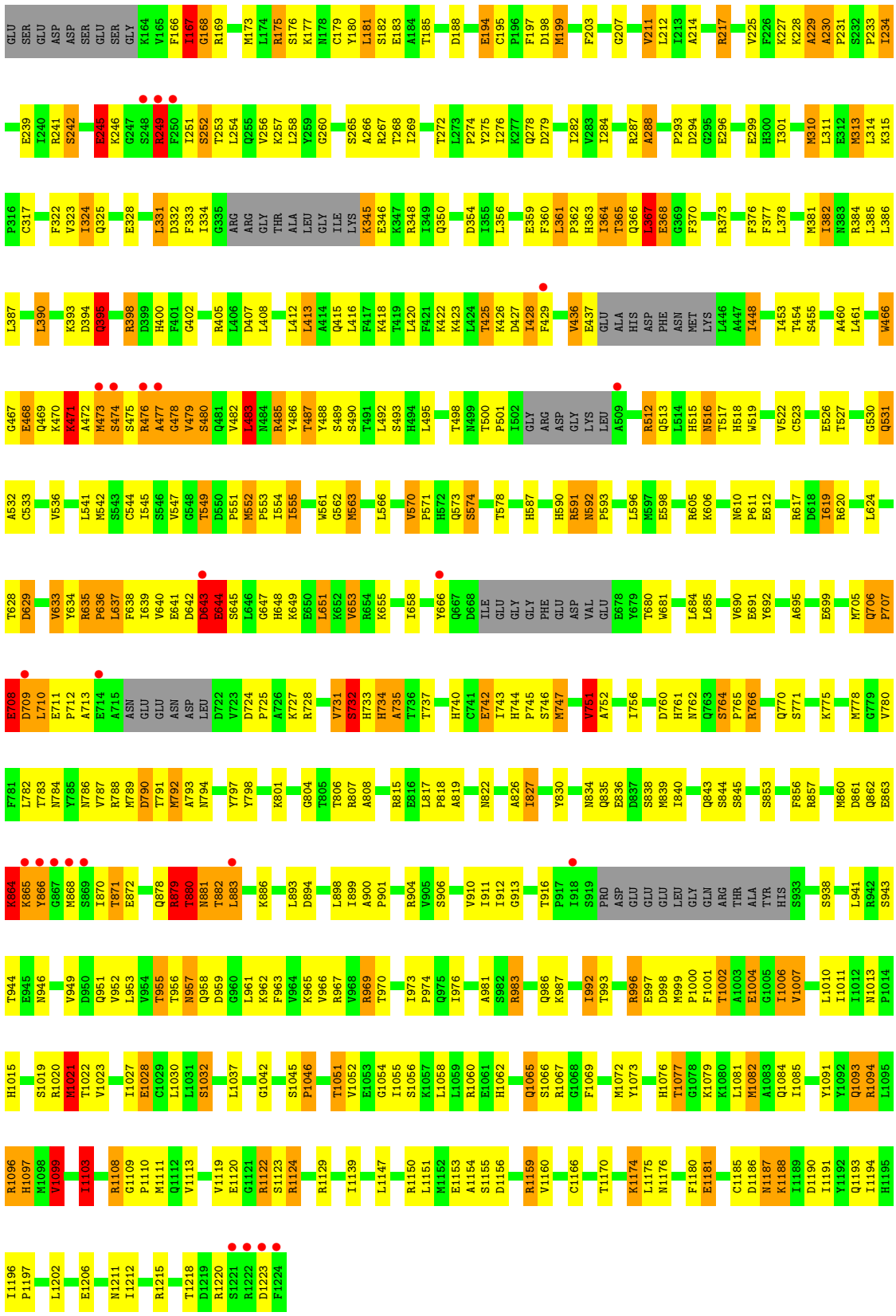




• Molecule 2: DNA-directed RNA polymerase II subunit RPB2

Chain B:





- Molecule 3: DNA-directed RNA polymerase II subunit RPB3

Chain C: 40% 32% 12% 16%

MET SER E3 E4 G5 P6 K9 I10 R11 K15 D16 N17 V18 D19 F20 I21 L22 S23 N24 V25 D26 L27 A28 M29 S32 R35 V36 M37 I38 A39 E40 I41 P42 T43 L44 A45 I46 D47 S48 T53 N54 T55 T56 V57 L58 E61 F62 I63 R66 L67 G68 L69 I70

Q73 S74 M75 D76 I77 L80 E81 E89 C92 D93 V97 V98 L99 T100 L101 Q102 E106 S109 T110 T111 N112 K116 I120 V121 S122 N123 L124 M125 G126 R127 N128 I129 I133 D136 K137 N140 G141 V142 L143 I144 C145 K146 L147 R148 K149 G150 Q151

K154 C157 K160 K161 G162 I163 A164 H167 A168 K169 W170 G171 P172 A173 A174 A175 I176 E177 F178 E179 Y180 D181 P182 W183 N184 K185 L186 K187 H188 T189 D190 Y191 W192 S197 W201 P202 Q203 S204 K205 N206 D211 N214 E215 K222 A223 Q224 A225 D226 T227 F228 Y229 M230

N231 V235 G236 S237 I238 P239 V240 D241 Q242 V243 V244 V245 R246 D249 T250 L251 Q252 K253 K254 V255 I258 L259 L260 A261 L262 T263 Q264 D268 LYS VAL ASN PHE ALA SER GLY ASP ASN ASN THR ALA SER ASN MET LEU GLY SER ASN GLU ASP VAL MET MET THR GLY ALA GLU

GLN ASP PRO TYR SER ASN ALA SER GLN MET GLY ASN THR GLY SER GLY GLY TYR ASP ASN ALA TRP

- Molecule 4: DNA-directed RNA polymerases I, II, and III subunit RPABC1

Chain E: 2% 57% 34% 8%

MET D2 Q3 E4 I9 W13 R14 A15 F16 V19 M22 V23 T31 Q32 E36 L37 E40 A44 S49 M50 G51 Q54 R55 K56 M57 M58 S59 P64 I65 E66 F72 G76 S77 L78 W79 V80 E81 P86 S87 V88 G89 V90 K91 T92 M93 K94

T95 F96 V97 I98 H99 I100 Q101 E102 K103 N104 F105 F110 I116 T117 P118 S119 A120 M121 K122 L123 S126 I127 P128 P129 A130 T131 T134 F135 N136 E137 L140 I144 T145 H146 H147 E148 L149 V150 P151 K152 L156 S157 S158 D159 E160 K161 R162 E163 L164 L165 K166 R167 Y168

R169 L175 Q179 D182 Y187 L190 K191 R192 V196 K197 I198 I199 R200 K201 S202 E203 T204 S205 Y208 Y211 R212 M215

- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain F: 29% 20% 5% • 46%

MET SER ASP TYR GLU GLU ALA PHE ASN ASP GLY ASN GLU ASN PHE GLU ASP PHE ASP VAL GLU HIS PHE SER ASP GLU GLU THR TYR GLU GLU LYS PRO GLN PHE LYS ASP GLY GLU THR THR ASP ALA ASN GLY LYS THR ILE VAL THR GLY GLY ASN GLY PRO GLU ASP PHE GLN GLN

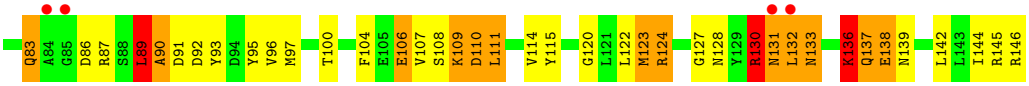
HIS GLU GLN ILE ARG ARG LYS THR LEU LYS GLU K72 A73 I74 P75 K76 R79 A80 T81 T82 P83 T86 K87 Y88 E89 R90 A91 R92 I93 R97 V109 D110 L111 E112 G113 E114 T115 D116 R119 E124 I130 P131 L132 V133 I134 R135 R136 D140 F143 E144 D145

W146 S147 V148 E149 E150 D154 L155

- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC3

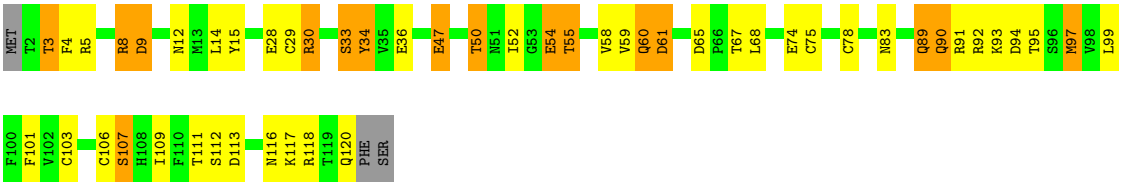
Chain H: 3% 45% 32% 13% • 9%

MET S2 N3 T4 L5 Q11 V15 D16 P17 G18 R19 Y20 N21 C24 R25 I26 S30 T31 T32 Q33 D34 Q35 C36 K37 L38 T39 L40 D41 V44 F47 L55 T58 I59 A60 S61 S62 L63 ASN LEU GLU ASP THR PRO ALA ASN ASP SER SER ALA T76 R77 S78



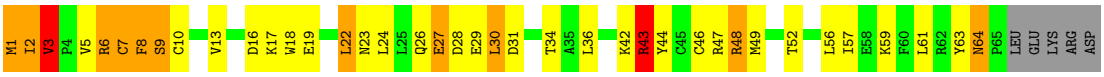
• Molecule 7: DNA-directed RNA polymerase II subunit RPB9

Chain I:



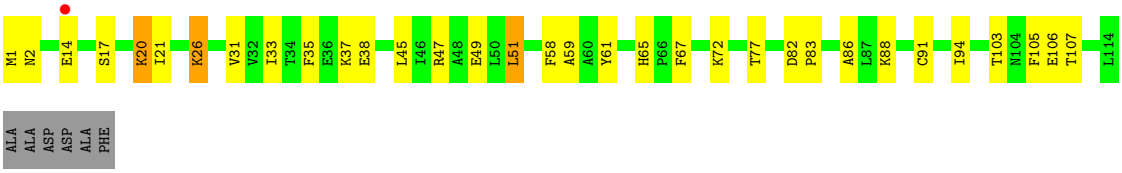
• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J:



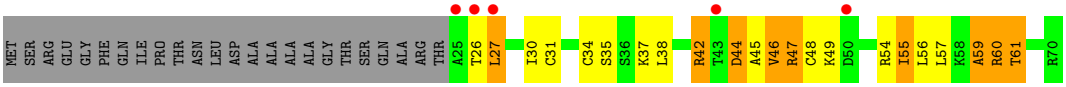
• Molecule 9: DNA-directed RNA polymerase II subunit RPB11

Chain K:



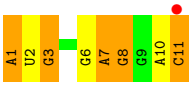
• Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC4

Chain L:



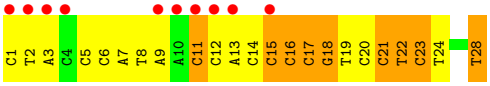
• Molecule 11: RNA (5'-R(*AP*UP*GP*GP*AP*GP*AP*GP*GP*AP*C)-3')

Chain R:



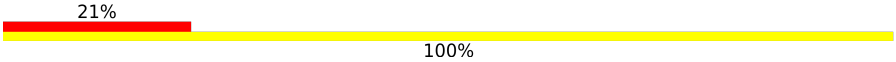
• Molecule 12: DNA (28-MER)

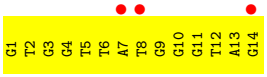
Chain T:



• Molecule 13: DNA (5'-D(*GP*TP*GP*GP*TP*TP*AP*TP*GP*GP*GP*TP*AP*G)-3')

Chain N:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	169.48Å 223.12Å 193.81Å 90.00° 101.47° 90.00°	Depositor
Resolution (Å)	40.00 – 3.18 36.31 – 3.18	Depositor EDS
% Data completeness (in resolution range)	98.6 (40.00-3.18) 98.6 (36.31-3.18)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$< I/\sigma(I) >$ [1]	2.51 (at 3.18Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.207 , 0.255 0.222 , 0.257	Depositor DCC
R_{free} test set	5827 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	77.3	Xtriage
Anisotropy	0.083	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 57.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	29241	wwPDB-VP
Average B, all atoms (Å^2)	116.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.62% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, C7P, MG

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	0.73	1/11163 (0.0%)	0.87	8/15091 (0.1%)
2	B	0.84	2/8963 (0.0%)	0.94	11/12086 (0.1%)
3	C	0.84	1/2133 (0.0%)	0.93	0/2891
4	E	0.60	0/1788	0.75	1/2406 (0.0%)
5	F	0.71	0/691	0.79	0/933
6	H	0.69	0/1086	0.91	1/1470 (0.1%)
7	I	0.81	1/989 (0.1%)	0.94	1/1331 (0.1%)
8	J	0.85	0/541	1.01	2/727 (0.3%)
9	K	0.74	0/937	0.82	0/1265
10	L	0.88	0/365	1.10	0/485
11	R	1.25	0/270	2.01	15/421 (3.6%)
12	T	1.34	5/612 (0.8%)	2.03	35/937 (3.7%)
13	N	0.50	0/329	0.94	0/509
All	All	0.79	10/29867 (0.0%)	0.96	74/40552 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
2	B	0	5
4	E	0	1
6	H	0	3
8	J	0	1
10	L	0	1
All	All	0	14

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	T	18	DG	C8-N7	9.27	1.36	1.30
12	T	21	DC	C3'-O3'	-6.85	1.35	1.44
12	T	18	DG	C6-N1	-6.38	1.35	1.39
12	T	18	DG	N9-C4	-5.70	1.33	1.38
1	A	795	GLU	CG-CD	5.61	1.60	1.51
12	T	19	DT	C3'-O3'	-5.54	1.36	1.44
3	C	92	CYS	CB-SG	-5.45	1.73	1.81
2	B	477	ALA	CA-CB	5.31	1.63	1.52
2	B	183	GLU	CG-CD	5.28	1.59	1.51
7	I	107	SER	CB-OG	5.04	1.48	1.42

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	T	18	DG	N3-C4-C5	-16.47	120.37	128.60
12	T	18	DG	C2-N3-C4	14.35	119.07	111.90
12	T	18	DG	C5-C6-N1	12.95	117.97	111.50
12	T	18	DG	N3-C4-N9	11.38	132.83	126.00
12	T	18	DG	O4'-C1'-N9	10.61	115.43	108.00
12	T	18	DG	O4'-C4'-C3'	-10.30	99.82	106.00
12	T	23	DC	O4'-C1'-N1	9.31	114.51	108.00
12	T	21	DC	O4'-C4'-C3'	-9.12	100.53	106.00
2	B	883	LEU	CA-CB-CG	9.10	136.23	115.30
11	R	8	G	C4'-C3'-C2'	-8.88	93.72	102.60
12	T	18	DG	C5-C6-O6	-8.82	123.31	128.60
12	T	20	DC	C4'-C3'-C2'	-8.45	95.49	103.10
1	A	702	LEU	CA-CB-CG	8.14	134.02	115.30
2	B	211	VAL	CB-CA-C	-8.07	96.07	111.40
2	B	167	ILE	CB-CA-C	-7.55	96.51	111.60
12	T	19	DT	C4-C5-C7	7.49	123.50	119.00
12	T	18	DG	C4'-C3'-C2'	-7.43	96.41	103.10
2	B	651	LEU	CA-CB-CG	7.42	132.35	115.30
11	R	11	C	C6-N1-C2	-7.41	117.33	120.30
11	R	11	C	O4'-C1'-N1	6.86	113.69	108.20
12	T	16	DC	C1'-O4'-C4'	-6.86	103.24	110.10
11	R	3	G	O4'-C1'-N9	6.84	113.67	108.20
8	J	3	VAL	CB-CA-C	-6.79	98.50	111.40
12	T	16	DC	O4'-C1'-N1	6.75	112.72	108.00
12	T	16	DC	O4'-C1'-C2'	-6.61	100.61	105.90
1	A	597	LEU	CB-CA-C	-6.61	97.65	110.20
1	A	936	LEU	CA-CB-CG	6.50	130.25	115.30
2	B	478	GLY	N-CA-C	-6.45	96.98	113.10
12	T	18	DG	C1'-O4'-C4'	-6.30	103.80	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	H	89	LEU	CA-CB-CG	6.16	129.47	115.30
12	T	22	DT	N3-C4-O4	6.14	123.58	119.90
11	R	1	A	O4'-C1'-N9	5.98	112.98	108.20
11	R	11	C	C3'-C2'-C1'	5.98	106.28	101.50
12	T	16	DC	P-O3'-C3'	5.95	126.84	119.70
12	T	17	DC	C4'-C3'-C2'	-5.91	97.78	103.10
12	T	19	DT	C6-C5-C7	-5.90	119.36	122.90
2	B	128	LEU	CA-CB-CG	5.89	128.84	115.30
11	R	8	G	C1'-O4'-C4'	-5.88	105.20	109.90
12	T	19	DT	O4'-C1'-N1	5.83	112.08	108.00
1	A	509	LEU	CA-CB-CG	5.81	128.66	115.30
12	T	18	DG	C6-N1-C2	-5.75	121.65	125.10
12	T	17	DC	C6-N1-C2	-5.73	118.01	120.30
11	R	10	A	C4'-C3'-C2'	-5.67	96.93	102.60
12	T	11	DC	O4'-C1'-N1	5.65	111.95	108.00
11	R	6	G	O4'-C1'-N9	5.63	112.70	108.20
4	E	175	LEU	CA-CB-CG	5.62	128.22	115.30
11	R	7	A	P-O3'-C3'	-5.57	113.02	119.70
2	B	390	LEU	CA-CB-CG	5.54	128.05	115.30
12	T	15	DC	O4'-C1'-N1	5.53	111.87	108.00
12	T	18	DG	N7-C8-N9	-5.48	110.36	113.10
1	A	821	ARG	NE-CZ-NH1	-5.47	117.56	120.30
12	T	22	DT	C4'-C3'-C2'	-5.46	98.18	103.10
11	R	7	A	OP1-P-O3'	5.45	117.20	105.20
12	T	28	DT	O4'-C4'-C3'	5.45	109.27	106.00
12	T	11	DC	C1'-O4'-C4'	-5.44	104.66	110.10
2	B	37	PHE	N-CA-C	-5.39	96.44	111.00
12	T	19	DT	C4'-C3'-C2'	-5.39	98.25	103.10
11	R	11	C	C4'-C3'-C2'	-5.39	97.21	102.60
7	I	78	CYS	CA-CB-SG	5.38	123.68	114.00
2	B	866	TYR	N-CA-C	5.36	125.47	111.00
12	T	17	DC	C2-N1-C1'	5.29	124.62	118.80
12	T	18	DG	N9-C1'-C2'	-5.29	102.54	112.60
2	B	1099	VAL	CB-CA-C	-5.27	101.39	111.40
11	R	7	A	C3'-C2'-C1'	5.25	105.70	101.50
11	R	2	U	O4'-C1'-N1	5.25	112.40	108.20
12	T	18	DG	C8-N9-C4	5.19	108.47	106.40
12	T	24	DT	C5-C4-O4	-5.16	121.29	124.90
1	A	598	LEU	N-CA-CB	5.13	120.65	110.40
2	B	766	ARG	NE-CZ-NH2	-5.11	117.75	120.30
11	R	3	G	N1-C6-O6	5.09	122.95	119.90
8	J	43	ARG	NE-CZ-NH1	-5.08	117.76	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1067	LEU	CA-CB-CG	5.05	126.91	115.30
1	A	399	HIS	C-N-CD	5.02	138.95	128.40
12	T	17	DC	O4'-C1'-C2'	-5.01	101.89	105.90

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1391	ARG	Peptide
1	A	252	PHE	Peptide
1	A	71	GLN	Peptide
2	B	1076	HIS	Peptide
2	B	245	GLU	Peptide
2	B	265	SER	Peptide
2	B	644	GLU	Peptide
2	B	882	THR	Peptide
4	E	157	SER	Peptide
6	H	136	LYS	Peptide
6	H	138	GLU	Peptide
6	H	61	SER	Peptide
8	J	64	ASN	Peptide
10	L	42	ARG	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10969	0	11071	589	0
2	B	8792	0	8824	445	0
3	C	2095	0	2051	114	0
4	E	1752	0	1776	63	0
5	F	679	0	701	26	0
6	H	1068	0	1040	69	0
7	I	971	0	927	36	0
8	J	532	0	543	40	0
9	K	919	0	929	23	0
10	L	363	0	387	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	R	240	0	122	2	0
12	T	550	0	316	66	0
13	N	293	0	161	75	0
14	A	2	0	0	0	0
14	B	1	0	0	0	0
14	C	1	0	0	0	0
14	I	2	0	0	0	0
14	J	1	0	0	1	0
14	L	1	0	0	0	0
15	A	1	0	0	0	0
16	T	9	0	5	0	0
All	All	29241	0	28853	1398	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 24.

