Full wwPDB X-ray Structure Validation Report (i)

Aug 25, 2026 – 02:04 am BST

PDB ID	:	4V8S / pdb_00004v8s
Title	:	Archaeal RNAP-DNA binary complex at 4.32Ang
Authors	:	Wojtas, M.N.; Mogni, M.; Millet, O.; Bell, S.D.; Abrescia, N.G.A.
Deposited on	:	2012-07-12
Resolution	:	4.32 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 (1)) were used in the production of this report:

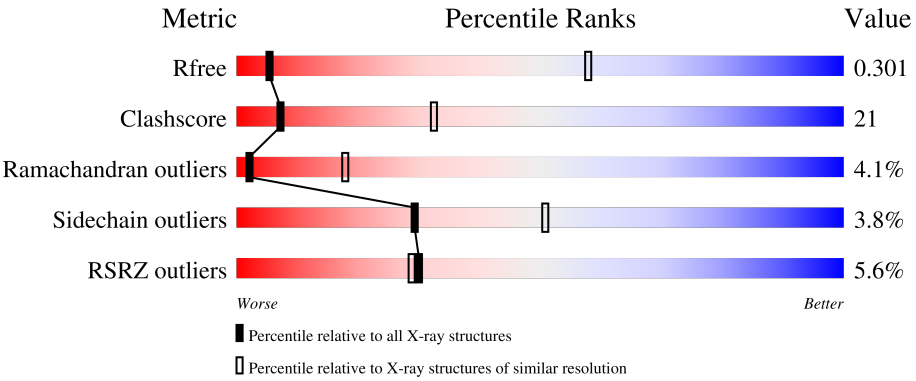
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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 4.32 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}	180053	1056 (4.72-3.90)
Clashscore	190562	1101 (4.72-3.90)
Ramachandran outliers	187476	1003 (4.72-3.90)
Sidechain outliers	187428	1010 (4.76-3.88)
RSRZ outliers	180081	1053 (4.72-3.90)

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	AC	14	57% 36% 7%
1	BR	14	50% 50%
2	AD	16	19% 25% 69% 6%
2	BS	16	6% 31% 69%
3	AI	95	2% 61% 24% . 12%

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Mol	Chain	Length	Quality of chain
3	BK	95	3% 65% 20% 12%
4	AJ	104	% 20% 21% 6% 53%
4	BQ	104	20% 21% 7% 52%
5	AM	92	3% 77% 22%
5	BL	92	8% 77% 22%
6	AO	66	5% 55% 36% 8%
6	BN	66	2% 58% 33% 8%
7	AR	1131	6% 65% 29%
7	BB	1131	6% 64% 29%
8	AS	265	3% 72% 26%
8	BD	265	5% 72% 27%
9	AT	180	2% 56% 37% 5%
9	BE	180	5% 57% 36% 5%
10	AU	113	3% 50% 36% 7% 7%
10	BF	113	2% 48% 35% 11% 7%
11	AV	132	5% 39% 42% 14%
11	BG	132	6% 38% 43% 14%
12	AW	880	5% 60% 34% 5%
12	BA	880	6% 60% 35%
13	AX	48	50% 40% 8%
13	BP	48	4% 50% 40% 8%
14	AY	395	6% 54% 36% 5%
14	BC	395	6% 56% 34% 5% 5%
15	AZ	84	4% 62% 26% 10%
15	BH	84	5% 62% 26% 10%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	SF4	AS	1001	-	-	X	-
17	SF4	BD	1001	-	-	X	-

2 Entry composition (i)

There are 18 unique types of molecules in this entry. The entry contains 111598 atoms, of which 56187 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a DNA chain called 5'-D(*TP*CP*TP*TP*AP*TP*AP*CP*TP*CP*TP*AP *TP*CP)-3'.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	P			
1	AC	13	411	127	151	38	82	13	0	0	0
1	BR	14	Total	C	H	N	O	P	0	0	0
			441	136	162	41	88	14			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	P			
2	AD	15	485	150	170	63	87	15	0	0	0
2	BS	16	Total	C	H	N	O	P	0	0	0
			517	160	181	68	92	16			

- Molecule 3 is a protein called DNA-DIRECTED RNA POLYMERASE SUBUNIT K.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
3	AI	84	1390	431	717	123	118	1	0	0	0
3	BK	84	Total	C	H	N	O	S	0	0	0
			1390	431	717	123	118	1			

- Molecule 4 is a protein called RNA POLYMERASE SUBUNIT 13.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
4	AJ	49	830	264	413	70	82	1	0	0	0
4	BQ	50	Total	C	H	N	O	S	0	0	0
			845	269	419	71	85	1			

- Molecule 5 is a protein called DNA-DIRECTED RNA POLYMERASE SUBUNIT L.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
5	AM	91	Total	C	H	N	O	S	0	0	0
			1449	454	742	114	137	2			
5	BL	91	Total	C	H	N	O	S	0	0	0
			1449	454	742	114	137	2			

- Molecule 6 is a protein called DNA-DIRECTED RNA POLYMERASE SUBUNIT N.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
6	AO	65	Total	C	H	N	O	S	0	0	0
			1058	332	537	94	88	7			
6	BN	65	Total	C	H	N	O	S	0	0	0
			1058	332	537	94	88	7			

- Molecule 7 is a protein called DNA-DIRECTED RNA POLYMERASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
7	AR	1103	Total	C	H	N	O	S	0	0	0
			17665	5548	8909	1552	1627	29			
7	BB	1103	Total	C	H	N	O	S	0	0	0
			17665	5548	8909	1552	1627	29			

- Molecule 8 is a protein called DNA-DIRECTED RNA POLYMERASE SUBUNIT D.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
8	AS	262	Total	C	H	N	O	S	0	0	0
			4215	1339	2128	337	398	13			
8	BD	262	Total	C	H	N	O	S	0	0	0
			4215	1339	2128	337	398	13			