All (1398) 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)
12:T:2:DT:H2"	12:T:3:DA:C5'	1.47	1.44
12:T:2:DT:C2'	12:T:3:DA:H5'	1.42	1.43
1:A:567:LYS:CG	1:A:568:PRO:HD2	1.60	1.30
13:N:1:DG:H2"	13:N:2:DT:C7	1.71	1.19
12:T:8:DT:H2"	12:T:9:DA:C8	1.79	1.18
1:A:567:LYS:HB3	6:H:96:VAL:H	1.03	1.17
1:A:567:LYS:HG3	1:A:568:PRO:CD	1.78	1.13
13:N:1:DG:H2"	13:N:2:DT:C5	1.84	1.12
1:A:320:ARG:HG3	1:A:320:ARG:HH11	1.12	1.11
5:F:93:ILE:HD11	5:F:134:ILE:HD11	1.28	1.10
1:A:423:ASP:O	1:A:424:ILE:HB	1.50	1.09
12:T:1:DC:H2"	12:T:2:DT:OP2	1.45	1.08
12:T:7:DA:C2	12:T:8:DT:C4	2.41	1.07
1:A:1116:LEU:HD13	1:A:1329:THR:HG23	1.29	1.06
1:A:630:ILE:HD12	1:A:630:ILE:H	1.21	1.06
1:A:567:LYS:HB3	6:H:96:VAL:N	1.72	1.05
1:A:315:LEU:HB3	1:A:316:GLN:HA	1.39	1.04
1:A:214:ILE:HG22	1:A:215:SER:H	1.21	1.04
1:A:53:LEU:HD23	1:A:54:ASN:H	1.19	1.02
1:A:412:ARG:HG3	1:A:412:ARG:HH11	1.22	1.01
13:N:4:DG:H1'	13:N:5:DT:H5"	1.44	1.00
2:B:25:ILE:HG23	2:B:29:ASP:HB2	1.43	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:344:ARG:HG3	1:A:344:ARG:HH11	1.23	0.99
2:B:485:ARG:HG2	2:B:485:ARG:HH11	1.27	0.99
1:A:503:GLN:NE2	5:F:90:ARG:HH21	1.58	0.99
1:A:853:ASP:OD1	1:A:855:THR:HB	1.63	0.98
1:A:855:THR:HG21	1:A:857:ARG:HE	1.27	0.98
13:N:4:DG:C2	13:N:5:DT:C2	2.51	0.98
4:E:90:VAL:HG23	4:E:123:LEU:HD21	1.47	0.96
12:T:2:DT:H2'	12:T:3:DA:C8	2.00	0.96
3:C:73:GLN:HE21	3:C:75:MET:H	0.99	0.95
13:N:4:DG:N2	13:N:5:DT:C2	2.33	0.95
2:B:744:HIS:CD2	2:B:746:SER:H	1.85	0.95
2:B:744:HIS:HD2	2:B:746:SER:H	1.02	0.95
4:E:15:ALA:O	4:E:19:VAL:HG23	1.67	0.94
7:I:111:THR:HG22	7:I:113:ASP:H	1.32	0.94
1:A:961:ARG:HH11	1:A:961:ARG:HB3	1.30	0.94
1:A:1364:ASN:ND2	1:A:1366:ARG:HG2	1.82	0.94
13:N:3:DG:H2"	13:N:4:DG:OP2	1.67	0.94
13:N:1:DG:C2'	13:N:2:DT:C7	2.46	0.93
3:C:222:LYS:HA	3:C:222:LYS:HE3	1.47	0.93
1:A:1116:LEU:HD13	1:A:1329:THR:CG2	1.98	0.93
1:A:780:VAL:HG22	2:B:699:GLU:OE2	1.70	0.92
2:B:423:LYS:O	2:B:427:ASP:HB2	1.70	0.91
2:B:175:ARG:HH11	2:B:175:ARG:HG3	1.35	0.91
2:B:801:LYS:O	8:J:52:THR:HG23	1.69	0.91
2:B:363:HIS:O	2:B:364:ILE:HB	1.69	0.91
2:B:778:MET:HE1	2:B:853:SER:HB3	1.51	0.91
1:A:1029:ARG:HH11	1:A:1029:ARG:CG	1.83	0.90
13:N:4:DG:C6	13:N:5:DT:C4	2.59	0.90
13:N:13:DA:H8	13:N:13:DA:OP2	1.54	0.90
1:A:503:GLN:HE21	5:F:90:ARG:HH21	1.18	0.90
12:T:8:DT:C2'	12:T:9:DA:C8	2.54	0.90
12:T:6:DC:C2	12:T:7:DA:N7	2.40	0.89
1:A:351:THR:HG23	2:B:1103:ILE:HG12	1.54	0.89
1:A:380:VAL:HG12	1:A:428:TYR:HA	1.54	0.89
2:B:175:ARG:HH11	2:B:175:ARG:CG	1.86	0.88
1:A:313:GLN:HB2	1:A:322:VAL:HG22	1.54	0.88
1:A:436:ILE:HD11	1:A:491:VAL:HG11	1.53	0.88
2:B:260:GLY:O	2:B:267:ARG:HD3	1.72	0.88
12:T:7:DA:C2	12:T:8:DT:N3	2.42	0.88
6:H:40:LEU:HD13	6:H:123:MET:HB2	1.55	0.88
10:L:47:ARG:NH1	10:L:54:ARG:HE	1.70	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:783:THR:HG21	1:A:796:SER:O	1.75	0.87
8:J:44:TYR:HA	8:J:47:ARG:HB3	1.55	0.87
1:A:567:LYS:HG3	1:A:568:PRO:HD2	0.89	0.87
1:A:412:ARG:HH11	1:A:412:ARG:CG	1.87	0.87
2:B:986:GLN:NE2	2:B:1022:THR:HG21	1.90	0.87
12:T:8:DT:H2"	12:T:9:DA:H8	1.39	0.87
1:A:532:ARG:HH11	1:A:532:ARG:CG	1.88	0.86
1:A:171:GLN:HG2	1:A:172:PRO:HD2	1.56	0.86
13:N:6:DT:C2	13:N:7:DA:C5	2.63	0.86
2:B:175:ARG:HG3	2:B:175:ARG:NH1	1.90	0.86
1:A:1161:THR:HG22	1:A:1163:ILE:H	1.38	0.86
13:N:5:DT:H2"	13:N:6:DT:C6	2.11	0.86
6:H:89:LEU:HD23	6:H:92:ASP:H	1.40	0.85
2:B:635:ARG:HG2	2:B:635:ARG:O	1.76	0.85
2:B:63:ILE:O	2:B:67:SER:HB2	1.77	0.85
1:A:901:LEU:H	1:A:926:GLN:HE21	1.20	0.85
13:N:5:DT:H2'	13:N:6:DT:H71	1.57	0.85
1:A:630:ILE:HD12	1:A:630:ILE:N	1.92	0.85
1:A:567:LYS:CB	1:A:568:PRO:CD	2.55	0.84
12:T:6:DC:C2	12:T:7:DA:C8	2.66	0.84
13:N:13:DA:OP2	13:N:13:DA:C8	2.30	0.84
2:B:120:ARG:HD2	2:B:955:THR:HG21	1.57	0.84
1:A:412:ARG:HG3	1:A:412:ARG:NH1	1.88	0.84
2:B:1051:THR:HG22	2:B:1054:GLY:H	1.42	0.84
13:N:12:DT:H2"	13:N:13:DA:OP2	1.75	0.84
1:A:567:LYS:CG	1:A:568:PRO:CD	2.47	0.83
12:T:6:DC:H2"	12:T:7:DA:OP2	1.77	0.83
3:C:54:ASN:OD1	3:C:56:THR:HB	1.79	0.83
2:B:822:ASN:HD22	8:J:52:THR:HG21	1.43	0.83
1:A:567:LYS:HB2	1:A:568:PRO:CD	2.09	0.82
1:A:821:ARG:O	1:A:825:ILE:HG12	1.79	0.82
1:A:902:LEU:HD11	1:A:926:GLN:HG3	1.60	0.82
2:B:1002:THR:HG23	2:B:1004:GLU:H	1.44	0.82
1:A:244:PRO:HB2	1:A:245:PRO:HD3	1.62	0.82
2:B:747:MET:HA	2:B:747:MET:CE	2.08	0.82
1:A:50:ILE:HG22	1:A:52:GLY:H	1.44	0.82
1:A:1116:LEU:CD1	1:A:1329:THR:HG23	2.08	0.82
2:B:732:SER:HB2	2:B:734:HIS:NE2	1.94	0.82
1:A:472:LEU:O	1:A:475:THR:HB	1.79	0.81
1:A:344:ARG:HG3	1:A:344:ARG:NH1	1.91	0.81
8:J:23:ASN:HB3	8:J:27:GLU:OE2	1.80	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:503:GLN:NE2	5:F:90:ARG:NH2	2.28	0.81
3:C:73:GLN:NE2	3:C:75:MET:H	1.76	0.81
3:C:37:MET:HA	3:C:41:ILE:HD11	1.61	0.81
3:C:73:GLN:HE21	3:C:75:MET:N	1.76	0.81
13:N:1:DG:H2"	13:N:2:DT:H71	1.58	0.81
2:B:541:LEU:HD12	2:B:747:MET:HE1	1.62	0.80
1:A:565:ILE:HG23	1:A:567:LYS:HE3	1.62	0.80
2:B:230:ALA:H	2:B:231:PRO:CD	1.95	0.80
1:A:261:ASP:OD2	1:A:323:LYS:HD2	1.82	0.80
12:T:6:DC:H1'	12:T:7:DA:C8	2.18	0.79
1:A:902:LEU:CD1	1:A:926:GLN:HG3	2.12	0.79
2:B:378:LEU:O	2:B:382:ILE:HG12	1.82	0.79
1:A:57:ARG:HA	1:A:68:GLN:HB3	1.65	0.79
1:A:315:LEU:CB	1:A:316:GLN:HA	2.11	0.79
1:A:351:THR:CG2	2:B:1103:ILE:HG12	2.12	0.79
1:A:320:ARG:HG3	1:A:320:ARG:NH1	1.91	0.79
1:A:567:LYS:CB	1:A:568:PRO:HD2	2.12	0.79
13:N:5:DT:C2'	13:N:6:DT:H71	2.12	0.79
1:A:115:LEU:HD22	1:A:119:ASN:HB2	1.65	0.79
13:N:6:DT:O2	13:N:7:DA:C5	2.36	0.79
2:B:732:SER:HB2	2:B:734:HIS:CD2	2.19	0.78
6:H:89:LEU:CD2	6:H:92:ASP:H	1.96	0.78
7:I:92:ARG:HG2	7:I:93:LYS:H	1.47	0.78
2:B:29:ASP:HB3	2:B:658:ILE:HG12	1.63	0.78
1:A:53:LEU:HD23	1:A:54:ASN:N	1.98	0.78
1:A:567:LYS:CB	6:H:96:VAL:H	1.92	0.78
1:A:630:ILE:H	1:A:630:ILE:CD1	1.97	0.78
13:N:5:DT:H2'	13:N:6:DT:C7	2.14	0.78
13:N:6:DT:C2	13:N:7:DA:C6	2.71	0.78
4:E:116:ILE:CG2	4:E:121:MET:HG3	2.15	0.77
1:A:1364:ASN:HD22	1:A:1366:ARG:HG2	1.46	0.77
1:A:1364:ASN:HD21	1:A:1366:ARG:HH11	1.30	0.77
1:A:265:LYS:C	1:A:267:ALA:H	1.86	0.77
1:A:37:PHE:HB2	1:A:52:GLY:HA3	1.67	0.76
1:A:296:LEU:HG	1:A:296:LEU:O	1.83	0.76
1:A:901:LEU:HB2	1:A:926:GLN:HG2	1.67	0.76
1:A:214:ILE:HG22	1:A:215:SER:N	1.99	0.76
1:A:855:THR:CG2	1:A:857:ARG:HE	1.97	0.76
1:A:1322:ILE:HG12	1:A:1323:ASP:N	2.00	0.76
2:B:644:GLU:HA	2:B:644:GLU:OE1	1.84	0.76
2:B:778:MET:CE	2:B:853:SER:HB3	2.14	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1029:ARG:HH11	1:A:1029:ARG:HG3	1.50	0.76
1:A:315:LEU:HB3	1:A:316:GLN:CA	2.14	0.76
8:J:7:CYS:HA	8:J:49:MET:HG2	1.66	0.76
13:N:4:DG:C2	13:N:5:DT:N1	2.54	0.76
1:A:741:ASN:HD22	1:A:744:LYS:H	1.31	0.76
4:E:19:VAL:O	4:E:23:VAL:HG23	1.86	0.76
1:A:114:LEU:O	1:A:115:LEU:HG	1.86	0.76
1:A:55:ASP:O	1:A:56:PRO:C	2.22	0.75
2:B:590:HIS:HD2	2:B:596:LEU:HD22	1.50	0.75
7:I:8:ARG:O	7:I:9:ASP:HB2	1.85	0.75
13:N:13:DA:H2"	13:N:14:DG:C8	2.20	0.75
2:B:515:HIS:HD2	2:B:517:THR:H	1.34	0.75
1:A:67:CYS:O	1:A:68:GLN:HG3	1.87	0.75
1:A:1063:MET:SD	1:A:1436:ILE:HG13	2.26	0.75
2:B:416:LEU:HD11	2:B:460:ALA:CB	2.17	0.75
9:K:65:HIS:HD2	9:K:67:PHE:H	1.30	0.75
1:A:1383:SER:O	1:A:1388:GLY:HA3	1.86	0.75
2:B:100:PRO:O	2:B:101:MET:HG3	1.86	0.74
3:C:148:ARG:HG2	3:C:149:LYS:N	2.02	0.74
2:B:641:GLU:HB3	2:B:643:ASP:OD1	1.87	0.74
3:C:123:ASN:HD21	3:C:125:MET:HB3	1.52	0.74
7:I:92:ARG:HG2	7:I:93:LYS:N	2.00	0.74
1:A:882:SER:HB3	1:A:953:ASN:OD1	1.88	0.74
2:B:254:LEU:HD23	2:B:381:MET:HE1	1.68	0.74
1:A:565:ILE:HG23	1:A:567:LYS:HG2	1.70	0.74
2:B:241:ARG:HA	2:B:253:THR:HG22	1.69	0.74
12:T:6:DC:N1	12:T:7:DA:N7	2.35	0.74
1:A:265:LYS:HZ1	1:A:302:THR:HG23	1.52	0.74
1:A:244:PRO:HB2	1:A:245:PRO:CD	2.17	0.74
1:A:961:ARG:HB3	1:A:961:ARG:NH1	2.01	0.74
2:B:969:ARG:NH1	3:C:61:GLU:OE1	2.21	0.74
1:A:108:MET:O	1:A:109:HIS:HB2	1.87	0.74
1:A:1206:ASP:H	1:A:1274:ARG:HH12	1.34	0.74
4:E:147:HIS:HD2	4:E:149:LEU:H	1.35	0.73
1:A:961:ARG:HH11	1:A:961:ARG:CB	1.99	0.73
2:B:129:PHE:CE2	2:B:166:PHE:HB2	2.23	0.73
2:B:1103:ILE:O	2:B:1103:ILE:HG22	1.86	0.73
1:A:392:VAL:HG11	1:A:424:ILE:HG21	1.70	0.73
3:C:116:LYS:HD3	3:C:140:ASN:HB3	1.68	0.73
1:A:596:THR:O	1:A:598:LEU:N	2.22	0.73
6:H:47:PHE:HB3	6:H:95:TYR:CD1	2.23	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1435:PRO:O	1:A:1436:ILE:HD12	1.89	0.73
2:B:642:ASP:HB3	2:B:649:LYS:HG3	1.70	0.73
2:B:900:ALA:HB3	10:L:61:THR:HG23	1.69	0.73
1:A:1129:GLU:HA	1:A:1132:LYS:HE2	1.71	0.73
4:E:198:ILE:CD1	4:E:212:ARG:HG3	2.17	0.73
2:B:29:ASP:OD2	2:B:655:LYS:HE2	1.89	0.73
6:H:2:SER:O	6:H:3:ASN:HB2	1.88	0.73
1:A:68:GLN:HE21	1:A:70:CYS:HB3	1.54	0.72
1:A:317:LYS:O	12:T:28:DT:H4'	1.89	0.72
1:A:1430:LEU:O	2:B:1196:ILE:HG22	1.88	0.72
2:B:287:ARG:NH2	2:B:294:ASP:OD2	2.23	0.72
1:A:869:GLY:O	4:E:204:THR:HG21	1.90	0.72
1:A:709:THR:HB	1:A:712:GLU:H	1.54	0.72
2:B:516:ASN:H	2:B:516:ASN:HD22	1.36	0.72
12:T:6:DC:C1'	12:T:7:DA:C8	2.72	0.72
1:A:215:SER:C	1:A:217:LYS:H	1.92	0.72
1:A:553:VAL:HG23	1:A:652:VAL:CG2	2.20	0.72
2:B:485:ARG:HH11	2:B:485:ARG:CG	2.02	0.72
1:A:946:VAL:HG22	4:E:201:LYS:HD3	1.71	0.72
2:B:229:ALA:HB1	2:B:231:PRO:HD2	1.70	0.72
2:B:881:ASN:HA	2:B:883:LEU:HD23	1.72	0.72
2:B:345:LYS:O	2:B:348:ARG:HG2	1.89	0.72
2:B:428:ILE:HG13	2:B:448:ILE:HD13	1.71	0.72
2:B:636:PRO:HB3	2:B:743:ILE:HG13	1.71	0.71
12:T:8:DT:O4	13:N:7:DA:N1	2.23	0.71
1:A:423:ASP:O	1:A:424:ILE:CB	2.32	0.71
13:N:1:DG:C2'	13:N:2:DT:H73	2.19	0.71
13:N:4:DG:C1'	13:N:5:DT:H5"	2.20	0.71
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.73	0.71
7:I:5:ARG:HD3	7:I:36:GLU:OE2	1.90	0.71
12:T:9:DA:C2	13:N:7:DA:C2	2.78	0.71
1:A:871:ASP:OD1	1:A:1366:ARG:NH2	2.23	0.71
3:C:148:ARG:HG2	3:C:149:LYS:H	1.55	0.71
12:T:7:DA:N1	12:T:8:DT:C4	2.59	0.71
1:A:256:GLN:HA	1:A:257:ARG:HB3	1.72	0.71
1:A:567:LYS:HE2	6:H:97:MET:HG2	1.72	0.71
2:B:1187:ASN:HD21	2:B:1190:ASP:H	1.38	0.71
13:N:6:DT:N3	13:N:7:DA:N6	2.38	0.71
1:A:1029:ARG:HH11	1:A:1029:ARG:HG2	1.55	0.70
2:B:25:ILE:CG2	2:B:29:ASP:HB2	2.20	0.70
13:N:4:DG:N1	13:N:5:DT:C4	2.60	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:922:ASP:O	1:A:923:LEU:HG	1.92	0.70
1:A:532:ARG:HH11	1:A:532:ARG:HG2	1.56	0.70
2:B:408:LEU:HD21	2:B:545:ILE:HD13	1.73	0.70
12:T:1:DC:C2'	12:T:2:DT:OP2	2.30	0.70
2:B:986:GLN:HE21	2:B:1022:THR:HG21	1.55	0.70
1:A:726:ARG:HG2	1:A:726:ARG:O	1.90	0.70
3:C:162:GLY:HA3	3:C:170:TRP:CE2	2.25	0.70
3:C:69:LEU:HB2	8:J:5:VAL:CG1	2.21	0.70
3:C:32:SER:O	3:C:36:VAL:HG23	1.91	0.69
3:C:56:THR:CG2	3:C:58:LEU:H	2.05	0.69
1:A:86:LEU:HD12	1:A:236:LEU:O	1.91	0.69
2:B:744:HIS:HD2	2:B:746:SER:N	1.84	0.69
1:A:55:ASP:O	1:A:57:ARG:N	2.25	0.69
1:A:650:GLN:O	1:A:654:ASN:HB2	1.92	0.69
1:A:1029:ARG:HG2	1:A:1029:ARG:NH1	2.06	0.69
6:H:63:LEU:C	6:H:90:ALA:HB3	2.12	0.69
1:A:42:ASP:HB3	1:A:45:GLN:HA	1.74	0.69
4:E:116:ILE:HG21	4:E:121:MET:HG3	1.75	0.69
2:B:167:ILE:HD13	2:B:167:ILE:N	2.07	0.69
12:T:6:DC:N1	12:T:7:DA:C8	2.60	0.69
1:A:134:ARG:HD3	1:A:221:SER:O	1.92	0.69
3:C:70:ILE:HD11	3:C:144:ILE:HD11	1.73	0.69
2:B:778:MET:HE1	2:B:853:SER:CB	2.23	0.69
3:C:27:LEU:HD12	3:C:228:PHE:HE2	1.56	0.69
3:C:142:VAL:H	8:J:16:ASP:HB3	1.58	0.68
2:B:254:LEU:HD23	2:B:381:MET:CE	2.23	0.68
3:C:66:ARG:NH2	8:J:3:VAL:O	2.26	0.68
4:E:72:PHE:CE2	4:E:157:SER:HB3	2.28	0.68
1:A:64:ASN:O	1:A:66:LYS:N	2.27	0.68
1:A:1206:ASP:H	1:A:1274:ARG:NH1	1.90	0.68
2:B:121:ASN:HD22	2:B:207:GLY:HA3	1.59	0.68
1:A:91:PHE:HB2	1:A:297:GLN:OE1	1.94	0.68
1:A:260:ASP:OD1	1:A:261:ASP:N	2.25	0.68
1:A:875:ALA:HB2	1:A:1366:ARG:HD2	1.74	0.68
1:A:901:LEU:H	1:A:926:GLN:NE2	1.92	0.68
1:A:1134:ILE:O	1:A:1138:ILE:HG12	1.94	0.68
13:N:9:DG:H2"	13:N:10:DG:C8	2.29	0.68
1:A:399:HIS:O	1:A:401:GLY:N	2.27	0.68
1:A:1325:THR:HG22	1:A:1326:ARG:HG3	1.76	0.68
1:A:1437:GLY:O	1:A:1439:GLY:N	2.27	0.68
13:N:2:DT:H2"	13:N:3:DG:C8	2.28	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:476:ARG:O	2:B:478:GLY:N	2.26	0.68
1:A:50:ILE:HG22	1:A:52:GLY:N	2.09	0.67
13:N:4:DG:N1	13:N:5:DT:N3	2.41	0.67
1:A:90:VAL:HB	1:A:297:GLN:NE2	2.09	0.67
3:C:99:LEU:HD23	3:C:99:LEU:N	2.08	0.67
6:H:63:LEU:C	6:H:90:ALA:CB	2.62	0.67
1:A:51:GLY:HA2	1:A:56:PRO:HG3	1.74	0.67
1:A:1189:SER:OG	1:A:1190:PRO:HD2	1.94	0.67
2:B:1077:THR:HG23	2:B:1079:LYS:H	1.59	0.67
1:A:343:LYS:NZ	2:B:1156:ASP:OD2	2.28	0.67
1:A:532:ARG:HH11	1:A:532:ARG:HG3	1.58	0.67
1:A:858:ASN:C	1:A:858:ASN:HD22	1.98	0.67
1:A:1336:MET:CE	1:A:1380:GLY:HA2	2.24	0.67
3:C:22:LEU:HD22	3:C:25:VAL:HG21	1.77	0.67
1:A:70:CYS:HA	2:B:1174:LYS:HD3	1.77	0.67
1:A:256:GLN:HB3	1:A:257:ARG:HD2	1.77	0.67
2:B:640:VAL:HG12	2:B:640:VAL:O	1.93	0.67
1:A:500:GLU:OE2	1:A:1438:THR:HG21	1.95	0.67
2:B:211:VAL:O	2:B:480:SER:HA	1.93	0.67
13:N:4:DG:C5	13:N:5:DT:C5	2.83	0.67
13:N:9:DG:H2"	13:N:10:DG:N7	2.09	0.67
1:A:53:LEU:CD2	1:A:54:ASN:H	2.03	0.67
1:A:1397:LEU:HB2	1:A:1426:GLU:OE2	1.94	0.67
4:E:147:HIS:CD2	4:E:149:LEU:H	2.12	0.67
2:B:843:GLN:HB2	2:B:993:THR:HB	1.77	0.66
2:B:880:THR:CG2	2:B:880:THR:O	2.43	0.66
1:A:542:GLU:OE1	1:A:569:LYS:NZ	2.28	0.66
1:A:609:ASP:O	1:A:611:GLN:N	2.28	0.66
2:B:788:ARG:NH1	2:B:790:ASP:OD1	2.28	0.66
7:I:111:THR:CG2	7:I:113:ASP:HB3	2.25	0.66
9:K:49:GLU:HG3	9:K:94:ILE:CG1	2.25	0.66
1:A:875:ALA:HA	1:A:878:ILE:HD12	1.77	0.66
1:A:1206:ASP:N	1:A:1274:ARG:HH12	1.92	0.66
13:N:6:DT:N3	13:N:7:DA:C6	2.64	0.66
1:A:1029:ARG:O	1:A:1033:GLN:HB2	1.96	0.66
2:B:470:LYS:O	2:B:471:LYS:HG3	1.96	0.66
2:B:1084:GLN:NE2	3:C:192:TRP:H	1.94	0.66
12:T:6:DC:H1'	12:T:7:DA:H8	1.59	0.66
1:A:378:GLU:OE1	1:A:434:ARG:NH1	2.27	0.65
2:B:1028:GLU:O	2:B:1032:SER:HB2	1.95	0.65
3:C:56:THR:HG22	3:C:58:LEU:H	1.59	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:761:MET:HG3	2:B:1021:MET:HG2	1.77	0.65
1:A:871:ASP:HB3	4:E:204:THR:HG23	1.78	0.65
2:B:230:ALA:H	2:B:231:PRO:HD3	1.60	0.65
1:A:1116:LEU:H	1:A:1308:THR:HB	1.61	0.65
2:B:365:THR:HG23	2:B:367:LEU:H	1.61	0.65
5:F:93:ILE:HD11	5:F:134:ILE:CD1	2.16	0.65
1:A:6:TYR:HD2	1:A:7:SER:N	1.94	0.65
1:A:545:GLN:HG2	1:A:549:MET:HE3	1.79	0.65
3:C:69:LEU:HB2	8:J:5:VAL:HG11	1.77	0.65
1:A:470:LEU:HD21	1:A:487:MET:CE	2.25	0.65
1:A:1438:THR:H	5:F:88:TYR:HB3	1.60	0.65
1:A:269:ILE:HD11	1:A:300:VAL:HA	1.78	0.65
2:B:1023:VAL:O	2:B:1027:ILE:HG13	1.97	0.65
1:A:12:ARG:HB3	2:B:1218:THR:HB	1.79	0.65
1:A:1336:MET:HE1	1:A:1380:GLY:HA2	1.77	0.65
1:A:1341:ILE:HG22	4:E:182:ASP:OD2	1.95	0.65
2:B:299:GLU:OE2	2:B:571:PRO:HD2	1.97	0.65
1:A:541:ILE:HG22	1:A:546:VAL:HG23	1.79	0.65
1:A:1036:ARG:HG3	1:A:1036:ARG:HH11	1.62	0.65
1:A:567:LYS:HD3	6:H:95:TYR:CG	2.31	0.64
2:B:282:ILE:HD12	2:B:382:ILE:HD12	1.79	0.64
4:E:55:ARG:C	4:E:57:MET:H	2.00	0.64
4:E:64:PRO:CG	4:E:76:GLY:HA2	2.26	0.64
6:H:89:LEU:O	6:H:91:ASP:N	2.30	0.64
2:B:747:MET:HA	2:B:747:MET:HE3	1.77	0.64
3:C:222:LYS:HA	3:C:222:LYS:CE	2.21	0.64
1:A:537:ARG:HD3	6:H:120:GLY:O	1.96	0.64
1:A:809:THR:HB	1:A:810:PRO:HD2	1.78	0.64
2:B:770:GLN:CG	2:B:770:GLN:O	2.45	0.64
2:B:955:THR:HG23	10:L:54:ARG:O	1.96	0.64
1:A:185:TRP:HZ3	1:A:200:ARG:HG2	1.62	0.64
1:A:1111:MET:HE1	1:A:1330:ASN:OD1	1.97	0.64
2:B:25:ILE:HG22	2:B:26:THR:N	2.12	0.64
2:B:102:VAL:HG11	2:B:122:LEU:HD13	1.78	0.64
4:E:135:PHE:HD2	4:E:140:LEU:HD21	1.61	0.64
7:I:8:ARG:O	7:I:9:ASP:CB	2.45	0.64
13:N:4:DG:C4	13:N:5:DT:C6	2.85	0.64
1:A:451:HIS:CD2	1:A:1074:GLU:HG3	2.33	0.64
1:A:470:LEU:HD21	1:A:487:MET:HE3	1.79	0.64
1:A:1156:PRO:O	1:A:1158:PRO:HD3	1.98	0.64
2:B:541:LEU:HD12	2:B:747:MET:CE	2.26	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:351:THR:HG22	1:A:352:VAL:H	1.63	0.64
1:A:928:LEU:O	1:A:931:GLU:HB3	1.98	0.64
1:A:1291:VAL:HG22	1:A:1292:PRO:HD2	1.80	0.64
2:B:167:ILE:O	2:B:168:GLY:O	2.15	0.64
1:A:445:ASN:HB2	1:A:455:MET:HE2	1.80	0.64
12:T:6:DC:C2	12:T:7:DA:C5	2.86	0.64
1:A:353:ILE:HD13	1:A:487:MET:CE	2.28	0.63
3:C:123:ASN:ND2	3:C:125:MET:HB3	2.13	0.63
2:B:822:ASN:O	8:J:48:ARG:NH1	2.31	0.63
6:H:131:ASN:C	6:H:133:ASN:H	2.02	0.63
6:H:89:LEU:C	6:H:91:ASP:H	2.02	0.63
2:B:864:LYS:HD2	2:B:865:LYS:N	2.13	0.63
1:A:870:GLU:OE1	4:E:202:SER:HB2	1.98	0.63
2:B:482:VAL:O	2:B:483:LEU:O	2.16	0.63
4:E:198:ILE:HD11	4:E:212:ARG:HG3	1.80	0.63
1:A:353:ILE:HG22	1:A:468:PHE:HB2	1.80	0.63
1:A:532:ARG:CG	1:A:532:ARG:NH1	2.55	0.63
1:A:567:LYS:HB2	1:A:568:PRO:HD3	1.79	0.63
1:A:828:ALA:HB1	2:B:530:GLY:HA2	1.80	0.63
2:B:770:GLN:O	2:B:770:GLN:HG3	1.98	0.63
1:A:114:LEU:HD12	1:A:145:LYS:HB3	1.80	0.63
1:A:874:ASP:HB2	1:A:1058:VAL:HG23	1.81	0.63
1:A:1173:HIS:O	1:A:1174:PHE:HB3	1.99	0.63
3:C:177:GLU:HG3	3:C:231:ASN:HB3	1.80	0.63
8:J:46:CYS:SG	14:J:101:ZN:ZN	1.85	0.63
1:A:1140:HIS:HB2	1:A:1276:VAL:O	1.99	0.63
2:B:732:SER:CB	2:B:734:HIS:CD2	2.82	0.62
2:B:899:ILE:HG21	2:B:949:VAL:HG21	1.80	0.62
2:B:25:ILE:HD11	2:B:653:VAL:HB	1.81	0.62
2:B:363:HIS:O	2:B:364:ILE:CB	2.45	0.62
1:A:1155:ASP:OD2	1:A:1161:THR:HG23	1.98	0.62
1:A:261:ASP:HB3	1:A:323:LYS:HG3	1.82	0.62
1:A:567:LYS:HB2	6:H:95:TYR:HA	1.80	0.62
2:B:516:ASN:H	2:B:516:ASN:ND2	1.97	0.62
1:A:567:LYS:CE	6:H:97:MET:HG2	2.29	0.62
1:A:768:GLN:CG	1:A:816:HIS:HA	2.29	0.62
2:B:203:PHE:HE1	2:B:212:LEU:HD12	1.64	0.62
6:H:89:LEU:CD2	6:H:92:ASP:N	2.62	0.62
13:N:4:DG:N3	13:N:5:DT:C6	2.67	0.62
1:A:565:ILE:HG23	1:A:567:LYS:CE	2.30	0.62
2:B:25:ILE:HG23	2:B:29:ASP:CB	2.25	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:473:MET:C	2:B:475:SER:H	2.02	0.62
1:A:1410:PHE:HD2	2:B:1212:ILE:HD11	1.64	0.62
6:H:83:GLN:HB3	6:H:86:ASP:OD1	2.00	0.62
12:T:6:DC:C2'	12:T:7:DA:OP2	2.48	0.62
1:A:265:LYS:NZ	1:A:302:THR:HG23	2.15	0.61
1:A:795:GLU:HG3	2:B:731:VAL:HG11	1.82	0.61
1:A:1435:PRO:C	1:A:1436:ILE:HD12	2.21	0.61
8:J:8:PHE:H	8:J:49:MET:HE3	1.65	0.61
13:N:4:DG:N2	13:N:5:DT:O2	2.33	0.61
1:A:22:PHE:HB2	2:B:1211:ASN:OD1	2.00	0.61
1:A:320:ARG:HH11	1:A:320:ARG:CG	2.02	0.61
1:A:369:SER:HB3	9:K:2:ASN:OD1	1.99	0.61
2:B:361:LEU:HD21	2:B:377:PHE:CD2	2.36	0.61
2:B:708:GLU:O	2:B:710:LEU:N	2.33	0.61
2:B:880:THR:O	2:B:880:THR:HG23	1.99	0.61
2:B:1159:ARG:HG3	2:B:1193:GLN:HE21	1.66	0.61
1:A:57:ARG:CA	1:A:68:GLN:HB3	2.30	0.61
1:A:1308:THR:CG2	1:A:1310:GLY:O	2.49	0.61
2:B:638:PHE:CD2	2:B:653:VAL:HG21	2.35	0.61
2:B:879:ARG:HG2	2:B:880:THR:N	2.15	0.61
4:E:77:SER:HB2	4:E:105:PHE:HD2	1.65	0.61
12:T:2:DT:OP2	12:T:2:DT:H71	2.00	0.61
6:H:26:ILE:O	6:H:39:THR:HA	2.00	0.61
1:A:508:PRO:O	1:A:511:ILE:HG13	2.00	0.61
2:B:766:ARG:NH2	2:B:1020:ARG:HG2	2.16	0.61
2:B:751:VAL:CG1	2:B:752:ALA:N	2.63	0.61
3:C:74:SER:O	3:C:77:ILE:HB	2.01	0.61
1:A:1424:VAL:HG11	2:B:1139:ILE:HD13	1.82	0.61
2:B:422:LYS:O	2:B:425:THR:HG22	2.01	0.61
12:T:7:DA:H2"	12:T:8:DT:H5"	1.82	0.61
1:A:106:VAL:HG21	1:A:214:ILE:HD12	1.81	0.60
1:A:331:GLY:O	1:A:332:LYS:HB3	1.99	0.60
1:A:567:LYS:NZ	6:H:95:TYR:CZ	2.59	0.60
2:B:570:VAL:HB	2:B:573:GLN:HG2	1.84	0.60
6:H:145:ARG:HD2	6:H:146:ARG:HD2	1.83	0.60
1:A:901:LEU:N	1:A:926:GLN:HE21	1.95	0.60
1:A:929:LEU:HD21	1:A:983:ILE:HG23	1.83	0.60
1:A:4:GLN:HE22	2:B:1159:ARG:H	1.50	0.60
1:A:283:GLY:O	1:A:285:PRO:HD3	2.02	0.60
2:B:95:ILE:HD12	2:B:130:VAL:HG22	1.83	0.60
2:B:482:VAL:C	2:B:483:LEU:O	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:111:THR:CG2	7:I:113:ASP:H	2.12	0.60
13:N:1:DG:H2'	13:N:2:DT:H73	1.82	0.60
2:B:864:LYS:HD3	2:B:870:ILE:O	2.02	0.60
1:A:53:LEU:HD11	1:A:266:LEU:O	2.01	0.60
2:B:173:MET:O	2:B:176:SER:HB3	2.02	0.60
2:B:797:TYR:O	8:J:1:MET:HG3	2.01	0.60
2:B:570:VAL:HG21	2:B:573:GLN:HE21	1.67	0.60
2:B:1001:PHE:HE1	3:C:178:PHE:HB3	1.66	0.60
4:E:179:GLN:O	4:E:182:ASP:HB2	2.01	0.60
8:J:48:ARG:HE	8:J:49:MET:HE2	1.66	0.59
1:A:666:ILE:HD11	2:B:1030:LEU:HD13	1.83	0.59
1:A:715:GLU:O	1:A:719:VAL:HG23	2.02	0.59
2:B:234:ILE:HG21	2:B:257:LYS:HD3	1.85	0.59
1:A:848:ILE:HG21	1:A:1370:LEU:HD11	1.83	0.59
1:A:963:ILE:HD13	1:A:1048:ASN:HB3	1.83	0.59
1:A:1256:GLU:HA	1:A:1259:MET:HB2	1.85	0.59
1:A:809:THR:HB	1:A:810:PRO:CD	2.32	0.59
1:A:858:ASN:HD22	1:A:860:LEU:H	1.50	0.59
2:B:185:THR:O	2:B:188:ASP:HB2	2.01	0.59
2:B:293:PRO:HG2	2:B:296:GLU:HB3	1.84	0.59
3:C:3:GLU:HG3	3:C:4:GLU:N	2.17	0.59
3:C:20:PHE:HE1	3:C:22:LEU:HD12	1.67	0.59
12:T:8:DT:H3	13:N:7:DA:H2	1.46	0.59
13:N:4:DG:C2	13:N:5:DT:C6	2.91	0.59
2:B:313:MET:CE	2:B:390:LEU:HG	2.33	0.59
2:B:373:ARG:HD2	2:B:566:LEU:HD23	1.85	0.59
1:A:265:LYS:C	1:A:267:ALA:N	2.55	0.59
2:B:1153:GLU:N	2:B:1153:GLU:OE2	2.36	0.59
8:J:57:ILE:O	8:J:61:LEU:HG	2.01	0.59
1:A:353:ILE:HD13	1:A:487:MET:HE2	1.84	0.59
1:A:503:GLN:HE22	5:F:90:ARG:NH2	1.99	0.59
2:B:747:MET:HA	2:B:747:MET:HE2	1.85	0.59
2:B:953:LEU:HD11	10:L:55:ILE:HG22	1.85	0.59
3:C:260:LEU:HG	3:C:264:GLN:HE21	1.67	0.59