- Molecule 9 is a protein called RNA POLYMERASE SUBUNIT 7.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
9	AT	171	Total	C	H	N	O	S	0	0	0
			2772	874	1413	229	251	5			
9	BE	171	Total	C	H	N	O	S	0	0	0
			2771	874	1412	229	251	5			

- Molecule 10 is a protein called RNA POLYMERASE SUBUNIT 4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
10	AU	105	Total	C	H	N	O	S	0	0	0
			1667	519	840	134	171	3			

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
10	BF	105	Total	C	H	N	O	S	0	0	0
			1667	519	840	134	171	3			

- Molecule 11 is a protein called RNA POLYMERASE SUBUNIT 8.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
11	AV	113	Total	C	H	N	O	S	0	0	0
			1816	572	915	152	173	4			
11	BG	113	Total	C	H	N	O	S	0	0	0
			1816	572	915	152	173	4			

- Molecule 12 is a protein called DNA-DIRECTED RNA POLYMERASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
12	AW	872	Total	C	H	N	O	S	0	0	0
			13987	4424	7030	1225	1282	26			
12	BA	872	Total	C	H	N	O	S	0	0	0
			13987	4424	7030	1225	1282	26			

- Molecule 13 is a protein called DNA-DIRECTED RNA POLYMERASE SUBUNIT P.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
13	AX	44	Total	C	H	N	O	S	0	0	0
			744	236	387	62	54	5			
13	BP	44	Total	C	H	N	O	S	0	0	0
			744	236	387	62	54	5			

- Molecule 14 is a protein called DNA-DIRECTED RNA POLYMERASE SUBUNIT A".

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
14	AY	376	Total	C	H	N	O	S	0	0	0
			5974	1840	3068	493	564	9			
14	BC	376	Total	C	H	N	O	S	0	0	0
			5974	1840	3068	493	564	9			

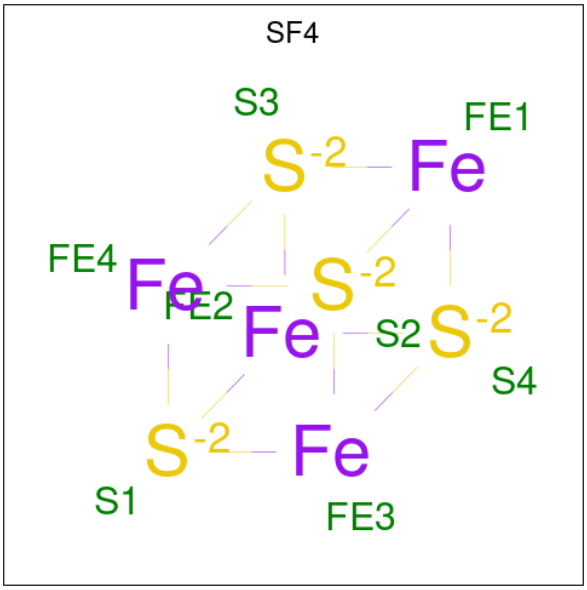
- Molecule 15 is a protein called DNA-DIRECTED RNA POLYMERASE SUBUNIT H.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	AZ	76	Total	C	H	N	O	0	0	0
			1284	405	660	111	108			
15	BH	76	Total	C	H	N	O	0	0	0
			1284	405	660	111	108			

- Molecule 16 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	AO	1	Total Zn 1 1	0	0
16	AR	1	Total Zn 1 1	0	0
16	AW	3	Total Zn 3 3	0	0
16	AX	1	Total Zn 1 1	0	0
16	BA	3	Total Zn 3 3	0	0
16	BB	1	Total Zn 1 1	0	0
16	BN	1	Total Zn 1 1	0	0
16	BP	1	Total Zn 1 1	0	0

- Molecule 17 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	AS	1	Total Fe S 7 3 4	0	0
17	BD	1	Total Fe S 7 3 4	0	0

- Molecule 18 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	AW	1	Total Mg 1 1	0	0
18	BA	1	Total Mg 1 1	0	0

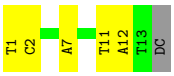
3 Residue-property plots (i)

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: 5'-D(*TP*CP*TP*TP*AP*TP*AP*CP*TP*CP*TP*AP*TP*CP)-3'

Chain AC:

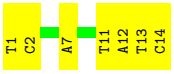




• Molecule 1: 5'-D(*TP*CP*TP*TP*AP*TP*AP*CP*TP*CP*TP*AP*TP*CP)-3'

Chain BR:

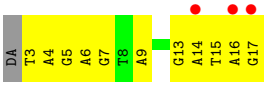




• Molecule 2: 5'-D(*AP*TP*AP*GP*AP*GP*TP*AP*TP*AP*AP*GP*AP*TP *AP*G)-3'

Chain AD:

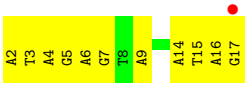




• Molecule 2: 5'-D(*AP*TP*AP*GP*AP*GP*TP*AP*TP*AP*AP*GP*AP*TP *AP*G)-3'

Chain BS:

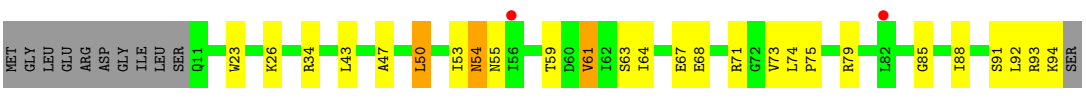




• Molecule 3: DNA-DIRECTED RNA POLYMERASE SUBUNIT K

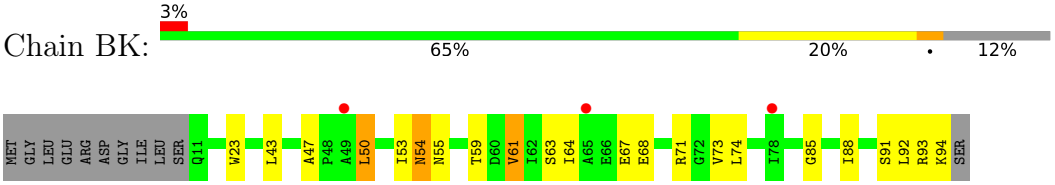
Chain AI:





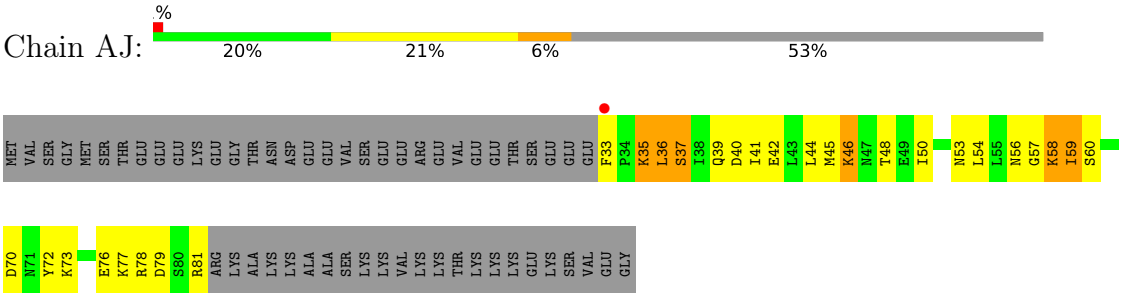
• Molecule 3: DNA-DIRECTED RNA POLYMERASE SUBUNIT K

Chain BK:



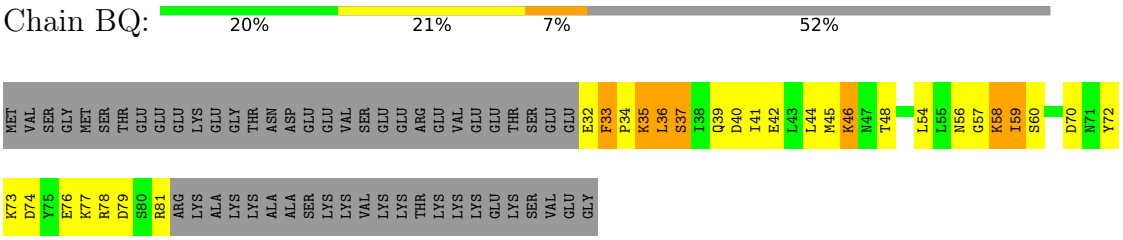
• Molecule 4: RNA POLYMERASE SUBUNIT 13

Chain AJ:



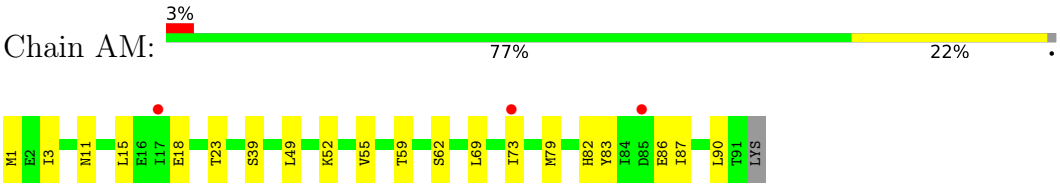
• Molecule 4: RNA POLYMERASE SUBUNIT 13

Chain BQ:



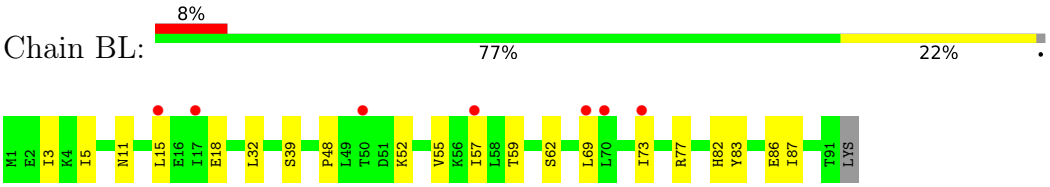
• Molecule 5: DNA-DIRECTED RNA POLYMERASE SUBUNIT L

Chain AM:



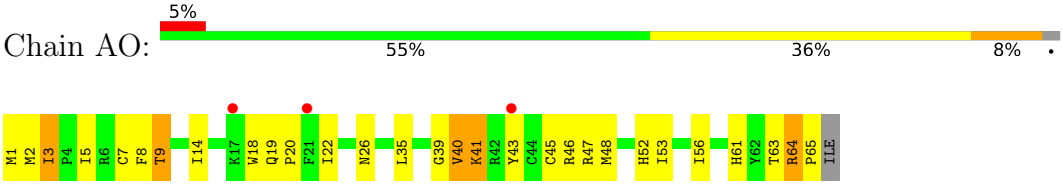
• Molecule 5: DNA-DIRECTED RNA POLYMERASE SUBUNIT L

Chain BL:



• Molecule 6: DNA-DIRECTED RNA POLYMERASE SUBUNIT N

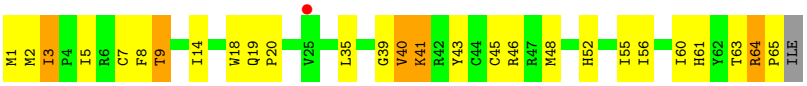
Chain AO:



• Molecule 6: DNA-DIRECTED RNA POLYMERASE SUBUNIT N

Chain BN:

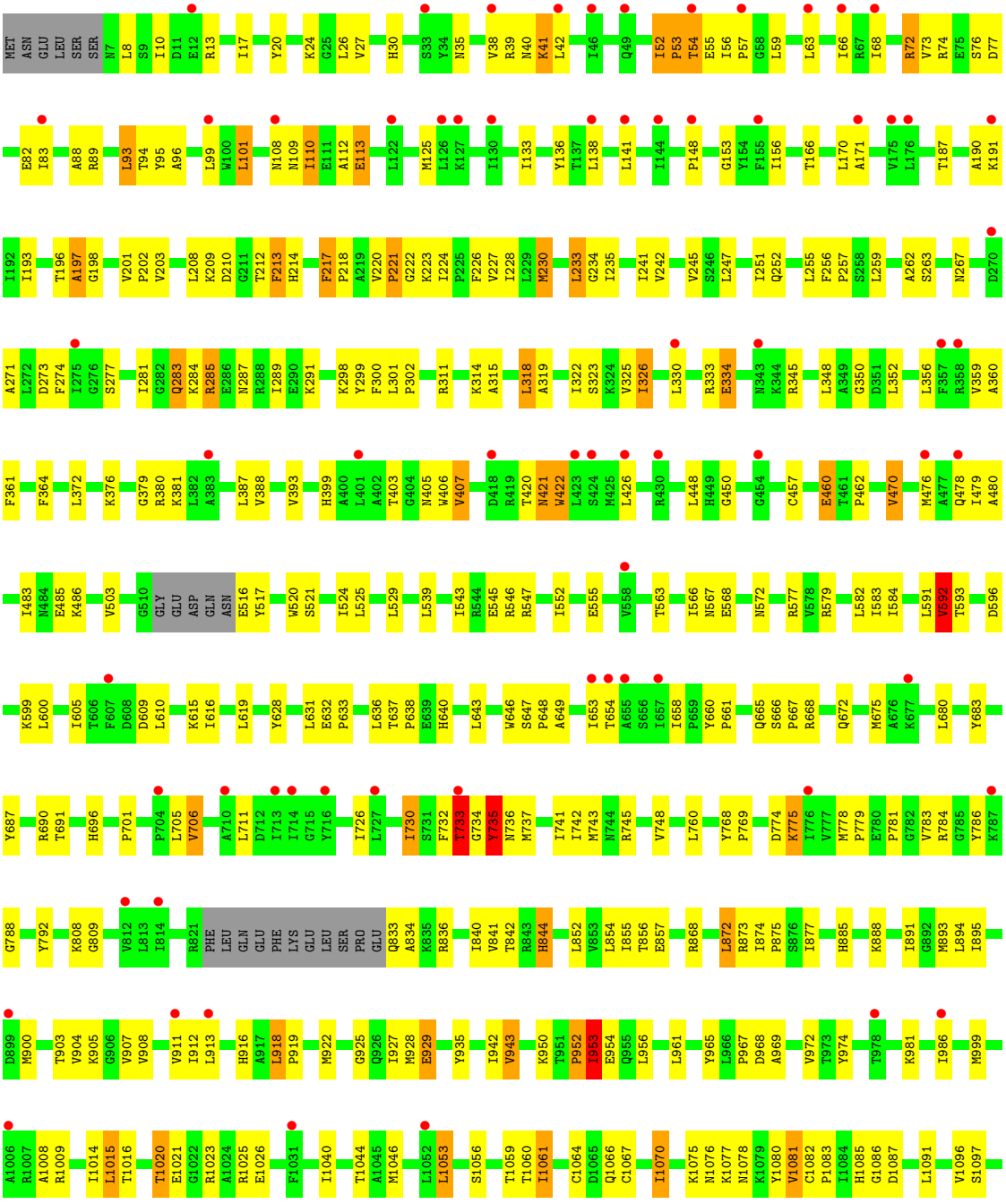


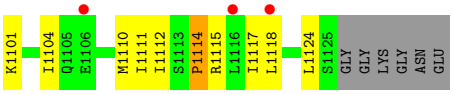


• Molecule 7: DNA-DIRECTED RNA POLYMERASE

Chain AR:



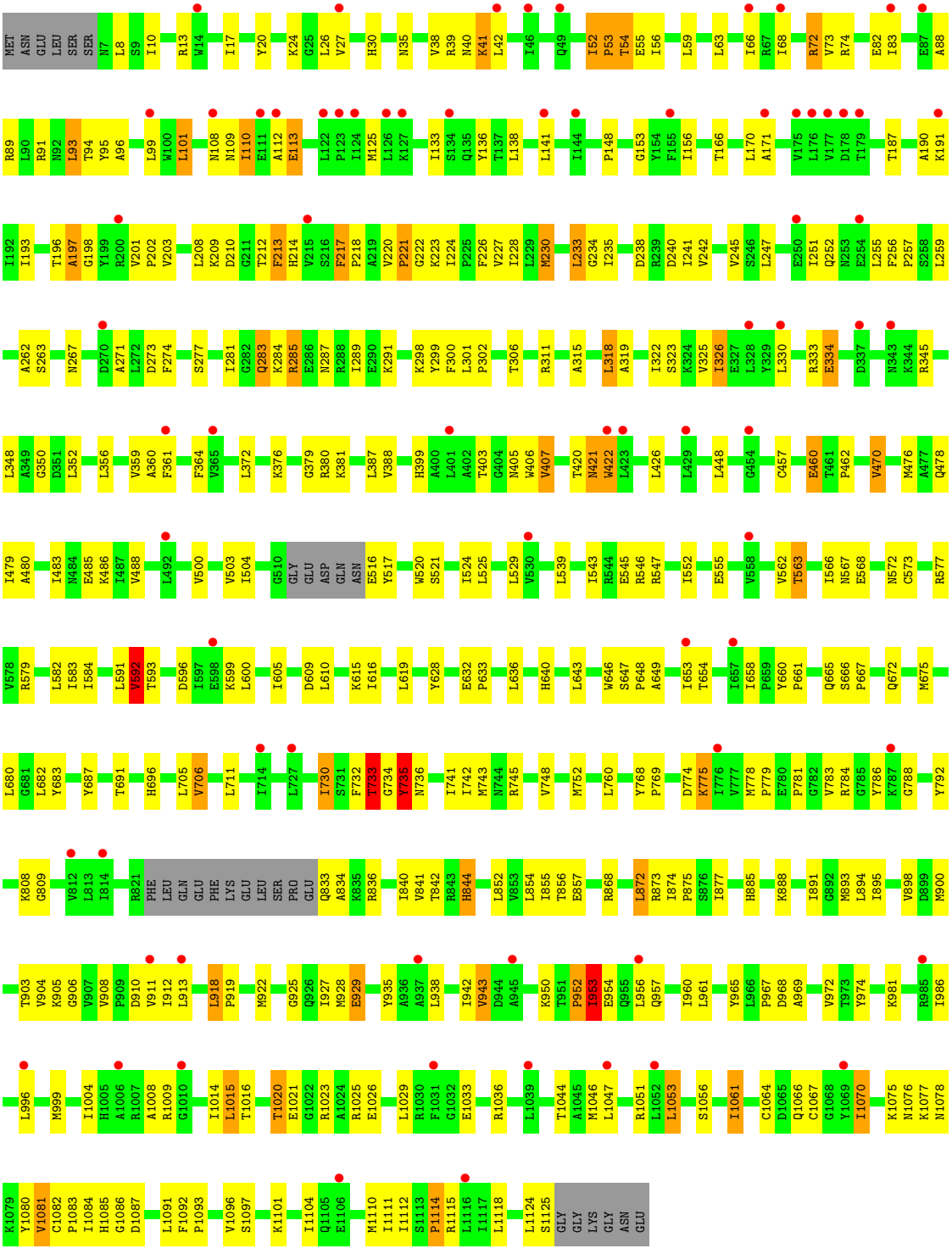




• Molecule 7: DNA-DIRECTED RNA POLYMERASE

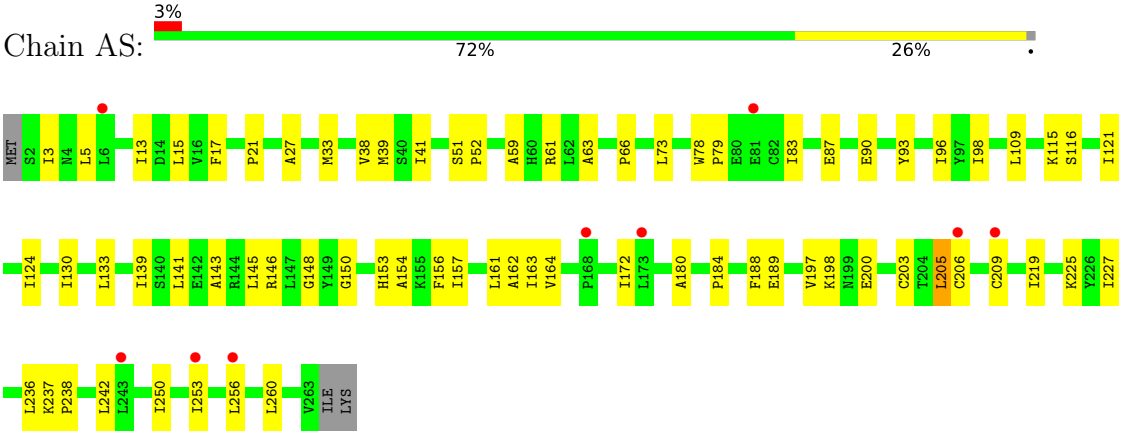
Chain BB:





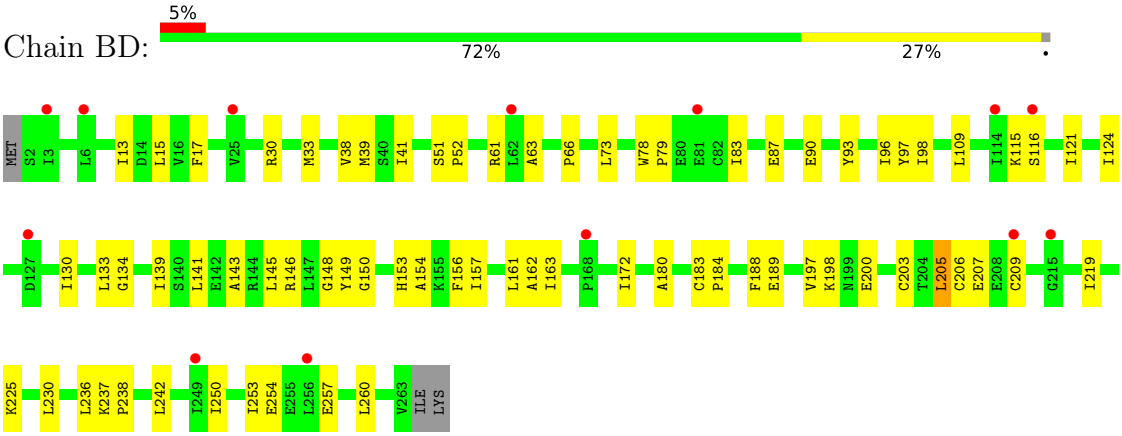
• Molecule 8: DNA-DIRECTED RNA POLYMERASE SUBUNIT D

Chain AS:



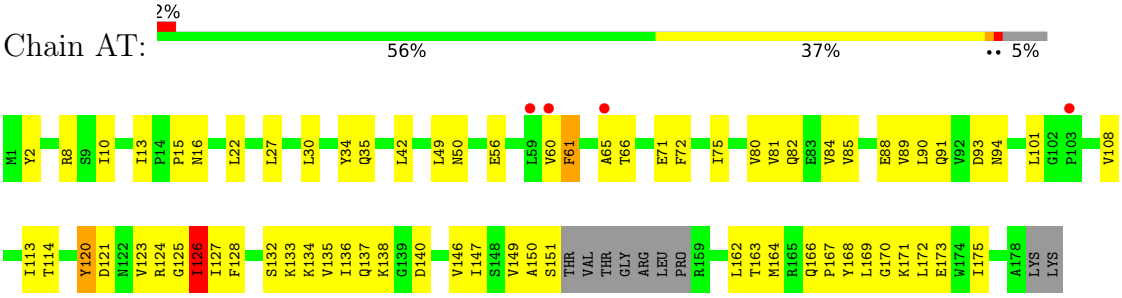
• Molecule 8: DNA-DIRECTED RNA POLYMERASE SUBUNIT D