4:E:96:PHE:C	4:E:98:ILE:H	2.07	0.59
5:F:93:ILE:CD1	5:F:134:ILE:HD11	2.17	0.59
13:N:1:DG:C2'	13:N:2:DT:H71	2.25	0.59
1:A:173:THR:HB	1:A:184:SER:HB3	1.84	0.58
1:A:765:VAL:HG22	1:A:800:VAL:HB	1.84	0.58
1:A:995:GLU:OE2	1:A:995:GLU:HA	2.01	0.58
2:B:322:PHE:CZ	7:I:30:ARG:HG2	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:647:GLY:C	2:B:648:HIS:ND1	2.57	0.58
2:B:1081:LEU:O	3:C:189:THR:HG23	2.03	0.58
4:E:13:TRP:O	4:E:16:PHE:HB3	2.03	0.58
4:E:135:PHE:CD2	4:E:140:LEU:HD21	2.38	0.58
5:F:109:VAL:HG22	5:F:124:GLU:HG3	1.85	0.58
12:T:12:DC:H2"	12:T:13:DA:C8	2.37	0.58
1:A:929:LEU:HD21	1:A:983:ILE:CG2	2.34	0.58
2:B:998:ASP:OD1	3:C:35:ARG:NH2	2.29	0.58
8:J:16:ASP:OD1	8:J:17:LYS:HG2	2.04	0.58
3:C:102:GLN:HG2	3:C:154:LYS:HD3	1.86	0.58
6:H:83:GLN:O	6:H:87:ARG:HG3	2.03	0.58
7:I:47:GLU:OE1	7:I:50:THR:HG22	2.02	0.58
13:N:1:DG:C2'	13:N:2:DT:C5	2.76	0.58
1:A:261:ASP:HB3	1:A:323:LYS:CG	2.33	0.58
1:A:215:SER:C	1:A:217:LYS:N	2.57	0.58
1:A:215:SER:O	1:A:217:LYS:N	2.37	0.58
2:B:882:THR:H	2:B:883:LEU:HB3	1.67	0.58
2:B:1166:CYS:O	2:B:1215:ARG:HD3	2.04	0.58
12:T:8:DT:C4	13:N:7:DA:N1	2.72	0.58
13:N:6:DT:H1'	13:N:7:DA:C8	2.38	0.58
1:A:317:LYS:HB3	12:T:28:DT:O3'	2.04	0.58
1:A:532:ARG:HG3	1:A:532:ARG:NH1	2.14	0.58
1:A:1312:ASN:O	1:A:1316:VAL:HG23	2.04	0.58
4:E:127:ILE:O	4:E:127:ILE:HG12	2.04	0.58
1:A:563:PRO:HB2	1:A:565:ILE:O	2.04	0.57
1:A:1342:GLU:OE2	4:E:212:ARG:NH1	2.37	0.57
1:A:567:LYS:CD	6:H:95:TYR:CD1	2.87	0.57
2:B:555:ILE:HD12	2:B:587:HIS:CE1	2.39	0.57
7:I:111:THR:HG21	7:I:113:ASP:HB3	1.86	0.57
12:T:3:DA:H8	12:T:3:DA:OP2	1.87	0.57
1:A:492:PRO:HB2	1:A:497:THR:CG2	2.33	0.57
2:B:778:MET:CE	2:B:853:SER:CB	2.83	0.57
3:C:184:ASN:OD1	3:C:187:LYS:HA	2.04	0.57
1:A:37:PHE:HB2	1:A:52:GLY:CA	2.33	0.57
1:A:567:LYS:HD3	6:H:95:TYR:CD1	2.39	0.57
1:A:1308:THR:HG21	1:A:1310:GLY:O	2.04	0.57
2:B:249:ARG:HG3	2:B:251:ILE:HG12	1.85	0.57
2:B:590:HIS:CD2	2:B:596:LEU:HD22	2.37	0.57
2:B:1077:THR:CG2	2:B:1079:LYS:H	2.18	0.57
2:B:899:ILE:HG22	2:B:900:ALA:N	2.20	0.57
6:H:115:TYR:CE2	6:H:124:ARG:HG3	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:868:TYR:CE1	1:A:1064:VAL:HG21	2.39	0.57
1:A:1293:SER:HB2	1:A:1299:VAL:HG23	1.87	0.57
2:B:269:ILE:HD11	2:B:386:LEU:HD21	1.87	0.57
6:H:131:ASN:O	6:H:133:ASN:N	2.36	0.57
1:A:332:LYS:H	1:A:337:ARG:HB2	1.69	0.57
1:A:302:THR:HA	1:A:305:ASP:O	2.05	0.57
1:A:304:MET:O	1:A:324:SER:HB2	2.05	0.57
1:A:365:GLY:O	1:A:468:PHE:HA	2.05	0.57
2:B:122:LEU:CD2	2:B:958:GLN:HB2	2.35	0.57
2:B:1082:MET:O	3:C:189:THR:HG22	2.05	0.57
1:A:211:PHE:O	1:A:214:ILE:HG12	2.05	0.56
2:B:195:CYS:HB3	2:B:782:LEU:HD22	1.87	0.56
1:A:457:ALA:HB3	1:A:506:ALA:HA	1.87	0.56
2:B:996:ARG:HH22	3:C:173:ALA:HB1	1.71	0.56
8:J:24:LEU:HB3	8:J:30:LEU:HD12	1.86	0.56
1:A:780:VAL:CG2	2:B:699:GLU:OE2	2.48	0.56
1:A:1319:VAL:HG12	1:A:1320:PRO:O	2.05	0.56
1:A:1342:GLU:HG2	4:E:212:ARG:HH11	1.69	0.56
3:C:185:LYS:NZ	3:C:211:ASP:O	2.31	0.56
6:H:47:PHE:CB	6:H:95:TYR:CD1	2.87	0.56
7:I:120:GLN:OE1	7:I:120:GLN:HA	2.05	0.56
12:T:7:DA:OP2	12:T:7:DA:H8	1.89	0.56
1:A:1338:VAL:HG12	1:A:1339:LEU:HD23	1.88	0.56
2:B:31:TRP:HA	2:B:34:ILE:HD12	1.88	0.56
2:B:37:PHE:O	2:B:38:PHE:HB2	2.06	0.56
2:B:708:GLU:O	2:B:709:ASP:C	2.44	0.56
2:B:1096:ARG:O	2:B:1097:HIS:CD2	2.59	0.56
1:A:768:GLN:HG3	1:A:816:HIS:HA	1.88	0.56
2:B:65:GLU:N	2:B:67:SER:HB3	2.21	0.56
2:B:515:HIS:H	2:B:518:HIS:CD2	2.24	0.56
2:B:1065:GLN:NE2	2:B:1069:PHE:HD1	2.03	0.56
1:A:541:ILE:N	1:A:541:ILE:HD12	2.20	0.56
1:A:1436:ILE:O	1:A:1437:GLY:C	2.43	0.56
6:H:44:VAL:O	6:H:44:VAL:CG1	2.53	0.56
7:I:111:THR:HG22	7:I:113:ASP:N	2.11	0.56
12:T:11:DC:C5	12:T:12:DC:N4	2.74	0.56
2:B:519:TRP:HZ2	2:B:705:MET:HE3	1.70	0.56
2:B:636:PRO:O	2:B:691:GLU:O	2.24	0.56
4:E:117:THR:O	4:E:119:SER:N	2.39	0.56
6:H:17:PRO:O	6:H:19:ARG:N	2.38	0.56
1:A:424:ILE:HG22	1:A:424:ILE:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1332:PHE:CE1	1:A:1348:LEU:HD13	2.40	0.56
2:B:58:THR:O	2:B:62:ILE:HG12	2.04	0.56
2:B:278:GLN:HG2	2:B:279:ASP:H	1.70	0.56
2:B:911:ILE:HG22	2:B:912:ILE:HG13	1.87	0.56
2:B:1084:GLN:HE22	3:C:192:TRP:N	2.04	0.56
1:A:224:PHE:CE2	1:A:231:PRO:HG3	2.41	0.56
1:A:777:PHE:CD1	1:A:781:ASP:HA	2.40	0.56
1:A:399:HIS:O	1:A:400:PRO:C	2.41	0.55
4:E:64:PRO:CD	4:E:76:GLY:HA2	2.36	0.55
12:T:6:DC:C6	12:T:7:DA:N7	2.74	0.55
1:A:541:ILE:HG22	1:A:546:VAL:CG2	2.36	0.55
13:N:4:DG:C4	13:N:5:DT:C5	2.94	0.55
1:A:345:VAL:HB	2:B:1154:ALA:HB1	1.87	0.55
1:A:414:ASP:OD1	1:A:416:ARG:HG2	2.06	0.55
1:A:709:THR:HG23	7:I:94:ASP:HA	1.88	0.55
1:A:907:THR:HG22	1:A:908:LEU:N	2.21	0.55
5:F:132:LEU:O	5:F:148:VAL:HG23	2.07	0.55
1:A:76:GLU:OE2	2:B:1159:ARG:NH1	2.40	0.55
1:A:381:THR:HG23	1:A:383:TYR:H	1.72	0.55
2:B:492:LEU:HB3	2:B:751:VAL:HG21	1.88	0.55
2:B:642:ASP:HA	2:B:649:LYS:HA	1.89	0.55
6:H:104:PHE:CZ	6:H:136:LYS:HA	2.42	0.55
2:B:1065:GLN:HE22	2:B:1067:ARG:HB2	1.70	0.55
1:A:754:SER:N	1:A:757:ASN:HD22	2.04	0.55
2:B:526:GLU:HG3	2:B:771:SER:HB3	1.89	0.55
5:F:73:ALA:O	5:F:74:ILE:HG12	2.06	0.55
6:H:109:LYS:NZ	6:H:111:LEU:HD12	2.20	0.55
2:B:203:PHE:CE1	2:B:212:LEU:HD12	2.41	0.55
2:B:999:MET:HG3	2:B:1000:PRO:HD2	1.88	0.55
4:E:116:ILE:HG22	4:E:121:MET:HG3	1.85	0.55
7:I:15:TYR:CE1	7:I:30:ARG:HD3	2.41	0.55
7:I:47:GLU:OE1	7:I:50:THR:CG2	2.54	0.55
1:A:482:PHE:HB2	2:B:838:SER:HB3	1.87	0.55
1:A:401:GLY:CA	1:A:435:HIS:HD2	2.20	0.55
3:C:251:LEU:O	3:C:255:VAL:HG23	2.07	0.55
13:N:4:DG:C6	13:N:5:DT:C5	2.95	0.55
3:C:162:GLY:HA3	3:C:170:TRP:CD2	2.41	0.55
4:E:54:GLN:HA	4:E:54:GLN:OE1	2.05	0.55
2:B:1072:MET:HE1	2:B:1085:ILE:HG21	1.88	0.54
1:A:244:PRO:O	1:A:246:VAL:N	2.39	0.54
1:A:261:ASP:HB3	1:A:323:LYS:CD	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:100:ILE:O	4:E:101:GLN:C	2.45	0.54
5:F:110:ASP:O	5:F:111:LEU:C	2.46	0.54
12:T:6:DC:C4	12:T:7:DA:N6	2.75	0.54
1:A:645:LEU:HD11	1:A:649:ILE:HD11	1.89	0.54
1:A:265:LYS:O	1:A:267:ALA:N	2.40	0.54
1:A:574:GLY:O	1:A:577:ILE:HD12	2.06	0.54
1:A:786:HIS:HE1	2:B:742:GLU:OE1	1.91	0.54
1:A:1431:GLY:HA3	2:B:1197:PRO:HD3	1.88	0.54
6:H:108:SER:O	6:H:109:LYS:HB2	2.07	0.54
13:N:6:DT:O2	13:N:7:DA:C4	2.60	0.54
1:A:86:LEU:HD13	1:A:90:VAL:HG22	1.89	0.54
1:A:361:LEU:HD22	1:A:646:PHE:CD1	2.43	0.54
1:A:586:ILE:HD11	1:A:637:LYS:HG3	1.90	0.54
1:A:1155:ASP:OD1	1:A:1162:VAL:HG23	2.07	0.54
12:T:2:DT:O2	13:N:13:DA:N1	2.40	0.54
1:A:424:ILE:O	1:A:424:ILE:CG2	2.54	0.54
9:K:47:ARG:HH11	9:K:47:ARG:HB3	1.72	0.54
1:A:56:PRO:O	1:A:58:LEU:N	2.41	0.54
1:A:84:ILE:HD11	1:A:270:LEU:HG	1.90	0.54
1:A:372:LYS:HA	1:A:435:HIS:ND1	2.23	0.54
2:B:1002:THR:HG23	2:B:1004:GLU:N	2.20	0.54
7:I:92:ARG:CG	7:I:93:LYS:H	2.20	0.54
12:T:7:DA:N1	12:T:8:DT:O4	2.40	0.54
2:B:322:PHE:HZ	7:I:30:ARG:HG2	1.72	0.54
3:C:22:LEU:CD2	3:C:25:VAL:HG21	2.37	0.54
1:A:364:VAL:O	1:A:364:VAL:HG13	2.06	0.54
1:A:984:LYS:O	1:A:988:LEU:HB3	2.08	0.54
2:B:473:MET:O	2:B:475:SER:N	2.41	0.54
12:T:6:DC:C1'	12:T:7:DA:H8	2.17	0.54
1:A:565:ILE:HG12	1:A:567:LYS:NZ	2.23	0.53
1:A:1400:CYS:O	1:A:1405:THR:HG23	2.07	0.53
3:C:141:GLY:O	3:C:142:VAL:HB	2.07	0.53
1:A:315:LEU:HD12	1:A:319:GLY:O	2.07	0.53
1:A:565:ILE:CG2	1:A:567:LYS:HG2	2.38	0.53
1:A:751:SER:OG	2:B:1015:HIS:HE1	1.92	0.53
1:A:608:ILE:O	1:A:609:ASP:O	2.26	0.53
1:A:1230:GLU:O	1:A:1233:ASP:HB2	2.08	0.53
2:B:1084:GLN:HG2	3:C:201:TRP:CH2	2.43	0.53
3:C:56:THR:HG22	3:C:58:LEU:N	2.22	0.53
9:K:61:TYR:HA	9:K:72:LYS:O	2.08	0.53
1:A:305:ASP:HA	1:A:326:ARG:HB2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:THR:HG22	1:A:44:THR:O	2.08	0.53
1:A:335:ARG:O	1:A:335:ARG:HG3	2.09	0.53
2:B:1065:GLN:NE2	2:B:1067:ARG:HB2	2.23	0.53
2:B:1096:ARG:O	2:B:1097:HIS:CG	2.61	0.53
3:C:175:ALA:HB3	8:J:43:ARG:CZ	2.39	0.53
13:N:6:DT:H2"	13:N:7:DA:OP2	2.09	0.53
1:A:218:ASP:O	1:A:222:LEU:HG	2.09	0.53
1:A:848:ILE:HD11	1:A:1374:VAL:HG21	1.90	0.53
9:K:21:ILE:HG12	9:K:33:ILE:HG12	1.91	0.53
2:B:254:LEU:CD2	2:B:381:MET:HE3	2.39	0.53
2:B:541:LEU:CD1	2:B:747:MET:HE1	2.36	0.53
13:N:6:DT:C4	13:N:7:DA:N6	2.77	0.53
2:B:65:GLU:H	2:B:67:SER:HB3	1.73	0.53
13:N:5:DT:C2'	13:N:6:DT:C7	2.81	0.53
1:A:215:SER:HB3	1:A:218:ASP:HB2	1.90	0.53
4:E:55:ARG:O	4:E:57:MET:N	2.42	0.53
12:T:3:DA:N1	13:N:12:DT:C4	2.77	0.53
1:A:828:ALA:CB	2:B:530:GLY:HA2	2.38	0.52
2:B:637:LEU:HD13	2:B:740:HIS:HB3	1.91	0.52
2:B:751:VAL:HG13	2:B:752:ALA:N	2.23	0.52
4:E:32:GLN:HE21	4:E:32:GLN:HA	1.74	0.52
12:T:2:DT:H2'	12:T:3:DA:H8	1.65	0.52
1:A:550:LEU:HD11	1:A:580:VAL:HG21	1.90	0.52
6:H:83:GLN:O	6:H:86:ASP:HB3	2.10	0.52
12:T:21:DC:H2"	12:T:22:DT:H5'	1.90	0.52
1:A:577:ILE:HD12	1:A:578:LEU:H	1.73	0.52
2:B:256:VAL:HG11	2:B:382:ILE:HD13	1.92	0.52
1:A:870:GLU:HB2	4:E:204:THR:HG21	1.91	0.52
2:B:332:ASP:C	2:B:334:ILE:H	2.12	0.52
8:J:1:MET:N	8:J:57:ILE:H	2.07	0.52
1:A:307:ASP:O	1:A:308:ILE:C	2.48	0.52
11:R:7:A:H2'	11:R:8:G:O4'	2.10	0.52
1:A:91:PHE:HA	1:A:235:ILE:HG22	1.92	0.52
2:B:114:PRO:HG2	2:B:181:LEU:HD11	1.91	0.52
2:B:487:THR:HG23	2:B:488:TYR:N	2.25	0.52
2:B:635:ARG:O	2:B:636:PRO:O	2.26	0.52
4:E:156:LEU:HD23	4:E:197:LYS:HB2	1.92	0.52
1:A:1194:ARG:NH2	1:A:1237:ILE:HD13	2.24	0.52
2:B:325:GLN:NE2	7:I:12:ASN:OD1	2.43	0.52
6:H:40:LEU:CD1	6:H:123:MET:HB2	2.32	0.52
12:T:7:DA:OP2	12:T:7:DA:H2'	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:3:DG:C2'	13:N:4:DG:OP2	2.50	0.52
1:A:1032:LEU:O	1:A:1036:ARG:HG2	2.10	0.52
6:H:104:PHE:CD2	6:H:114:VAL:HG12	2.44	0.52
12:T:8:DT:N3	13:N:7:DA:C2	2.74	0.52
1:A:511:ILE:O	1:A:519:PRO:HA	2.10	0.52
1:A:855:THR:HG21	1:A:857:ARG:NE	2.11	0.52
2:B:25:ILE:HG22	2:B:26:THR:O	2.10	0.52
2:B:986:GLN:HE21	2:B:1022:THR:CG2	2.23	0.52
2:B:1103:ILE:O	2:B:1122:ARG:NH1	2.42	0.52
3:C:69:LEU:CB	8:J:5:VAL:CG1	2.88	0.52
1:A:276:LEU:HD11	1:A:293:GLU:HG2	1.92	0.51
1:A:1193:LEU:HD12	1:A:1194:ARG:N	2.25	0.51
3:C:147:LEU:HB3	3:C:151:GLN:HB2	1.92	0.51
1:A:289:ILE:O	1:A:293:GLU:HG3	2.10	0.51
1:A:404:TYR:HA	1:A:413:ILE:O	2.11	0.51
2:B:62:ILE:HG23	2:B:418:LYS:HG3	1.91	0.51
2:B:169:ARG:HG3	2:B:454:THR:HG23	1.91	0.51
3:C:242:GLN:HE21	3:C:246:ARG:HE	1.57	0.51
2:B:254:LEU:CD2	2:B:381:MET:CE	2.87	0.51
2:B:487:THR:CG2	2:B:488:TYR:N	2.73	0.51
2:B:605:ARG:HH21	2:B:639:ILE:HG12	1.76	0.51
2:B:681:TRP:O	2:B:684:LEU:HB2	2.10	0.51
9:K:83:PRO:O	9:K:86:ALA:HB3	2.10	0.51
1:A:23:SER:O	1:A:26:GLU:N	2.43	0.51
1:A:1067:LEU:HD12	1:A:1067:LEU:O	2.10	0.51
1:A:1355:VAL:HG12	1:A:1356:ILE:HD13	1.92	0.51
2:B:911:ILE:HG23	2:B:966:VAL:HG11	1.92	0.51
4:E:164:LEU:HD13	4:E:211:TYR:CE2	2.46	0.51
9:K:37:LYS:O	9:K:38:GLU:HG2	2.11	0.51
10:L:44:ASP:O	10:L:46:VAL:N	2.43	0.51
1:A:40:THR:HG21	1:A:259:GLU:CD	2.31	0.51
2:B:313:MET:HE3	2:B:390:LEU:HG	1.93	0.51
2:B:489:SER:HA	2:B:492:LEU:HB2	1.93	0.51
1:A:24:PRO:HB3	1:A:237:THR:HB	1.92	0.51
1:A:30:ILE:HG12	2:B:1170:THR:HG21	1.92	0.51
1:A:856:THR:HB	1:A:865:GLN:HB2	1.93	0.51
6:H:5:LEU:HD11	6:H:61:SER:HB3	1.93	0.51
7:I:60:GLN:HE21	7:I:60:GLN:HA	1.75	0.51
12:T:7:DA:C2	12:T:8:DT:C5	2.97	0.51
1:A:401:GLY:C	1:A:435:HIS:CD2	2.84	0.51
2:B:789:MET:HE2	2:B:965:LYS:HB2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:952:VAL:HG13	2:B:966:VAL:HG22	1.93	0.51
9:K:49:GLU:HG3	9:K:94:ILE:HG13	1.93	0.51
12:T:3:DA:C2	13:N:12:DT:N3	2.73	0.51
1:A:596:THR:C	1:A:598:LEU:H	2.14	0.51
1:A:858:ASN:ND2	1:A:860:LEU:H	2.08	0.51
1:A:870:GLU:HG2	4:E:208:TYR:CG	2.46	0.51
2:B:487:THR:H	2:B:490:SER:HB3	1.76	0.51
2:B:639:ILE:HD11	2:B:691:GLU:HB2	1.91	0.51
3:C:133:ILE:CD1	3:C:237:SER:HA	2.41	0.51
2:B:485:ARG:HG2	2:B:485:ARG:NH1	2.08	0.51
12:T:7:DA:N3	12:T:8:DT:C5	2.78	0.51
1:A:507:VAL:N	1:A:508:PRO:CD	2.73	0.51
1:A:1121:GLU:O	1:A:1124:HIS:O	2.29	0.51
6:H:2:SER:HA	6:H:62:SER:HB3	1.93	0.51
6:H:109:LYS:HB2	6:H:110:ASP:O	2.11	0.51
6:H:41:ASP:OD2	6:H:122:LEU:N	2.39	0.50
7:I:111:THR:HG22	7:I:113:ASP:HB3	1.93	0.50
13:N:12:DT:H1'	13:N:13:DA:C8	2.46	0.50
13:N:13:DA:H8	13:N:13:DA:P	2.35	0.50
1:A:276:LEU:HD13	1:A:292:ALA:O	2.11	0.50
2:B:120:ARG:CD	2:B:955:THR:HG21	2.35	0.50
4:E:97:VAL:HG12	4:E:97:VAL:O	2.11	0.50
1:A:693:VAL:HG21	1:A:721:PHE:HE1	1.75	0.50
2:B:398:ARG:HB3	2:B:398:ARG:NH1	2.27	0.50
6:H:131:ASN:OD1	6:H:132:LEU:N	2.42	0.50
9:K:49:GLU:HG3	9:K:94:ILE:HG12	1.92	0.50
1:A:920:LEU:HD23	1:A:921:GLY:N	2.27	0.50
2:B:839:MET:CE	2:B:1010:LEU:HD21	2.41	0.50
1:A:256:GLN:CA	1:A:257:ARG:HB3	2.41	0.50
1:A:343:LYS:HZ1	2:B:1197:PRO:HB3	1.74	0.50
1:A:472:LEU:HD11	2:B:835:GLN:NE2	2.27	0.50
1:A:553:VAL:CG2	1:A:652:VAL:CG2	2.88	0.50
1:A:647:GLY:O	1:A:651:LYS:HG3	2.11	0.50
1:A:868:TYR:CZ	1:A:1064:VAL:HG21	2.46	0.50
1:A:1101:LEU:HD13	1:A:1355:VAL:HG11	1.94	0.50
2:B:28:GLU:C	2:B:30:SER:H	2.14	0.50
2:B:911:ILE:HD11	2:B:941:LEU:HD23	1.92	0.50
12:T:7:DA:C2	12:T:8:DT:C2	3.00	0.50
1:A:87:ALA:HB3	1:A:276:LEU:HD23	1.94	0.50
1:A:731:ARG:HG3	1:A:755:PHE:CZ	2.46	0.50
2:B:176:SER:O	2:B:182:SER:HB3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:89:LEU:C	6:H:91:ASP:N	2.63	0.50
13:N:5:DT:H2"	13:N:6:DT:C5	2.46	0.50
1:A:114:LEU:HD11	1:A:171:GLN:HE21	1.77	0.50
1:A:219:PHE:O	1:A:222:LEU:N	2.43	0.50
1:A:482:PHE:CD1	2:B:836:GLU:HB2	2.46	0.50
2:B:789:MET:HE2	2:B:965:LYS:CB	2.42	0.50
2:B:981:ALA:O	2:B:1093:GLN:HG2	2.11	0.50
5:F:79:ARG:HG2	5:F:144:GLU:HB3	1.93	0.50
6:H:106:GLU:C	6:H:108:SER:H	2.14	0.50
12:T:14:DC:H2"	12:T:15:DC:OP2	2.12	0.50
3:C:124:LEU:HD22	3:C:129:ILE:HG22	1.93	0.50
4:E:179:GLN:HA	4:E:179:GLN:NE2	2.27	0.50
1:A:65:LEU:O	1:A:66:LYS:HG3	2.11	0.50
2:B:63:ILE:O	2:B:67:SER:CB	2.55	0.50
2:B:797:TYR:CE2	3:C:62:PHE:CD2	3.00	0.50
4:E:72:PHE:HE2	4:E:157:SER:HB3	1.77	0.50
12:T:5:DC:C4	12:T:6:DC:C4	2.99	0.50
1:A:50:ILE:C	1:A:52:GLY:H	2.15	0.49
1:A:1053:PHE:O	1:A:1056:SER:N	2.36	0.49
7:I:59:VAL:HG12	7:I:61:ASP:H	1.76	0.49
1:A:852:TYR:CE2	1:A:1060:PRO:HB2	2.46	0.49
2:B:636:PRO:HB3	2:B:637:LEU:HA	1.93	0.49
1:A:560:ILE:N	6:H:78:SER:HB2	2.28	0.49
1:A:1198:ASP:O	1:A:1202:MET:HG2	2.12	0.49
2:B:471:LYS:HD2	2:B:471:LYS:O	2.11	0.49
2:B:563:MET:HG3	2:B:563:MET:O	2.13	0.49
2:B:574:SER:HB3	2:B:591:ARG:HH22	1.78	0.49
2:B:863:GLU:OE1	2:B:962:LYS:HB3	2.12	0.49
12:T:6:DC:N3	12:T:7:DA:C5	2.79	0.49
1:A:567:LYS:HD2	6:H:95:TYR:CD1	2.48	0.49
1:A:907:THR:HG22	1:A:908:LEU:H	1.78	0.49
1:A:1410:PHE:CD2	2:B:1212:ILE:HD11	2.45	0.49
2:B:1096:ARG:O	2:B:1097:HIS:CB	2.59	0.49
3:C:76:ASP:OD2	3:C:128:ASN:HB3	2.12	0.49
7:I:99:LEU:HB2	7:I:112:SER:HB3	1.93	0.49
1:A:303:TYR:O	1:A:303:TYR:CG	2.66	0.49
1:A:518:LYS:HB2	1:A:519:PRO:HD2	1.93	0.49
1:A:697:ALA:HB2	1:A:702:LEU:HD23	1.93	0.49
1:A:1194:ARG:HH21	1:A:1237:ILE:HD13	1.76	0.49
2:B:361:LEU:N	2:B:362:PRO:HD3	2.27	0.49
7:I:47:GLU:HG2	7:I:50:THR:HG23	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:4:DG:C2'	13:N:5:DT:H5"	2.42	0.49
1:A:350:ARG:HG3	1:A:488:ASN:OD1	2.13	0.49
2:B:356:LEU:HA	2:B:360:PHE:HB3	1.95	0.49
2:B:487:THR:HG22	2:B:489:SER:N	2.28	0.49
7:I:33:SER:O	7:I:34:TYR:O	2.30	0.49
3:C:18:VAL:HG22	3:C:240:VAL:HB	1.95	0.49
4:E:59:SER:HB3	4:E:81:GLU:HA	1.95	0.49
1:A:103:CYS:O	1:A:174:ILE:HD12	2.13	0.49
1:A:470:LEU:HD21	1:A:487:MET:HE1	1.95	0.49
1:A:550:LEU:HG	1:A:556:TRP:CE2	2.47	0.49
1:A:560:ILE:H	6:H:78:SER:HB2	1.78	0.49
1:A:784:LEU:HB3	1:A:786:HIS:HD2	1.76	0.49
2:B:211:VAL:HG13	2:B:495:LEU:HD23	1.94	0.49
2:B:906:SER:HA	2:B:946:ASN:HB2	1.93	0.49
1:A:67:CYS:C	1:A:68:GLN:HG3	2.33	0.49
1:A:565:ILE:HG23	1:A:567:LYS:CG	2.40	0.49
2:B:487:THR:O	2:B:490:SER:HB3	2.12	0.49
6:H:109:LYS:HB3	6:H:110:ASP:CB	2.43	0.49
12:T:2:DT:C3'	12:T:3:DA:H5'	2.32	0.49
1:A:401:GLY:N	1:A:435:HIS:HD2	2.10	0.49
2:B:493:SER:OG	2:B:775:LYS:HE2	2.13	0.49
8:J:1:MET:HB2	8:J:56:LEU:HD12	1.94	0.49
1:A:494:SER:O	1:A:498:ARG:HG2	2.12	0.48
1:A:605:MET:HA	1:A:605:MET:CE	2.43	0.48
1:A:977:LYS:HE3	1:A:977:LYS:HA	1.94	0.48
1:A:1342:GLU:HG2	4:E:212:ARG:NH1	2.28	0.48
1:A:1386:ARG:HE	1:A:1403:GLU:HG2	1.78	0.48
2:B:197:PHE:CE1	2:B:817:LEU:HD11	2.48	0.48
1:A:590:ARG:O	1:A:591:PHE:HB2	2.12	0.48
1:A:1392:SER:O	1:A:1394:THR:N	2.46	0.48
2:B:25:ILE:CG2	2:B:26:THR:N	2.76	0.48
2:B:100:PRO:HD2	2:B:180:TYR:CE1	2.48	0.48
2:B:724:ASP:HB3	2:B:727:LYS:HG3	1.95	0.48
1:A:55:ASP:N	1:A:56:PRO:HD2	2.28	0.48
1:A:151:ASP:CG	1:A:163:SER:HA	2.34	0.48
1:A:218:ASP:O	1:A:222:LEU:CD1	2.61	0.48
1:A:353:ILE:HD13	1:A:487:MET:HE3	1.95	0.48
1:A:574:GLY:HA2	1:A:577:ILE:HD11	1.95	0.48
1:A:663:SER:HB2	2:B:827:ILE:O	2.13	0.48
1:A:869:GLY:O	1:A:870:GLU:HB2	2.12	0.48
2:B:562:GLY:HA3	2:B:590:HIS:CE1	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:760:ASP:OD1	2:B:760:ASP:N	2.36	0.48
6:H:91:ASP:O	6:H:92:ASP:OD2	2.31	0.48
12:T:7:DA:C4	12:T:8:DT:C5	3.01	0.48
13:N:2:DT:H2"	13:N:3:DG:O5'	2.13	0.48
1:A:605:MET:HA	1:A:605:MET:HE2	1.95	0.48
1:A:800:VAL:HA	1:A:812:GLU:HG2	1.96	0.48
1:A:1293:SER:HB2	1:A:1299:VAL:CG2	2.43	0.48
1:A:1438:THR:N	5:F:88:TYR:HB3	2.27	0.48
2:B:65:GLU:CG	2:B:66:ASP:H	2.26	0.48
2:B:834:ASN:ND2	2:B:1011:ILE:HG22	2.29	0.48
2:B:973:ILE:HG23	2:B:974:PRO:HD2	1.94	0.48
2:B:1010:LEU:HD12	2:B:1010:LEU:HA	1.51	0.48
3:C:206:ASN:ND2	3:C:229:TYR:CB	2.76	0.48
1:A:546:VAL:O	1:A:550:LEU:HB2	2.12	0.48
1:A:1356:ILE:HD13	1:A:1356:ILE:N	2.28	0.48
2:B:840:ILE:HG12	2:B:992:ILE:HG22	1.95	0.48
8:J:8:PHE:H	8:J:49:MET:CE	2.26	0.48
1:A:868:TYR:CZ	1:A:1064:VAL:CG2	2.97	0.48
2:B:532:ALA:HB1	2:B:536:VAL:HG23	1.95	0.48
1:A:346:ASP:OD1	2:B:1108:ARG:HA	2.13	0.48
1:A:1110:ASN:ND2	1:A:1110:ASN:H	2.11	0.48
2:B:287:ARG:NH1	2:B:324:ILE:O	2.44	0.48
2:B:591:ARG:O	2:B:592:ASN:CB	2.61	0.48
2:B:806:THR:HG22	2:B:808:ALA:H	1.78	0.48
1:A:77:CYS:C	1:A:79:GLY:H	2.17	0.48
1:A:224:PHE:CZ	1:A:231:PRO:HG3	2.49	0.48
1:A:407:ARG:HD2	1:A:413:ILE:HD11	1.95	0.48
1:A:752:LYS:HD3	2:B:1019:SER:HB3	1.95	0.48
1:A:1364:ASN:HD22	1:A:1366:ARG:CG	2.22	0.48
1:A:1386:ARG:NE	1:A:1403:GLU:HG2	2.28	0.48
2:B:211:VAL:CG2	2:B:483:LEU:HD23	2.43	0.48
2:B:734:HIS:O	2:B:735:ALA:HB3	2.12	0.48
1:A:1159:ARG:NH1	1:A:1159:ARG:HB3	2.28	0.48
2:B:706:GLN:O	2:B:710:LEU:HB2	2.14	0.48
2:B:783:THR:HG22	8:J:63:TYR:HE1	1.79	0.48
3:C:99:LEU:HD23	3:C:99:LEU:H	1.77	0.48
5:F:116:ASP:HB3	5:F:119:ARG:HB2	1.95	0.48
6:H:15:VAL:HA	6:H:26:ILE:HD12	1.95	0.48
1:A:1098:VAL:N	1:A:1099:PRO:HD2	2.29	0.48
3:C:73:GLN:NE2	3:C:75:MET:N	2.49	0.48
3:C:262:LEU:CD1	9:K:88:LYS:HG2	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:567:LYS:HD2	6:H:95:TYR:CE1	2.49	0.47
1:A:629:LEU:HD22	1:A:633:VAL:HG23	1.94	0.47
1:A:871:ASP:HB3	4:E:205:SER:HB3	1.95	0.47
2:B:1037:LEU:HD13	2:B:1062:HIS:HB3	1.95	0.47
13:N:2:DT:C2'	13:N:3:DG:C8	2.95	0.47
1:A:8:SER:HB3	2:B:1180:PHE:HE1	1.79	0.47
1:A:664:THR:HG23	1:A:742:ASN:HB2	1.95	0.47
2:B:121:ASN:ND2	2:B:207:GLY:HA3	2.28	0.47
2:B:778:MET:HG2	2:B:794:ASN:HB3	1.96	0.47
12:T:5:DC:C5	12:T:6:DC:C4	3.03	0.47
1:A:852:TYR:CD2	1:A:1060:PRO:HB2	2.50	0.47
1:A:1312:ASN:ND2	1:A:1314:SER:OG	2.47	0.47
2:B:227:LYS:H	2:B:395:GLN:HG3	1.79	0.47
2:B:334:ILE:HG22	2:B:334:ILE:O	2.14	0.47
2:B:365:THR:HG23	2:B:367:LEU:N	2.28	0.47
1:A:974:ASP:OD1	1:A:977:LYS:HB2	2.14	0.47
1:A:1277:GLU:O	1:A:1278:ASN:HB2	2.13	0.47
2:B:515:HIS:CD2	2:B:517:THR:H	2.22	0.47
2:B:826:ALA:O	2:B:1011:ILE:HA	2.14	0.47
2:B:951:GLN:HG2	10:L:57:LEU:HD22	1.95	0.47
2:B:1110:PRO:O	2:B:1119:VAL:HG13	2.14	0.47
3:C:9:LYS:HB2	3:C:9:LYS:HE2	1.62	0.47
3:C:167:HIS:HD2	3:C:169:LYS:H	1.62	0.47
4:E:192:ARG:O	4:E:192:ARG:HG3	2.14	0.47
13:N:3:DG:OP2	13:N:3:DG:H2'	2.14	0.47
13:N:10:DG:H2"	13:N:11:DG:OP2	2.14	0.47
1:A:43:GLU:O	1:A:43:GLU:HG2	2.14	0.47
1:A:225:ASN:C	1:A:225:ASN:HD22	2.18	0.47
1:A:553:VAL:HG23	1:A:652:VAL:HG23	1.96	0.47
1:A:672:ASP:HB3	1:A:675:THR:H	1.79	0.47
3:C:172:PRO:O	3:C:235:VAL:HG23	2.14	0.47
1:A:100:LYS:HG3	1:A:181:LEU:HD22	1.95	0.47
1:A:261:ASP:HB3	1:A:323:LYS:HD2	1.96	0.47
1:A:550:LEU:HD12	1:A:550:LEU:HA	1.58	0.47
2:B:862:GLN:HE21	2:B:961:LEU:CD1	2.28	0.47
3:C:244:VAL:HG21	9:K:105:PHE:CZ	2.50	0.47
1:A:65:LEU:C	1:A:66:LYS:HG3	2.34	0.47
1:A:328:ARG:HD3	2:B:1206:GLU:OE1	2.14	0.47
1:A:492:PRO:CB	1:A:497:THR:HG23	2.44	0.47
1:A:754:SER:H	1:A:757:ASN:HD22	1.61	0.47
1:A:1293:SER:HB3	1:A:1297:GLU:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:29:MET:HA	9:K:45:LEU:CD1	2.45	0.47
4:E:167:ARG:HD3	4:E:167:ARG:HA	1.59	0.47
8:J:36:LEU:HD13	8:J:47:ARG:HG3	1.96	0.47
12:T:6:DC:N4	12:T:7:DA:N6	2.62	0.47
1:A:378:GLU:OE1	1:A:434:ARG:HD3	2.14	0.47
1:A:567:LYS:CB	6:H:95:TYR:HA	2.45	0.47
1:A:636:GLU:OE2	1:A:962:ARG:HD2	2.15	0.47
2:B:64:CYS:O	2:B:65:GLU:CD	2.53	0.47
2:B:620:ARG:CZ	7:I:68:LEU:HD21	2.44	0.47
1:A:208:LEU:HD21	1:A:212:LYS:NZ	2.30	0.47
1:A:499:ALA:O	1:A:503:GLN:HG2	2.14	0.47
1:A:896:ARG:HD2	1:A:897:TYR:CE1	2.50	0.47
1:A:969:GLN:C	1:A:971:PHE:H	2.18	0.47
2:B:475:SER:O	2:B:476:ARG:C	2.52	0.47
2:B:512:ARG:HB3	2:B:533:CYS:O	2.15	0.47
2:B:552:MET:N	2:B:553:PRO:HD2	2.30	0.47
2:B:797:TYR:CE2	3:C:62:PHE:HD2	2.32	0.47
2:B:807:ARG:HG2	2:B:1045:SER:OG	2.14	0.47
3:C:76:ASP:OD2	3:C:128:ASN:N	2.46	0.47
13:N:4:DG:N1	13:N:5:DT:C2	2.81	0.47
1:A:1128:GLN:HB2	1:A:1304:TRP:NE1	2.30	0.47
2:B:102:VAL:HG22	2:B:112:LEU:HB2	1.97	0.47
2:B:115:GLN:HE21	2:B:119:LEU:HD11	1.81	0.47
3:C:47:ASP:O	3:C:48:SER:HB2	2.15	0.47
10:L:47:ARG:NH1	10:L:54:ARG:NE	2.52	0.47
2:B:784:ASN:OD1	2:B:788:ARG:HD2	2.13	0.46
2:B:957:ASN:ND2	2:B:959:ASP:HB2	2.30	0.46
2:B:860:MET:HG2	2:B:861:ASP:H	1.80	0.46
4:E:64:PRO:HD3	4:E:76:GLY:HA2	1.97	0.46
9:K:51:LEU:CD1	9:K:59:ALA:HB3	2.45	0.46
1:A:596:THR:O	1:A:597:LEU:C	2.52	0.46
1:A:741:ASN:ND2	1:A:744:LYS:H	2.07	0.46
1:A:855:THR:HG22	1:A:857:ARG:HG3	1.96	0.46
1:A:899:VAL:HB	1:A:929:LEU:HD13	1.98	0.46
1:A:1423:GLY:O	1:A:1424:VAL:C	2.53	0.46
2:B:258:LEU:HD12	2:B:269:ILE:HG12	1.98	0.46
2:B:331:LEU:O	2:B:334:ILE:HB	2.15	0.46
2:B:744:HIS:O	2:B:747:MET:HB2	2.15	0.46
2:B:778:MET:O	2:B:819:ALA:HB1	2.16	0.46
5:F:113:GLY:O	5:F:115:THR:HG23	2.15	0.46
1:A:68:GLN:NE2	1:A:70:CYS:HB3	2.27	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:PRO:C	1:A:246:VAL:H	2.19	0.46
1:A:253:ASN:O	1:A:254:GLU:HB2	2.15	0.46
1:A:472:LEU:HD21	2:B:835:GLN:HB2	1.97	0.46
1:A:1166:ASP:HA	1:A:1169:ILE:HD13	1.98	0.46
6:H:93:TYR:HB3	6:H:144:ILE:O	2.16	0.46
1:A:225:ASN:C	1:A:225:ASN:ND2	2.69	0.46
1:A:372:LYS:HD3	1:A:397:ASN:HA	1.97	0.46
2:B:36:ALA:C	2:B:37:PHE:O	2.42	0.46
2:B:545:ILE:HG13	2:B:633:VAL:HG13	1.96	0.46
2:B:780:VAL:HG21	8:J:56:LEU:HD13	1.97	0.46
2:B:1079:LYS:HE2	3:C:188:HIS:CE1	2.51	0.46
6:H:131:ASN:C	6:H:133:ASN:N	2.69	0.46
1:A:68:GLN:C	1:A:70:CYS:H	2.19	0.46
1:A:1209:MET:SD	1:A:1236:LEU:HB3	2.55	0.46
1:A:1420:ASP:HB3	1:A:1422:ARG:HG2	1.97	0.46
2:B:217:ARG:NH1	2:B:407:ASP:OD1	2.48	0.46
2:B:485:ARG:CG	2:B:485:ARG:NH1	2.68	0.46
2:B:592:ASN:H	2:B:593:PRO:HD3	1.80	0.46
6:H:47:PHE:CB	6:H:95:TYR:HD1	2.27	0.46
6:H:137:GLN:C	6:H:139:ASN:H	2.18	0.46
9:K:20:LYS:O	9:K:33:ILE:HA	2.15	0.46
1:A:134:ARG:CD	1:A:221:SER:O	2.63	0.46
1:A:351:THR:HG21	1:A:466:SER:O	2.16	0.46
1:A:738:LYS:HB3	6:H:19:ARG:HH22	1.81	0.46
1:A:1308:THR:HG22	1:A:1310:GLY:O	2.14	0.46
1:A:1424:VAL:HG11	2:B:1139:ILE:CD1	2.46	0.46
2:B:1077:THR:HG23	2:B:1079:LYS:HB2	1.98	0.46
1:A:965:GLN:HA	1:A:968:GLN:HG2	1.98	0.46
2:B:198:ASP:OD1	2:B:485:ARG:NH2	2.46	0.46
2:B:1001:PHE:CE2	2:B:1073:TYR:HB2	2.50	0.46
13:N:4:DG:C5	13:N:5:DT:C7	2.98	0.46
1:A:351:THR:HG22	1:A:352:VAL:N	2.29	0.46
1:A:500:GLU:O	1:A:504:LEU:HB2	2.15	0.46
1:A:1412:ALA:HA	1:A:1417:GLU:HG3	1.97	0.46
1:A:1443:VAL:O	1:A:1444:MET:HG3	2.16	0.46
2:B:176:SER:OG	2:B:177:LYS:N	2.48	0.46
2:B:1065:GLN:HE21	2:B:1069:PHE:HD1	1.63	0.46
1:A:579:SER:HB3	1:A:611:GLN:HA	1.97	0.46
1:A:856:THR:O	1:A:856:THR:HG22	2.15	0.46
1:A:856:THR:HG22	1:A:864:ILE:HB	1.97	0.46
1:A:910:PRO:HA	1:A:916:GLY:HA3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1035:TYR:O	1:A:1037:LEU:N	2.49	0.46
2:B:416:LEU:HD11	2:B:460:ALA:HB3	1.94	0.46
2:B:642:ASP:CB	2:B:649:LYS:HG3	2.42	0.46
2:B:766:ARG:HA	2:B:766:ARG:HD3	1.74	0.46
2:B:864:LYS:HD2	2:B:865:LYS:H	1.81	0.46
2:B:996:ARG:HG3	2:B:1007:VAL:HG11	1.98	0.46
2:B:1187:ASN:HD22	2:B:1188:LYS:N	2.14	0.46
3:C:69:LEU:O	8:J:6:ARG:NH1	2.49	0.46
4:E:119:SER:HB2	13:N:12:DT:H5"	1.98	0.46
12:T:1:DC:N4	13:N:13:DA:N6	2.63	0.46
1:A:31:SER:CB	1:A:83:HIS:HD2	2.28	0.45
1:A:180:LYS:HE3	1:A:294:SER:HB3	1.97	0.45
1:A:1073:GLY:O	1:A:1076:ALA:HB3	2.16	0.45
2:B:830:TYR:CZ	2:B:1000:PRO:HD3	2.51	0.45
2:B:1159:ARG:HE	2:B:1193:GLN:NE2	2.15	0.45
5:F:130:ILE:HA	5:F:131:PRO:HD3	1.87	0.45
9:K:51:LEU:HD13	9:K:59:ALA:HB3	1.98	0.45
1:A:214:ILE:CG2	1:A:215:SER:N	2.70	0.45
1:A:360:GLU:HB2	1:A:363:GLN:HG3	1.98	0.45
1:A:492:PRO:HB2	1:A:497:THR:HG23	1.98	0.45
1:A:1107:VAL:HG23	1:A:1383:SER:HB3	1.97	0.45
2:B:230:ALA:N	2:B:231:PRO:CD	2.73	0.45
1:A:53:LEU:CD1	1:A:266:LEU:O	2.65	0.45
1:A:868:TYR:CE1	1:A:1064:VAL:CG2	2.98	0.45
2:B:486:TYR:CE2	2:B:1096:ARG:HG2	2.52	0.45
2:B:878:GLN:O	2:B:879:ARG:C	2.55	0.45
12:T:7:DA:C2'	12:T:8:DT:H5"	2.45	0.45
13:N:4:DG:H2"	13:N:5:DT:C5'	2.46	0.45
1:A:709:THR:CG2	7:I:94:ASP:HA	2.46	0.45
1:A:753:GLY:HA2	1:A:757:ASN:ND2	2.31	0.45
3:C:186:LEU:HB3	3:C:188:HIS:CD2	2.50	0.45
3:C:186:LEU:CB	3:C:188:HIS:HD2	2.29	0.45
1:A:351:THR:HG21	2:B:1103:ILE:HG12	1.96	0.45
1:A:852:TYR:O	5:F:81:THR:HG22	2.17	0.45
1:A:1372:VAL:O	1:A:1376:THR:HB	2.16	0.45
1:A:1444:MET:HB2	5:F:133:VAL:HG12	1.97	0.45
2:B:957:ASN:HD21	2:B:959:ASP:HB2	1.80	0.45
3:C:67:LEU:HD23	3:C:144:ILE:HD11	1.98	0.45
1:A:43:GLU:OE1	1:A:43:GLU:N	2.48	0.45
1:A:265:LYS:HZ1	1:A:303:TYR:N	2.14	0.45
1:A:962:ARG:O	1:A:966:ASN:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:65:GLU:HG2	2:B:66:ASP:H	1.80	0.45
2:B:175:ARG:HH11	2:B:175:ARG:HG2	1.78	0.45
2:B:680:THR:O	2:B:681:TRP:C	2.53	0.45
2:B:845:SER:HB2	8:J:8:PHE:HB3	1.98	0.45
2:B:872:GLU:HG2	2:B:916:THR:HB	1.99	0.45
3:C:238:ILE:HG23	3:C:242:GLN:HB2	1.99	0.45
12:T:2:DT:H3'	12:T:2:DT:H6	1.82	0.45
1:A:272:ALA:O	1:A:296:LEU:HB2	2.17	0.45
1:A:375:THR:HG21	1:A:433:GLU:OE1	2.16	0.45
1:A:472:LEU:HD11	2:B:835:GLN:HE22	1.80	0.45
1:A:1193:LEU:HD12	1:A:1193:LEU:C	2.36	0.45
2:B:118:ARG:HH22	2:B:194:GLU:CD	2.20	0.45
3:C:97:VAL:HG21	3:C:129:ILE:HG23	1.97	0.45
3:C:238:ILE:HD11	3:C:246:ARG:NH1	2.32	0.45
4:E:79:TRP:HB2	4:E:105:PHE:CD1	2.51	0.45
1:A:151:ASP:OD2	1:A:163:SER:HA	2.17	0.45
1:A:504:LEU:CD1	5:F:91:ALA:HB2	2.47	0.45
3:C:142:VAL:HG13	8:J:5:VAL:HG23	1.98	0.45
5:F:114:GLU:OE1	5:F:119:ARG:HG3	2.17	0.45
6:H:11:GLN:HE21	6:H:11:GLN:HB2	1.60	0.45
12:T:2:DT:O2	13:N:13:DA:C2	2.69	0.45
13:N:14:DG:OP2	13:N:14:DG:H2'	2.17	0.45
2:B:370:PHE:HD2	2:B:373:ARG:HG3	1.81	0.45
2:B:647:GLY:O	2:B:648:HIS:ND1	2.50	0.45
2:B:708:GLU:O	2:B:712:PRO:HD3	2.16	0.45
12:T:16:DC:H2"	12:T:17:DC:C5	2.52	0.45
1:A:313:GLN:HB3	1:A:314:ALA:H	1.42	0.45
1:A:1258:HIS:O	1:A:1262:LYS:NZ	2.47	0.45
2:B:167:ILE:HG21	2:B:453:ILE:HD12	1.99	0.45
4:E:55:ARG:C	4:E:57:MET:N	2.67	0.45
6:H:110:ASP:O	6:H:111:LEU:HG	2.16	0.45
6:H:127:GLY:HA3	6:H:130:ARG:CZ	2.47	0.45
13:N:5:DT:C2'	13:N:6:DT:C5	2.99	0.45
1:A:219:PHE:HB3	1:A:224:PHE:HB2	1.99	0.44
1:A:322:VAL:C	1:A:323:LYS:HD3	2.37	0.44
1:A:565:ILE:HG12	1:A:567:LYS:HZ1	1.82	0.44
2:B:1093:GLN:HG2	2:B:1093:GLN:H	1.70	0.44
3:C:99:LEU:N	3:C:99:LEU:CD2	2.76	0.44
4:E:96:PHE:C	4:E:98:ILE:N	2.70	0.44
5:F:136:ARG:O	5:F:143:PHE:HA	2.17	0.44
1:A:242:PRO:HA	1:A:243:PRO:HD3	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1130:GLN:O	1:A:1134:ILE:HD12	2.17	0.44
2:B:228:LYS:HB3	2:B:228:LYS:HE2	1.73	0.44
2:B:793:ALA:HB3	2:B:856:PHE:HB2	1.98	0.44
1:A:783:THR:CG2	1:A:784:LEU:N	2.80	0.44
1:A:1194:ARG:NH2	1:A:1237:ILE:CD1	2.80	0.44
1:A:1206:ASP:N	1:A:1206:ASP:OD2	2.51	0.44
2:B:764:SER:O	2:B:765:PRO:C	2.55	0.44
1:A:251:SER:HB2	11:R:1:A:N3	2.32	0.44
2:B:764:SER:O	2:B:766:ARG:N	2.51	0.44
2:B:382:ILE:HG12	2:B:382:ILE:H	1.65	0.44
2:B:420:LEU:HD23	2:B:420:LEU:HA	1.83	0.44
3:C:127:ARG:HE	3:C:127:ARG:HB2	1.54	0.44
8:J:22:LEU:HA	8:J:22:LEU:HD12	1.59	0.44
1:A:5:GLN:O	2:B:1159:ARG:NH2	2.50	0.44
1:A:417:TYR:O	1:A:418:SER:HB3	2.18	0.44
1:A:547:LEU:HB3	9:K:58:PHE:CE1	2.52	0.44
2:B:797:TYR:HB3	2:B:798:TYR:CD1	2.53	0.44
2:B:1181:GLU:H	2:B:1181:GLU:HG2	1.55	0.44
12:T:5:DC:C4	12:T:6:DC:N3	2.85	0.44
13:N:1:DG:H2"	13:N:2:DT:C6	2.46	0.44
1:A:1111:MET:HE2	1:A:1111:MET:HB2	1.73	0.44
2:B:857:ARG:O	2:B:967:ARG:HA	2.18	0.44
8:J:52:THR:HG22	8:J:52:THR:O	2.17	0.44
12:T:22:DT:C2'	12:T:23:DC:O5'	2.65	0.44
2:B:43:LEU:HD23	2:B:43:LEU:HA	1.76	0.44
2:B:217:ARG:NH2	2:B:405:ARG:HG3	2.33	0.44
4:E:190:LEU:HD11	4:E:196:VAL:HG13	2.00	0.44
4:E:197:LYS:HG3	4:E:211:TYR:CE2	2.53	0.44
1:A:472:LEU:HD21	2:B:835:GLN:CB	2.48	0.44
1:A:836:TYR:O	1:A:837:ILE:C	2.56	0.44
2:B:635:ARG:C	2:B:636:PRO:O	2.56	0.44
2:B:879:ARG:O	2:B:880:THR:C	2.56	0.44
2:B:1109:GLY:HA3	2:B:1110:PRO:HD2	1.67	0.44
1:A:114:LEU:HD11	1:A:171:GLN:NE2	2.33	0.43
1:A:260:ASP:CG	1:A:261:ASP:H	2.21	0.43
1:A:302:THR:HG21	1:A:313:GLN:OE1	2.18	0.43
1:A:835:GLY:HA3	12:T:18:DG:H1'	1.98	0.43
1:A:1312:ASN:OD1	1:A:1315:GLU:HG3	2.18	0.43
2:B:493:SER:HA	2:B:751:VAL:HG11	1.99	0.43
2:B:547:VAL:N	2:B:612:GLU:OE2	2.39	0.43
2:B:636:PRO:CB	2:B:637:LEU:HA	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:69:LEU:HB3	8:J:6:ARG:HD3	2.00	0.43
1:A:22:PHE:CB	2:B:1211:ASN:OD1	2.65	0.43
1:A:91:PHE:N	1:A:297:GLN:HE22	2.15	0.43
1:A:577:ILE:H	1:A:577:ILE:HG13	1.57	0.43
2:B:242:SER:HB2	2:B:252:SER:O	2.17	0.43
2:B:778:MET:CE	2:B:1094:ARG:HD3	2.48	0.43
2:B:913:GLY:HA2	2:B:938:SER:OG	2.18	0.43
3:C:112:ASN:HD21	3:C:146:LYS:HD3	1.83	0.43
3:C:129:ILE:HA	3:C:129:ILE:HD12	1.74	0.43
1:A:610:GLY:O	1:A:611:GLN:NE2	2.51	0.43
1:A:973:ILE:HD12	1:A:974:ASP:H	1.83	0.43
1:A:1155:ASP:HA	1:A:1156:PRO:HD3	1.75	0.43
2:B:96:TYR:HB2	2:B:129:PHE:HB2	2.01	0.43
2:B:470:LYS:C	2:B:472:ALA:H	2.22	0.43
2:B:724:ASP:HA	2:B:725:PRO:HD3	1.90	0.43
2:B:1084:GLN:NE2	3:C:192:TRP:N	2.60	0.43
1:A:269:ILE:HD13	1:A:300:VAL:HG22	2.00	0.43
1:A:533:LYS:HD3	1:A:745:GLN:NE2	2.33	0.43
1:A:598:LEU:HD23	1:A:598:LEU:HA	1.74	0.43
1:A:825:ILE:HD12	2:B:512:ARG:HB2	2.00	0.43
1:A:913:LEU:HD11	1:A:981:LEU:O	2.18	0.43
2:B:100:PRO:C	2:B:101:MET:HG3	2.38	0.43
3:C:231:ASN:C	3:C:231:ASN:ND2	2.71	0.43
4:E:88:VAL:HG11	4:E:110:PHE:CE2	2.53	0.43
13:N:7:DA:H2"	13:N:8:DT:C6	2.54	0.43
1:A:112:LYS:HG2	1:A:113:LEU:N	2.34	0.43
1:A:352:VAL:CG2	2:B:1099:VAL:HG13	2.48	0.43
1:A:858:ASN:C	1:A:858:ASN:ND2	2.70	0.43
1:A:1156:PRO:HD2	1:A:1157:ASP:H	1.83	0.43
2:B:549:THR:O	2:B:628:THR:CG2	2.67	0.43
2:B:983:ARG:NH1	2:B:1091:TYR:HB3	2.32	0.43
2:B:1058:LEU:HD23	2:B:1058:LEU:HA	1.87	0.43
3:C:56:THR:HG23	3:C:58:LEU:H	1.83	0.43
3:C:142:VAL:N	8:J:16:ASP:HB3	2.31	0.43
7:I:111:THR:CG2	7:I:113:ASP:CB	2.93	0.43
1:A:99:ILE:HD13	1:A:235:ILE:HG23	1.99	0.43
1:A:354:SER:HA	1:A:482:PHE:CD2	2.53	0.43
1:A:1015:VAL:O	1:A:1015:VAL:CG1	2.66	0.43
2:B:121:ASN:HD22	2:B:121:ASN:HA	1.61	0.43
5:F:83:PRO:HA	5:F:146:TRP:CZ3	2.53	0.43
1:A:596:THR:C	1:A:598:LEU:N	2.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:88:VAL:HG11	4:E:110:PHE:HE2	1.84	0.43
5:F:76:LYS:O	5:F:79:ARG:HD3	2.18	0.43
1:A:629:LEU:HD13	1:A:645:LEU:HD21	1.99	0.43
1:A:1143:LEU:HD23	1:A:1267:MET:O	2.19	0.43
2:B:483:LEU:HD23	2:B:483:LEU:HA	1.93	0.43
8:J:3:VAL:HG11	8:J:18:TRP:HB2	2.01	0.43
1:A:211:PHE:O	1:A:213:HIS:N	2.52	0.43
1:A:979:SER:OG	1:A:981:LEU:HD12	2.19	0.43
2:B:293:PRO:HG2	2:B:296:GLU:CB	2.48	0.43
2:B:1060:ARG:HD2	2:B:1060:ARG:HA	1.69	0.43
3:C:5:GLY:HA3	3:C:6:PRO:HD2	1.87	0.43
3:C:77:ILE:HD12	3:C:161:LYS:HG3	2.01	0.43
1:A:31:SER:OG	1:A:83:HIS:HD2	2.02	0.43
1:A:129:LYS:O	1:A:130:ASP:HB3	2.19	0.43
1:A:368:LYS:HB2	1:A:368:LYS:HE2	1.75	0.43
1:A:982:THR:O	1:A:983:ILE:C	2.57	0.43
2:B:64:CYS:O	2:B:65:GLU:HB3	2.18	0.43
2:B:229:ALA:HB1	2:B:231:PRO:CD	2.44	0.43
2:B:274:PRO:HB2	2:B:359:GLU:HB3	2.01	0.43
2:B:770:GLN:O	2:B:770:GLN:CD	2.57	0.43
2:B:801:LYS:O	8:J:52:THR:CG2	2.54	0.43
2:B:911:ILE:HD13	2:B:911:ILE:HG21	1.60	0.43
2:B:957:ASN:CG	2:B:958:GLN:N	2.73	0.43
1:A:19:PHE:HE1	1:A:1396:ALA:HB3	1.84	0.42
1:A:96:ILE:O	1:A:97:ALA:C	2.58	0.42
2:B:168:GLY:HA2	2:B:454:THR:OG1	2.19	0.42
2:B:634:TYR:CD1	2:B:692:TYR:HB3	2.54	0.42
13:N:6:DT:C2	13:N:7:DA:N7	2.87	0.42
1:A:981:LEU:HD21	1:A:1039:LYS:HA	2.02	0.42
1:A:1437:GLY:O	1:A:1440:ALA:N	2.43	0.42
4:E:22:MET:HB2	4:E:187:TYR:CE1	2.54	0.42
4:E:157:SER:O	4:E:159:ASP:N	2.52	0.42
1:A:313:GLN:HB2	1:A:322:VAL:CG2	2.37	0.42
1:A:836:TYR:CZ	1:A:840:ARG:HD2	2.53	0.42
1:A:992:ASP:O	1:A:995:GLU:HB2	2.19	0.42
1:A:1159:ARG:HB3	1:A:1159:ARG:HH11	1.84	0.42
2:B:642:ASP:O	2:B:644:GLU:N	2.52	0.42
3:C:226:ASP:O	3:C:227:THR:O	2.37	0.42
4:E:76:GLY:O	4:E:77:SER:C	2.58	0.42
4:E:122:LYS:HB3	4:E:123:LEU:HD23	2.02	0.42
4:E:157:SER:N	4:E:160:GLU:OE1	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:101:PHE:O	7:I:109:ILE:HA	2.20	0.42
1:A:269:ILE:CD1	1:A:300:VAL:HG22	2.49	0.42
1:A:323:LYS:O	1:A:324:SER:CB	2.66	0.42
1:A:535:THR:O	1:A:536:LEU:C	2.58	0.42
1:A:744:LYS:HE2	1:A:748:MET:HE3	2.00	0.42
3:C:246:ARG:HA	3:C:249:ASP:HB2	2.02	0.42
1:A:744:LYS:HE2	1:A:748:MET:CE	2.49	0.42
1:A:783:THR:HG23	1:A:815:PHE:HZ	1.84	0.42
1:A:969:GLN:O	1:A:971:PHE:N	2.52	0.42
2:B:212:LEU:HD23	2:B:480:SER:HB3	2.02	0.42
2:B:412:LEU:O	2:B:413:LEU:C	2.57	0.42
2:B:473:MET:C	2:B:475:SER:N	2.72	0.42
2:B:542:MET:SD	2:B:747:MET:HG3	2.59	0.42
3:C:63:ILE:HA	3:C:66:ARG:HG3	2.00	0.42
6:H:25:ARG:NH2	6:H:41:ASP:OD2	2.52	0.42
6:H:38:LEU:HG	6:H:39:THR:N	2.34	0.42
1:A:902:LEU:H	1:A:902:LEU:HG	1.37	0.42
2:B:254:LEU:HD21	2:B:381:MET:HE3	2.01	0.42
2:B:1002:THR:HG22	2:B:1006:ILE:H	1.85	0.42
2:B:1124:ARG:HE	2:B:1124:ARG:HB2	1.66	0.42
3:C:69:LEU:CB	8:J:5:VAL:HG13	2.50	0.42
3:C:142:VAL:H	8:J:16:ASP:CB	2.28	0.42
7:I:58:VAL:HG11	7:I:109:ILE:HD11	2.02	0.42
1:A:243:PRO:O	1:A:244:PRO:C	2.57	0.42
1:A:380:VAL:CG1	1:A:428:TYR:HA	2.37	0.42
2:B:515:HIS:HD2	2:B:517:THR:N	2.11	0.42
3:C:143:LEU:HG	8:J:2:ILE:HD11	2.00	0.42
6:H:109:LYS:HB3	6:H:110:ASP:CG	2.40	0.42
1:A:1060:PRO:HD2	5:F:86:THR:HG21	2.02	0.42
1:A:1115:SER:HB3	1:A:1330:ASN:ND2	2.35	0.42
1:A:1336:MET:HE2	1:A:1380:GLY:HA2	2.01	0.42
2:B:400:HIS:CE1	2:B:517:THR:HG21	2.55	0.42
2:B:413:LEU:HD23	2:B:413:LEU:HA	1.81	0.42
2:B:638:PHE:CE2	2:B:653:VAL:HG21	2.54	0.42
2:B:1027:ILE:HG23	2:B:1052:VAL:HG22	2.02	0.42
3:C:43:THR:HG22	3:C:44:LEU:N	2.35	0.42
1:A:257:ARG:HG2	1:A:258:GLY:N	2.34	0.42
2:B:35:SER:O	2:B:37:PHE:O	2.38	0.42
2:B:705:MET:HE2	2:B:745:PRO:HB3	2.02	0.42
2:B:756:ILE:HG12	2:B:770:GLN:HG2	2.01	0.42
2:B:1187:ASN:HD21	2:B:1190:ASP:N	2.12	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:190:ASP:C	3:C:190:ASP:OD1	2.58	0.42
4:E:3:GLN:HB2	4:E:4:GLU:H	1.63	0.42
6:H:107:VAL:HG12	6:H:107:VAL:O	2.20	0.42
10:L:27:LEU:HD22	10:L:37:LYS:NZ	2.35	0.42
2:B:120:ARG:HD2	2:B:955:THR:CG2	2.39	0.42
2:B:314:LEU:O	2:B:317:CYS:HB2	2.19	0.42
2:B:685:LEU:HD21	2:B:692:TYR:CE1	2.54	0.42
2:B:804:GLY:HA2	2:B:1042:GLY:O	2.20	0.42
2:B:862:GLN:HE21	2:B:961:LEU:HD13	1.85	0.42
13:N:4:DG:C2	13:N:5:DT:N3	2.80	0.42
1:A:99:ILE:CD1	1:A:235:ILE:HG23	2.50	0.41
1:A:312:PRO:C	1:A:313:GLN:HE21	2.23	0.41
1:A:775:ILE:H	1:A:775:ILE:HG12	1.69	0.41
1:A:808:LEU:O	2:B:728:ARG:NH1	2.53	0.41
1:A:821:ARG:HH11	1:A:821:ARG:HD3	1.69	0.41
1:A:943:LEU:O	1:A:946:VAL:N	2.51	0.41
2:B:310:MET:O	2:B:313:MET:HB2	2.21	0.41
10:L:59:ALA:O	10:L:60:ARG:HB3	2.19	0.41
1:A:804:TYR:O	2:B:761:HIS:ND1	2.48	0.41
2:B:288:ALA:HB1	2:B:331:LEU:HD13	2.02	0.41
2:B:301:ILE:HG21	2:B:314:LEU:HD11	2.02	0.41
2:B:1002:THR:HG21	2:B:1006:ILE:CG1	2.50	0.41
2:B:1056:SER:O	2:B:1066:SER:HB2	2.20	0.41
6:H:40:LEU:HD12	6:H:41:ASP:H	1.84	0.41
1:A:322:VAL:HB	1:A:323:LYS:H	1.29	0.41
2:B:35:SER:O	2:B:39:ARG:HB2	2.20	0.41
2:B:185:THR:HG23	2:B:188:ASP:OD2	2.21	0.41
12:T:7:DA:H2	12:T:8:DT:N3	2.07	0.41
1:A:785:PRO:HD2	1:A:786:HIS:CD2	2.55	0.41
2:B:122:LEU:HD21	2:B:958:GLN:HB2	2.02	0.41
2:B:195:CYS:SG	2:B:783:THR:HB	2.60	0.41
2:B:311:LEU:HB3	7:I:4:PHE:HZ	1.85	0.41
10:L:59:ALA:O	10:L:60:ARG:CB	2.68	0.41
1:A:53:LEU:HD23	1:A:54:ASN:HB3	2.01	0.41
1:A:573:SER:O	1:A:574:GLY:C	2.59	0.41
1:A:1060:PRO:HD2	5:F:86:THR:CG2	2.49	0.41
2:B:402:GLY:HA2	2:B:695:ALA:HB3	2.01	0.41
2:B:542:MET:SD	2:B:636:PRO:HG3	2.61	0.41
6:H:62:SER:HB2	6:H:63:LEU:H	1.41	0.41
13:N:12:DT:H2"	13:N:13:DA:C8	2.55	0.41
1:A:848:ILE:HD11	1:A:1374:VAL:CG2	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1392:SER:C	1:A:1394:THR:H	2.24	0.41
2:B:258:LEU:HB2	2:B:385:LEU:HD21	2.01	0.41
2:B:500:THR:HA	2:B:501:PRO:HD3	1.94	0.41
2:B:522:VAL:HG12	2:B:523:CYS:N	2.35	0.41
2:B:798:TYR:CZ	3:C:62:PHE:HE2	2.38	0.41
1:A:255:SER:O	1:A:256:GLN:HB2	2.21	0.41
1:A:335:ARG:NH1	2:B:1206:GLU:OE1	2.54	0.41
1:A:444:PHE:O	1:A:455:MET:HA	2.21	0.41
1:A:683:ILE:HD13	1:A:683:ILE:HA	1.72	0.41
1:A:1130:GLN:HE21	1:A:1130:GLN:HB3	1.71	0.41
1:A:1376:THR:HG23	4:E:212:ARG:HH22	1.85	0.41
2:B:551:PRO:C	2:B:553:PRO:HD2	2.41	0.41
2:B:898:LEU:HD23	2:B:898:LEU:HA	1.82	0.41
3:C:102:GLN:CG	3:C:154:LYS:HD3	2.48	0.41
1:A:7:SER:HB3	2:B:1193:GLN:OE1	2.19	0.41
1:A:149:GLU:HB3	1:A:150:THR:H	1.63	0.41
1:A:553:VAL:CG2	1:A:652:VAL:HG23	2.51	0.41
1:A:575:LYS:HD3	1:A:612:ILE:HD11	2.02	0.41
1:A:709:THR:HG21	7:I:93:LYS:O	2.20	0.41
2:B:28:GLU:C	2:B:30:SER:N	2.74	0.41
2:B:398:ARG:HB3	2:B:398:ARG:CZ	2.50	0.41
2:B:402:GLY:CA	2:B:695:ALA:HB3	2.51	0.41
2:B:635:ARG:O	2:B:636:PRO:C	2.59	0.41
2:B:956:THR:HB	10:L:46:VAL:HG21	2.03	0.41
6:H:44:VAL:O	6:H:44:VAL:HG12	2.19	0.41
7:I:54:GLU:O	7:I:89:GLN:HB2	2.20	0.41
8:J:1:MET:H2	8:J:57:ILE:H	1.66	0.41
1:A:23:SER:O	1:A:24:PRO:C	2.59	0.41
1:A:322:VAL:HG12	1:A:323:LYS:HE2	2.03	0.41
1:A:438:ASP:O	1:A:439:ASN:HB2	2.21	0.41
1:A:544:ASP:HB2	9:K:47:ARG:HH21	1.86	0.41
1:A:666:ILE:H	1:A:666:ILE:HG13	1.70	0.41
1:A:782:ARG:NH2	7:I:67:THR:CG2	2.84	0.41
1:A:834:THR:HG21	1:A:1077:THR:HA	2.03	0.41
1:A:1036:ARG:HG3	1:A:1036:ARG:NH1	2.31	0.41
1:A:1118:VAL:HB	1:A:1306:LEU:HB2	2.01	0.41
2:B:203:PHE:HE1	2:B:212:LEU:CD1	2.33	0.41
2:B:212:LEU:HD21	2:B:466:TRP:CH2	2.55	0.41
2:B:367:LEU:HB3	2:B:368:GLU:H	1.58	0.41
2:B:619:ILE:H	2:B:619:ILE:HG12	1.73	0.41
2:B:744:HIS:HA	2:B:745:PRO:HD2	1.96	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:834:ASN:O	2:B:1013:ASN:HB2	2.21	0.41
2:B:864:LYS:HG2	2:B:871:THR:HG23	2.03	0.41
2:B:893:LEU:HD21	2:B:910:VAL:HG12	2.03	0.41
3:C:73:GLN:NE2	3:C:75:MET:HB2	2.36	0.41
3:C:93:ASP:OD1	3:C:122:SER:HB2	2.21	0.41
3:C:133:ILE:HD13	3:C:237:SER:HA	2.03	0.41
3:C:259:LEU:HD12	3:C:259:LEU:HA	1.80	0.41
3:C:259:LEU:HD13	9:K:91:CYS:HB2	2.02	0.41
7:I:55:THR:O	7:I:55:THR:CG2	2.68	0.41
12:T:7:DA:C6	12:T:8:DT:O4	2.74	0.41
12:T:17:DC:H2'	12:T:17:DC:O2	2.21	0.41
1:A:40:THR:HG22	1:A:41:MET:HG3	2.02	0.41
1:A:851:HIS:CD2	1:A:857:ARG:HB2	2.55	0.41
2:B:619:ILE:HG13	7:I:65:ASP:HB2	2.03	0.41
2:B:817:LEU:N	2:B:818:PRO:CD	2.84	0.41
3:C:180:TYR:O	3:C:181:ASP:C	2.59	0.41
1:A:556:TRP:O	9:K:26:LYS:HD3	2.21	0.40
1:A:707:GLY:O	1:A:1281:ARG:HD2	2.22	0.40
1:A:1062:GLU:O	1:A:1064:VAL:N	2.53	0.40
1:A:1279:ILE:HD13	1:A:1279:ILE:N	2.36	0.40
1:A:1297:GLU:H	1:A:1297:GLU:CD	2.24	0.40
2:B:412:LEU:HA	2:B:412:LEU:HD23	1.83	0.40
2:B:610:ASN:HA	2:B:611:PRO:HD3	1.95	0.40
2:B:762:ASN:HD22	2:B:762:ASN:HA	1.66	0.40
3:C:46:ILE:HG23	3:C:157:CYS:HB3	2.03	0.40
3:C:57:VAL:HG11	8:J:57:ILE:HG13	2.02	0.40
6:H:30:SER:HB2	6:H:36:CYS:SG	2.61	0.40
10:L:48:CYS:O	10:L:49:LYS:HG2	2.21	0.40
12:T:7:DA:N3	12:T:8:DT:C6	2.89	0.40
1:A:86:LEU:CD1	1:A:236:LEU:O	2.67	0.40
1:A:541:ILE:HG23	1:A:545:GLN:NE2	2.37	0.40
1:A:1279:ILE:N	1:A:1279:ILE:CD1	2.84	0.40
2:B:605:ARG:NE	2:B:691:GLU:OE2	2.54	0.40
3:C:244:VAL:HG21	9:K:105:PHE:CE1	2.56	0.40
1:A:152:VAL:HA	1:A:153:PRO:HD3	1.92	0.40
1:A:632:VAL:HG13	1:A:962:ARG:HD3	2.02	0.40
3:C:80:LEU:O	3:C:161:LYS:HE2	2.21	0.40
3:C:236:GLY:C	3:C:238:ILE:H	2.23	0.40
3:C:262:LEU:HD13	9:K:88:LYS:HG2	2.02	0.40
10:L:55:ILE:O	10:L:56:LEU:HB2	2.20	0.40
1:A:43:GLU:OE1	1:A:46:THR:HB	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1129:GLU:HA	1:A:1132:LYS:CE	2.46	0.40
1:A:1169:ILE:H	1:A:1169:ILE:HD12	1.86	0.40
2:B:199:MET:SD	2:B:199:MET:N	2.95	0.40
2:B:214:ALA:HB2	2:B:408:LEU:HD13	2.03	0.40
2:B:578:THR:HB	2:B:593:PRO:HG3	2.04	0.40
2:B:706:GLN:O	2:B:707:PRO:C	2.58	0.40
2:B:801:LYS:O	2:B:801:LYS:HG2	2.21	0.40
3:C:44:LEU:HD12	3:C:160:LYS:O	2.20	0.40
3:C:76:ASP:HB2	3:C:129:ILE:HD13	2.04	0.40
3:C:258:ILE:HG12	9:K:35:PHE:HE2	1.87	0.40
4:E:204:THR:CG2	4:E:205:SER:N	2.85	0.40
6:H:106:GLU:OE1	6:H:108:SER:HA	2.21	0.40
8:J:30:LEU:HD22	8:J:34:THR:HG21	2.04	0.40
1:A:23:SER:HA	1:A:24:PRO:HD2	1.91	0.40
1:A:102:VAL:HG12	1:A:102:VAL:O	2.21	0.40
1:A:447:GLN:HB3	1:A:448:PRO:HA	2.03	0.40
1:A:664:THR:HA	1:A:742:ASN:HD22	1.86	0.40
1:A:1143:LEU:O	1:A:1146:VAL:HG23	2.22	0.40
1:A:1365:TYR:CD2	1:A:1365:TYR:C	2.94	0.40
2:B:492:LEU:HD23	2:B:492:LEU:HA	1.61	0.40
2:B:879:ARG:CG	2:B:880:THR:N	2.84	0.40
3:C:186:LEU:HB2	3:C:188:HIS:HD2	1.85	0.40
4:E:95:THR:O	4:E:98:ILE:HG22	2.21	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	1383/1733 (80%)	1094 (79%)	201 (14%)	88 (6%)	1 9
2	B	1088/1224 (89%)	900 (83%)	126 (12%)	62 (6%)	1 12

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	264/318 (83%)	226 (86%)	30 (11%)	8 (3%)	4	25
4	E	212/215 (99%)	173 (82%)	28 (13%)	11 (5%)	2	13
5	F	82/155 (53%)	63 (77%)	13 (16%)	6 (7%)	1	6
6	H	129/146 (88%)	94 (73%)	23 (18%)	12 (9%)	0	3
7	I	117/122 (96%)	97 (83%)	13 (11%)	7 (6%)	1	11
8	J	63/70 (90%)	52 (82%)	6 (10%)	5 (8%)	1	5
9	K	112/120 (93%)	105 (94%)	7 (6%)	0	100	100
10	L	44/70 (63%)	25 (57%)	10 (23%)	9 (20%)	0	0
All	All	3494/4173 (84%)	2829 (81%)	457 (13%)	208 (6%)	1	11

All (208) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	50	ILE
1	A	55	ASP
1	A	57	ARG
1	A	65	LEU
1	A	73	GLY
1	A	109	HIS
1	A	148	CYS
1	A	169	ASN
1	A	216	VAL
1	A	226	GLU
1	A	245	PRO
1	A	250	ILE
1	A	258	GLY
1	A	286	HIS
1	A	308	ILE
1	A	315	LEU
1	A	399	HIS
1	A	424	ILE
1	A	567	LYS
1	A	597	LEU
1	A	609	ASP
1	A	610	GLY
1	A	846	GLU
1	A	923	LEU
1	A	972	HIS
1	A	994	GLN

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Mol	Chain	Res	Type
1	A	1014	ALA
1	A	1036	ARG
1	A	1393	ASN
1	A	1403	GLU
1	A	1438	THR
2	B	65	GLU
2	B	168	GLY
2	B	229	ALA
2	B	230	ALA
2	B	245	GLU
2	B	266	ALA
2	B	395	GLN
2	B	436	VAL
2	B	469	GLN
2	B	473	MET
2	B	474	SER
2	B	477	ALA
2	B	483	LEU
2	B	531	GLN
2	B	592	ASN
2	B	629	ASP
2	B	636	PRO
2	B	645	SER
2	B	708	GLU
2	B	709	ASP
2	B	713	ALA
2	B	733	HIS
2	B	734	HIS
2	B	751	VAL
2	B	866	TYR
2	B	879	ARG
2	B	881	ASN
2	B	1046	PRO
2	B	1097	HIS
2	B	1223	ASP
3	C	173	ALA
4	E	49	SER
4	E	59	SER
4	E	118	PRO
5	F	73	ALA
6	H	90	ALA
6	H	109	LYS

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Mol	Chain	Res	Type
6	H	111	LEU
6	H	131	ASN
6	H	132	LEU
6	H	138	GLU
7	I	34	TYR
8	J	2	ILE
10	L	34	CYS
10	L	35	SER
10	L	45	ALA
10	L	59	ALA
10	L	60	ARG
1	A	130	ASP
1	A	224	PHE
1	A	257	ARG
1	A	266	LEU
1	A	298	PHE
1	A	309	ALA
1	A	322	VAL
1	A	324	SER
1	A	837	ILE
1	A	1123	GLY
1	A	1174	PHE
1	A	1234	GLU
1	A	1257	ASP
1	A	1388	GLY
1	A	1420	ASP
2	B	67	SER
2	B	249	ARG
2	B	288	ALA
2	B	466	TRP
2	B	643	ASP
2	B	737	THR
2	B	880	THR
2	B	1021	MET
2	B	1103	ILE
2	B	1185	CYS
3	C	48	SER
3	C	142	VAL
3	C	174	ALA
3	C	227	THR
4	E	56	LYS
4	E	77	SER

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Mol	Chain	Res	Type
5	F	111	LEU
6	H	3	ASN
6	H	62	SER
6	H	136	LYS
7	I	3	THR
7	I	9	ASP
7	I	54	GLU
7	I	97	MET
8	J	8	PHE
8	J	30	LEU
10	L	46	VAL
1	A	35	ILE
1	A	54	ASN
1	A	131	SER
1	A	142	CYS
1	A	214	ILE
1	A	251	SER
1	A	673	GLY
1	A	674	PRO
1	A	852	TYR
1	A	1127	ASP
1	A	1278	ASN
2	B	364	ILE
2	B	468	GLU
2	B	471	LYS
2	B	480	SER
2	B	555	ILE
2	B	732	SER
2	B	735	ALA
2	B	792	MET
2	B	864	LYS
4	E	101	GLN
4	E	158	SER
5	F	114	GLU
6	H	128	ASN
7	I	90	GLN
8	J	9	SER
8	J	19	GLU
10	L	44	ASP
1	A	48	ALA
1	A	49	LYS
1	A	69	THR

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Mol	Chain	Res	Type
1	A	147	VAL
1	A	178	GLY
1	A	219	PHE
1	A	220	THR
1	A	404	TYR
1	A	423	ASP
1	A	583	PRO
1	A	958	VAL
1	A	1093	LYS
2	B	367	LEU
2	B	479	VAL
2	B	561	TRP
2	B	644	GLU
2	B	711	GLU
2	B	1108	ARG
4	E	97	VAL
6	H	130	ARG
7	I	47	GLU
1	A	24	PRO
1	A	51	GLY
1	A	234	MET
1	A	254	GLU
1	A	903	ASN
1	A	970	THR
1	A	1151	GLU
2	B	333	PHE
2	B	413	LEU
2	B	476	ARG
2	B	707	PRO
3	C	214	ASN
3	C	215	GLU
4	E	36	GLU
6	H	18	GLY
10	L	26	THR
1	A	38	PRO
1	A	1062	GLU
2	B	233	PRO
2	B	1175	LEU
3	C	136	ASP
4	E	51	GLY
5	F	74	ILE
5	F	154	ASP

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Mol	Chain	Res	Type
1	A	79	GLY
1	A	244	PRO
1	A	1156	PRO
1	A	1424	VAL
1	A	1437	GLY
2	B	467	GLY
1	A	794	PRO
5	F	131	PRO
1	A	312	PRO
1	A	990	VAL
10	L	30	ILE
1	A	310	GLY
1	A	772	GLY
4	E	86	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	1218/1520 (80%)	974 (80%)	244 (20%)	1 6
2	B	960/1061 (90%)	772 (80%)	188 (20%)	1 7
3	C	234/274 (85%)	180 (77%)	54 (23%)	1 3
4	E	196/197 (100%)	160 (82%)	36 (18%)	1 8
5	F	74/137 (54%)	62 (84%)	12 (16%)	2 10
6	H	117/128 (91%)	95 (81%)	22 (19%)	1 7
7	I	113/116 (97%)	87 (77%)	26 (23%)	1 3
8	J	60/65 (92%)	42 (70%)	18 (30%)	0 1
9	K	99/102 (97%)	87 (88%)	12 (12%)	5 20
10	L	40/57 (70%)	33 (82%)	7 (18%)	2 9
All	All	3111/3657 (85%)	2492 (80%)	619 (20%)	1 6

All (619) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	TYR
1	A	12	ARG
1	A	18	GLN
1	A	22	PHE
1	A	30	ILE
1	A	47	ARG
1	A	49	LYS
1	A	54	ASN
1	A	55	ASP
1	A	61	ILE
1	A	64	ASN
1	A	65	LEU
1	A	68	GLN
1	A	69	THR
1	A	70	CYS
1	A	71	GLN
1	A	74	MET
1	A	80	HIS
1	A	93	VAL
1	A	109	HIS
1	A	114	LEU
1	A	132	LYS
1	A	144	THR
1	A	146	MET
1	A	147	VAL
1	A	148	CYS
1	A	162	VAL
1	A	169	ASN
1	A	170	THR
1	A	179	LEU
1	A	185	TRP
1	A	202	LEU
1	A	208	LEU
1	A	212	LYS
1	A	216	VAL
1	A	220	THR
1	A	222	LEU
1	A	225	ASN
1	A	227	VAL
1	A	250	ILE
1	A	257	ARG
1	A	264	PHE
1	A	287	HIS

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Mol	Chain	Res	Type
1	A	289	ILE
1	A	297	GLN
1	A	303	TYR
1	A	306	ASN
1	A	308	ILE
1	A	311	GLN
1	A	313	GLN
1	A	315	LEU
1	A	316	GLN
1	A	320	ARG
1	A	322	VAL
1	A	323	LYS
1	A	326	ARG
1	A	329	LEU
1	A	332	LYS
1	A	333	GLU
1	A	335	ARG
1	A	344	ARG
1	A	351	THR
1	A	353	ILE
1	A	369	SER
1	A	373	THR
1	A	375	THR
1	A	380	VAL
1	A	381	THR
1	A	383	TYR
1	A	403	LYS
1	A	412	ARG
1	A	416	ARG
1	A	419	LYS
1	A	424	ILE
1	A	434	ARG
1	A	436	ILE
1	A	443	LEU
1	A	451	HIS
1	A	452	LYS
1	A	454	SER
1	A	461	LYS
1	A	466	SER
1	A	469	ARG
1	A	470	LEU
1	A	472	LEU

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Mol	Chain	Res	Type
1	A	474	VAL
1	A	475	THR
1	A	497	THR
1	A	509	LEU
1	A	512	VAL
1	A	513	SER
1	A	518	LYS
1	A	532	ARG
1	A	542	GLU
1	A	544	ASP
1	A	560	ILE
1	A	567	LYS
1	A	577	ILE
1	A	589	GLN
1	A	590	ARG
1	A	595	THR
1	A	598	LEU
1	A	605	MET
1	A	612	ILE
1	A	618	GLU
1	A	629	LEU
1	A	637	LYS
1	A	663	SER
1	A	664	THR
1	A	666	ILE
1	A	670	ILE
1	A	672	ASP
1	A	681	GLU
1	A	682	THR
1	A	685	GLU
1	A	688	LYS
1	A	695	LYS
1	A	702	LEU
1	A	703	THR
1	A	709	THR
1	A	710	LEU
1	A	728	LYS
1	A	732	LEU
1	A	735	VAL
1	A	740	LEU
1	A	756	ILE
1	A	764	CYS

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Mol	Chain	Res	Type
1	A	765	VAL
1	A	768	GLN
1	A	769	SER
1	A	774	ARG
1	A	780	VAL
1	A	783	THR
1	A	801	GLU
1	A	803	SER
1	A	821	ARG
1	A	829	VAL
1	A	830	LYS
1	A	838	GLN
1	A	839	ARG
1	A	855	THR
1	A	856	THR
1	A	858	ASN
1	A	880	LYS
1	A	884	ASP
1	A	885	THR
1	A	886	ILE
1	A	895	LYS
1	A	896	ARG
1	A	902	LEU
1	A	904	THR
1	A	911	SER
1	A	914	GLU
1	A	919	ILE
1	A	922	ASP
1	A	926	GLN
1	A	932	GLU
1	A	940	ARG
1	A	941	LYS
1	A	949	ASP
1	A	961	ARG
1	A	965	GLN
1	A	966	ASN
1	A	976	THR
1	A	977	LYS
1	A	982	THR
1	A	995	GLU
1	A	996	ASN
1	A	1000	LEU

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Mol	Chain	Res	Type
1	A	1001	ARG
1	A	1017	LEU
1	A	1025	ARG
1	A	1029	ARG
1	A	1033	GLN
1	A	1034	GLU
1	A	1047	SER
1	A	1048	ASN
1	A	1050	GLU
1	A	1055	ARG
1	A	1058	VAL
1	A	1064	VAL
1	A	1081	LEU
1	A	1092	LYS
1	A	1093	LYS
1	A	1095	THR
1	A	1110	ASN
1	A	1111	MET
1	A	1116	LEU
1	A	1128	GLN
1	A	1130	GLN
1	A	1146	VAL
1	A	1159	ARG
1	A	1165	GLU
1	A	1171	GLN
1	A	1172	LEU
1	A	1187	GLN
1	A	1193	LEU
1	A	1205	LYS
1	A	1206	ASP
1	A	1208	THR
1	A	1219	THR
1	A	1231	ASP
1	A	1243	VAL
1	A	1257	ASP
1	A	1259	MET
1	A	1261	LYS
1	A	1262	LYS
1	A	1264	GLU
1	A	1267	MET
1	A	1269	GLU
1	A	1273	LEU

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Mol	Chain	Res	Type
1	A	1274	ARG
1	A	1277	GLU
1	A	1279	ILE
1	A	1280	GLU
1	A	1285	MET
1	A	1288	ASP
1	A	1291	VAL
1	A	1295	THR
1	A	1297	GLU
1	A	1299	VAL
1	A	1300	LYS
1	A	1322	ILE
1	A	1325	THR
1	A	1329	THR
1	A	1333	ILE
1	A	1334	ASP
1	A	1336	MET
1	A	1345	ARG
1	A	1354	ASN
1	A	1359	ASP
1	A	1366	ARG
1	A	1374	VAL
1	A	1376	THR
1	A	1385	THR
1	A	1391	ARG
1	A	1393	ASN
1	A	1400	CYS
1	A	1403	GLU
1	A	1406	VAL
1	A	1407	GLU
1	A	1422	ARG
1	A	1426	GLU
1	A	1445	ILE
2	B	20	ASP
2	B	28	GLU
2	B	46	GLN
2	B	58	THR
2	B	63	ILE
2	B	65	GLU
2	B	66	ASP
2	B	67	SER
2	B	70	ILE

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Mol	Chain	Res	Type
2	B	94	LYS
2	B	97	VAL
2	B	98	THR
2	B	102	VAL
2	B	108	VAL
2	B	120	ARG
2	B	133	LYS
2	B	134	LYS
2	B	167	ILE
2	B	175	ARG
2	B	179	CYS
2	B	181	LEU
2	B	194	GLU
2	B	199	MET
2	B	217	ARG
2	B	225	VAL
2	B	234	ILE
2	B	239	GLU
2	B	242	SER
2	B	245	GLU
2	B	246	LYS
2	B	249	ARG
2	B	252	SER
2	B	268	THR
2	B	272	THR
2	B	275	TYR
2	B	276	ILE
2	B	284	ILE
2	B	310	MET
2	B	313	MET
2	B	315	LYS
2	B	323	VAL
2	B	324	ILE
2	B	328	GLU
2	B	331	LEU
2	B	345	LYS
2	B	346	GLU
2	B	350	GLN
2	B	354	ASP
2	B	361	LEU
2	B	365	THR
2	B	366	GLN

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Mol	Chain	Res	Type
2	B	367	LEU
2	B	368	GLU
2	B	376	PHE
2	B	382	ILE
2	B	384	ARG
2	B	387	LEU
2	B	393	LYS
2	B	394	ASP
2	B	395	GLN
2	B	398	ARG
2	B	415	GLN
2	B	425	THR
2	B	426	LYS
2	B	428	ILE
2	B	429	PHE
2	B	436	VAL
2	B	437	GLU
2	B	448	ILE
2	B	455	SER
2	B	461	LEU
2	B	468	GLU
2	B	471	LYS
2	B	474	SER
2	B	479	VAL
2	B	483	LEU
2	B	485	ARG
2	B	487	THR
2	B	498	THR
2	B	512	ARG
2	B	513	GLN
2	B	516	ASN
2	B	527	THR
2	B	531	GLN
2	B	544	CYS
2	B	549	THR
2	B	552	MET
2	B	554	ILE
2	B	563	MET
2	B	570	VAL
2	B	574	SER
2	B	591	ARG
2	B	598	GLU

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Mol	Chain	Res	Type
2	B	606	LYS
2	B	617	ARG
2	B	619	ILE
2	B	624	LEU
2	B	629	ASP
2	B	633	VAL
2	B	635	ARG
2	B	637	LEU
2	B	643	ASP
2	B	644	GLU
2	B	651	LEU
2	B	653	VAL
2	B	666	TYR
2	B	690	VAL
2	B	706	GLN
2	B	708	GLU
2	B	710	LEU
2	B	731	VAL
2	B	732	SER
2	B	742	GLU
2	B	747	MET
2	B	751	VAL
2	B	764	SER
2	B	786	ASN
2	B	787	VAL
2	B	790	ASP
2	B	791	THR
2	B	792	MET
2	B	815	ARG
2	B	827	ILE
2	B	844	SER
2	B	864	LYS
2	B	865	LYS
2	B	868	MET
2	B	871	THR
2	B	879	ARG
2	B	880	THR
2	B	886	LYS
2	B	894	ASP
2	B	901	PRO
2	B	904	ARG
2	B	943	SER

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Mol	Chain	Res	Type
2	B	944	THR
2	B	955	THR
2	B	957	ASN
2	B	963	PHE
2	B	969	ARG
2	B	970	THR
2	B	976	ILE
2	B	983	ARG
2	B	987	LYS
2	B	992	ILE
2	B	996	ARG
2	B	997	GLU
2	B	1002	THR
2	B	1004	GLU
2	B	1006	ILE
2	B	1007	VAL
2	B	1021	MET
2	B	1028	GLU
2	B	1032	SER
2	B	1046	PRO
2	B	1051	THR
2	B	1055	ILE
2	B	1065	GLN
2	B	1077	THR
2	B	1082	MET
2	B	1093	GLN
2	B	1094	ARG
2	B	1096	ARG
2	B	1099	VAL
2	B	1103	ILE
2	B	1111	MET
2	B	1113	VAL
2	B	1120	GLU
2	B	1122	ARG
2	B	1123	SER
2	B	1124	ARG
2	B	1129	ARG
2	B	1147	LEU
2	B	1150	ARG
2	B	1151	LEU
2	B	1155	SER
2	B	1159	ARG

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Mol	Chain	Res	Type
2	B	1160	VAL
2	B	1174	LYS
2	B	1176	ASN
2	B	1181	GLU
2	B	1186	ASP
2	B	1187	ASN
2	B	1188	LYS
2	B	1191	ILE
2	B	1194	ILE
2	B	1202	LEU
2	B	1220	ARG
3	C	4	GLU
3	C	9	LYS
3	C	11	ARG
3	C	15	LYS
3	C	16	ASP
3	C	18	VAL
3	C	22	LEU
3	C	23	SER
3	C	25	VAL
3	C	35	ARG
3	C	41	ILE
3	C	53	THR
3	C	56	THR
3	C	57	VAL
3	C	69	LEU
3	C	77	ILE
3	C	81	GLU
3	C	89	GLU
3	C	99	LEU
3	C	100	THR
3	C	106	GLU
3	C	109	SER
3	C	110	THR
3	C	116	LYS
3	C	120	ILE
3	C	129	ILE
3	C	133	ILE
3	C	137	LYS
3	C	140	ASN
3	C	149	LYS
3	C	151	GLN

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Mol	Chain	Res	Type
3	C	154	LYS
3	C	170	TRP
3	C	177	GLU
3	C	183	TRP
3	C	186	LEU
3	C	189	THR
3	C	197	SER
3	C	203	GLN
3	C	204	SER
3	C	222	LYS
3	C	224	GLN
3	C	226	ASP
3	C	231	ASN
3	C	235	VAL
3	C	238	ILE
3	C	240	VAL
3	C	244	VAL
3	C	246	ARG
3	C	249	ASP
3	C	253	LYS
3	C	258	ILE
3	C	263	THR
3	C	268	ASP
4	E	3	GLN
4	E	9	ILE
4	E	31	THR
4	E	32	GLN
4	E	37	LEU
4	E	40	GLU
4	E	54	GLN
4	E	66	GLU
4	E	78	LEU
4	E	92	THR
4	E	94	LYS
4	E	95	THR
4	E	98	ILE
4	E	101	GLN
4	E	103	LYS
4	E	122	LYS
4	E	123	LEU
4	E	127	ILE
4	E	131	THR

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Mol	Chain	Res	Type
4	E	134	THR
4	E	137	GLU
4	E	144	ILE
4	E	146	HIS
4	E	150	VAL
4	E	152	LYS
4	E	162	ARG
4	E	165	LEU
4	E	169	ARG
4	E	179	GLN
4	E	191	LYS
4	E	192	ARG
4	E	200	ARG
4	E	201	LYS
4	E	202	SER
4	E	204	THR
4	E	215	MET
5	F	72	LYS
5	F	79	ARG
5	F	82	THR
5	F	97	ARG
5	F	111	LEU
5	F	112	GLU
5	F	119	ARG
5	F	133	VAL
5	F	140	ASP
5	F	149	GLU
5	F	150	GLU
5	F	155	LEU
6	H	2	SER
6	H	11	GLN
6	H	15	VAL
6	H	21	ASN
6	H	24	CYS
6	H	32	THR
6	H	34	ASP
6	H	55	LEU
6	H	58	THR
6	H	59	ILE
6	H	83	GLN
6	H	89	LEU
6	H	100	THR

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Mol	Chain	Res	Type
6	H	106	GLU
6	H	110	ASP
6	H	123	MET
6	H	124	ARG
6	H	130	ARG
6	H	133	ASN
6	H	136	LYS
6	H	137	GLN
6	H	142	LEU
7	I	3	THR
7	I	8	ARG
7	I	14	LEU
7	I	28	GLU
7	I	29	CYS
7	I	30	ARG
7	I	33	SER
7	I	50	THR
7	I	52	ILE
7	I	55	THR
7	I	60	GLN
7	I	61	ASP
7	I	74	GLU
7	I	75	CYS
7	I	83	ASN
7	I	89	GLN
7	I	90	GLN
7	I	91	ARG
7	I	95	THR
7	I	97	MET
7	I	103	CYS
7	I	106	CYS
7	I	107	SER
7	I	116	ASN
7	I	117	LYS
7	I	118	ARG
8	J	1	MET
8	J	3	VAL
8	J	6	ARG
8	J	7	CYS
8	J	9	SER
8	J	10	CYS
8	J	13	VAL

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Mol	Chain	Res	Type
8	J	22	LEU
8	J	26	GLN
8	J	27	GLU
8	J	28	ASP
8	J	29	GLU
8	J	31	ASP
8	J	42	LYS
8	J	43	ARG
8	J	48	ARG
8	J	59	LYS
8	J	64	ASN
9	K	1	MET
9	K	14	GLU
9	K	17	SER
9	K	20	LYS
9	K	26	LYS
9	K	31	VAL
9	K	51	LEU
9	K	77	THR
9	K	82	ASP
9	K	103	THR
9	K	106	GLU
9	K	107	THR
10	L	27	LEU
10	L	31	CYS
10	L	38	LEU
10	L	42	ARG
10	L	47	ARG
10	L	55	ILE
10	L	61	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (93) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	68	GLN
1	A	71	GLN
1	A	83	HIS
1	A	169	ASN
1	A	171	GLN
1	A	225	ASN
1	A	316	GLN

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Mol	Chain	Res	Type
1	A	394	ASN
1	A	435	HIS
1	A	451	HIS
1	A	503	GLN
1	A	517	ASN
1	A	545	GLN
1	A	611	GLN
1	A	741	ASN
1	A	742	ASN
1	A	745	GLN
1	A	757	ASN
1	A	768	GLN
1	A	786	HIS
1	A	858	ASN
1	A	906	HIS
1	A	926	GLN
1	A	968	GLN
1	A	975	HIS
1	A	1110	ASN
1	A	1124	HIS
1	A	1130	GLN
1	A	1171	GLN
1	A	1203	ASN
1	A	1270	ASN
1	A	1364	ASN
1	A	1393	ASN
1	A	1432	GLN
2	B	103	ASN
2	B	115	GLN
2	B	121	ASN
2	B	215	GLN
2	B	325	GLN
2	B	350	GLN
2	B	366	GLN
2	B	383	ASN
2	B	395	GLN
2	B	469	GLN
2	B	513	GLN
2	B	515	HIS
2	B	516	ASN
2	B	518	HIS
2	B	531	GLN

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Mol	Chain	Res	Type
2	B	573	GLN
2	B	587	HIS
2	B	590	HIS
2	B	657	HIS
2	B	686	ASN
2	B	744	HIS
2	B	762	ASN
2	B	794	ASN
2	B	822	ASN
2	B	843	GLN
2	B	862	GLN
2	B	957	ASN
2	B	975	GLN
2	B	1015	HIS
2	B	1065	GLN
2	B	1084	GLN
2	B	1093	GLN
2	B	1179	GLN
2	B	1187	ASN
2	B	1193	GLN
3	C	73	GLN
3	C	112	ASN
3	C	123	ASN
3	C	128	ASN
3	C	167	HIS
3	C	188	HIS
3	C	224	GLN
3	C	242	GLN
3	C	264	GLN
4	E	32	GLN
4	E	99	HIS
4	E	101	GLN
4	E	147	HIS
4	E	179	GLN
6	H	11	GLN
6	H	137	GLN
6	H	139	ASN
7	I	12	ASN
7	I	60	GLN
7	I	83	ASN
9	K	65	HIS
9	K	76	GLN

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Mol	Chain	Res	Type
9	K	89	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	R	10/11 (90%)	2 (20%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
11	R	3	G
11	R	11	C

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 10 ligands modelled in this entry, 9 are monoatomic - leaving 1 for Mogul analysis.

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	$\#\|Z\| > 2$
16	C7P	T	29	12	3,9,10	0.42	0	2,11,14	0.68	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
16	C7P	T	29	12	-	-	0/0/1/1

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 (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	1395/1733 (80%)	-0.25	22 (1%) 72 59	47, 104, 216, 308	0
2	B	1106/1224 (90%)	-0.34	24 (2%) 62 48	43, 86, 154, 209	0
3	C	266/318 (83%)	-0.43	0 100 100	62, 91, 135, 158	0
4	E	214/215 (99%)	-0.04	4 (1%) 66 53	81, 159, 225, 242	0
5	F	84/155 (54%)	-0.26	0 100 100	77, 110, 142, 150	0
6	H	133/146 (91%)	0.06	4 (3%) 50 34	101, 153, 199, 211	0
7	I	119/122 (97%)	-0.11	0 100 100	74, 118, 158, 172	0
8	J	65/70 (92%)	-0.65	0 100 100	56, 73, 100, 116	0
9	K	114/120 (95%)	-0.40	1 (0%) 84 75	59, 103, 131, 141	0
10	L	46/70 (65%)	0.40	5 (10%) 5 3	72, 144, 173, 182	0
11	R	11/11 (100%)	0.88	1 (9%) 9 5	141, 156, 210, 217	0
12	T	28/28 (100%)	1.91	10 (35%) 0 0	146, 286, 394, 400	0
13	N	14/14 (100%)	1.67	3 (21%) 0 0	309, 352, 380, 391	0
All	All	3595/4226 (85%)	-0.24	74 (2%) 63 49	43, 103, 203, 400	0

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1176	LEU	9.0
1	A	44	THR	7.7
2	B	866	TYR	7.7
2	B	1223	ASP	5.7
1	A	318	SER	5.6
1	A	69	THR	5.2
2	B	1224	PHE	5.1
1	A	150	THR	5.0
6	H	84	ALA	4.6

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Mol	Chain	Res	Type	RSRZ
2	B	477	ALA	4.6
1	A	316	GLN	4.6
10	L	27	LEU	4.5
1	A	149	GLU	4.4
12	T	3	DA	4.0
2	B	869	SER	4.0
10	L	26	THR	3.9
1	A	65	LEU	3.8
2	B	1221	SER	3.8
2	B	250	PHE	3.8
6	H	131	ASN	3.7
2	B	509	ALA	3.6
12	T	10	DA	3.5
6	H	85	GLY	3.4
12	T	2	DT	3.4
12	T	13	DA	3.4
2	B	476	ARG	3.4
2	B	474	SER	3.4
2	B	643	ASP	3.4
12	T	9	DA	3.3
2	B	865	LYS	3.2
12	T	12	DC	3.2
2	B	714	GLU	3.1
12	T	4	DC	3.1
12	T	11	DC	3.0
4	E	126	SER	3.0
2	B	1222	ARG	3.0
2	B	883	LEU	3.0
2	B	248	SER	3.0
10	L	43	THR	3.0
2	B	868	MET	3.0
10	L	50	ASP	3.0
12	T	1	DC	2.9
1	A	161	LEU	2.9
13	N	7	DA	2.7
13	N	14	DG	2.7
1	A	286	HIS	2.7
1	A	251	SER	2.6
1	A	141	LEU	2.6
1	A	71	GLN	2.6
2	B	709	ASP	2.6
2	B	666	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	867	GLY	2.5
1	A	118	HIS	2.5
1	A	254	GLU	2.5
4	E	44	ALA	2.4
13	N	8	DT	2.3
4	E	32	GLN	2.3
2	B	473	MET	2.3
1	A	250	ILE	2.3
12	T	15	DC	2.2
6	H	132	LEU	2.1
11	R	11	C	2.1
10	L	25	ALA	2.1
1	A	320	ARG	2.1
1	A	234	MET	2.1
1	A	1232	ASN	2.1
9	K	14	GLU	2.1
2	B	429	PHE	2.1
2	B	918	ILE	2.1
1	A	285	PRO	2.0
4	E	129	PRO	2.0
2	B	249	ARG	2.0
1	A	1286	LYS	2.0
1	A	164	ARG	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
15	MG	A	2001	1/1	0.84	0.08	67,67,67,67	0
14	ZN	A	1734	1/1	0.89	0.09	113,113,113,113	0
16	C7P	T	29	9/10	0.92	0.33	205,229,260,269	1
14	ZN	B	1307	1/1	0.95	0.04	92,92,92,92	0
14	ZN	J	101	1/1	0.96	0.06	61,61,61,61	0
14	ZN	L	105	1/1	0.96	0.05	101,101,101,101	1
14	ZN	A	1735	1/1	0.98	0.04	83,83,83,83	0
14	ZN	I	204	1/1	0.98	0.07	59,59,59,59	0
14	ZN	I	203	1/1	0.99	0.03	74,74,74,74	0
14	ZN	C	319	1/1	0.99	0.04	63,63,63,63	0

6.5 Other polymers (i)

There are no such residues in this entry.