Chain BD:



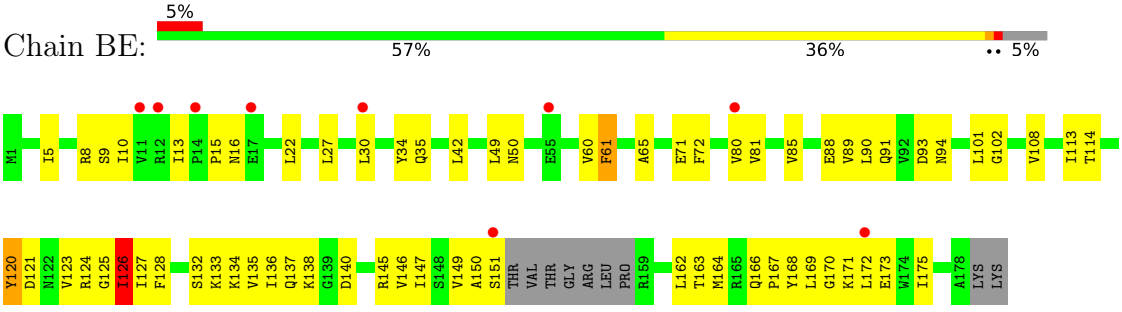
• Molecule 9: RNA POLYMERASE SUBUNIT 7

Chain AT:



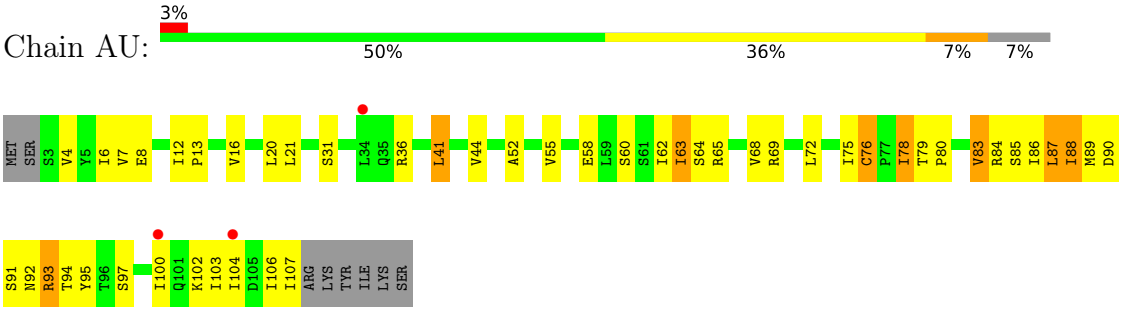
• Molecule 9: RNA POLYMERASE SUBUNIT 7

Chain BE:



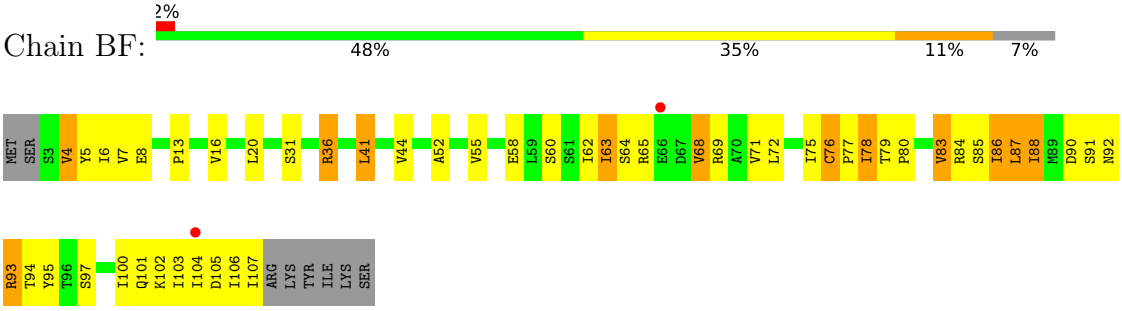
• Molecule 10: RNA POLYMERASE SUBUNIT 4

Chain AU:



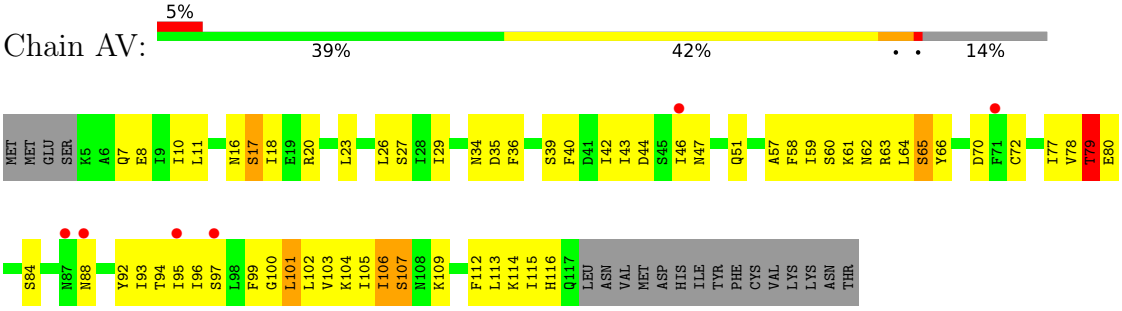
• Molecule 10: RNA POLYMERASE SUBUNIT 4

Chain BF:



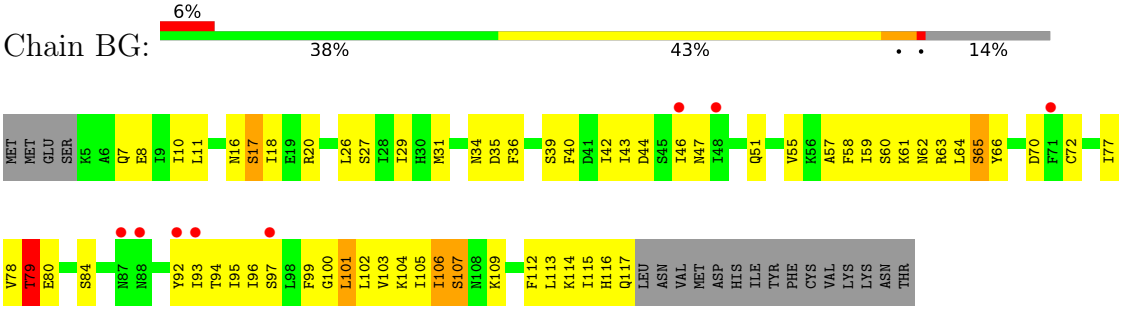
• Molecule 11: RNA POLYMERASE SUBUNIT 8

Chain AV:



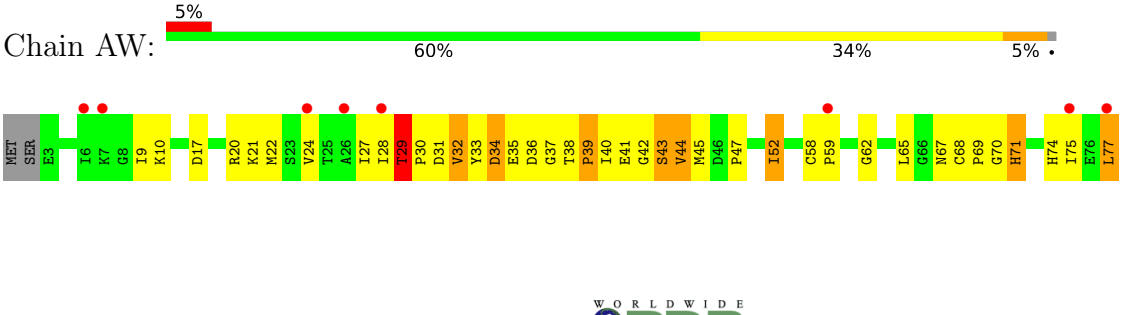
• Molecule 11: RNA POLYMERASE SUBUNIT 8

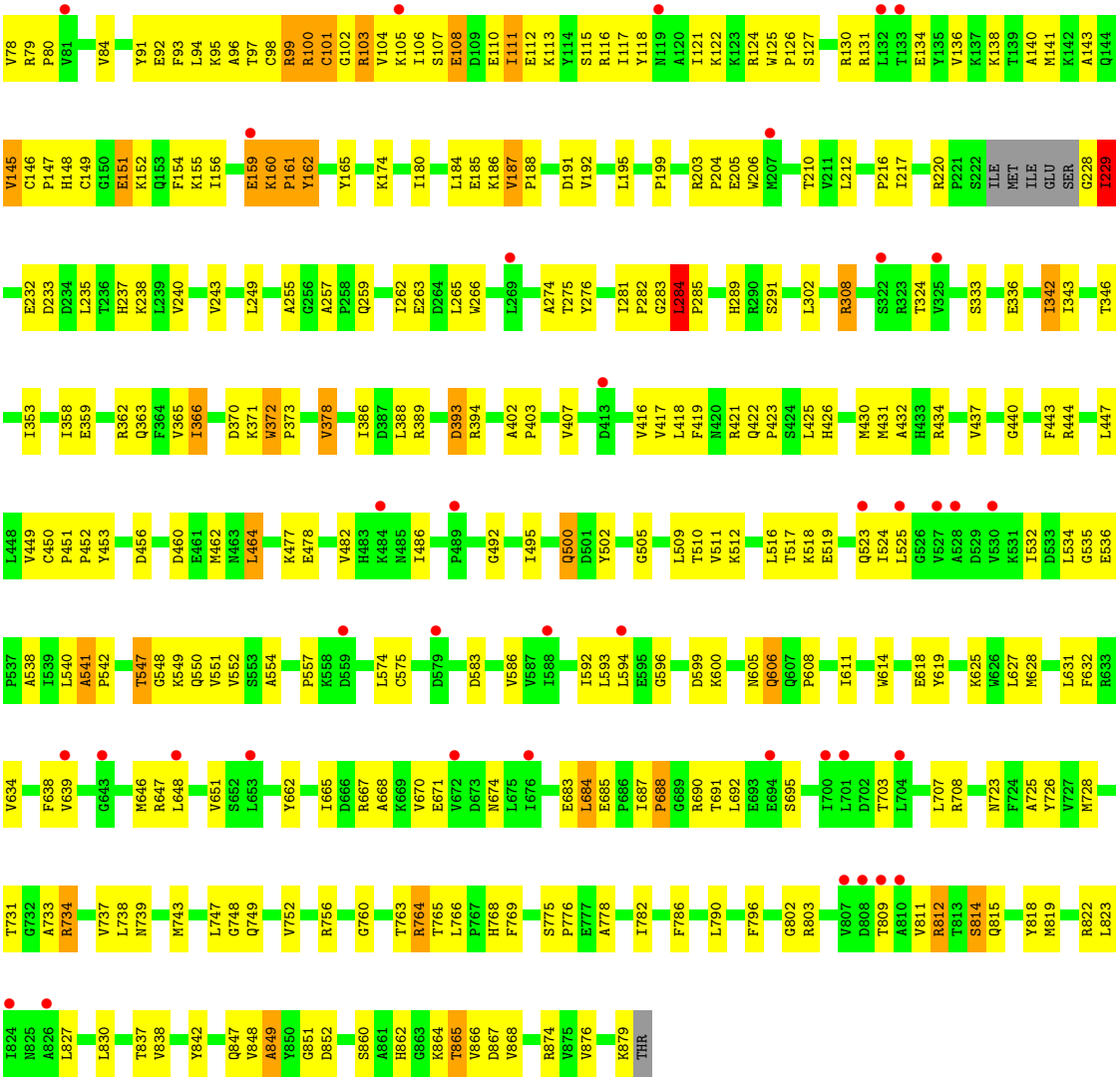
Chain BG:



• Molecule 12: DNA-DIRECTED RNA POLYMERASE

Chain AW:

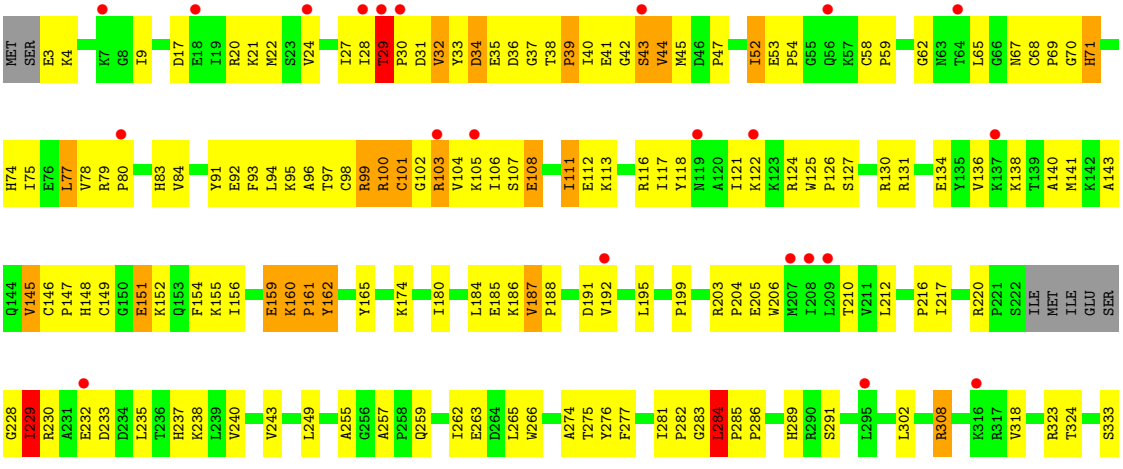


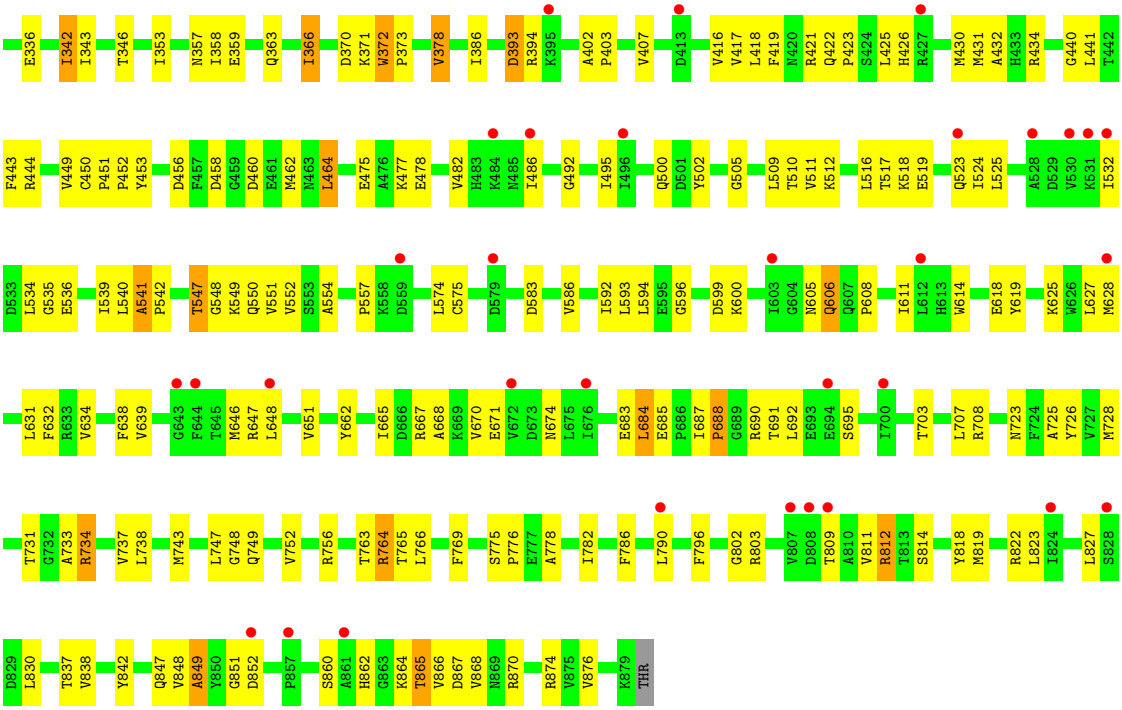


• Molecule 12: DNA-DIRECTED RNA POLYMERASE

Chain BA:



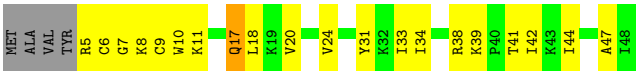




• Molecule 13: DNA-DIRECTED RNA POLYMERASE SUBUNIT P

Chain AX:

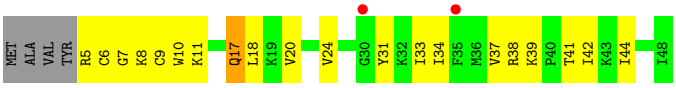




• Molecule 13: DNA-DIRECTED RNA POLYMERASE SUBUNIT P

Chain BP:

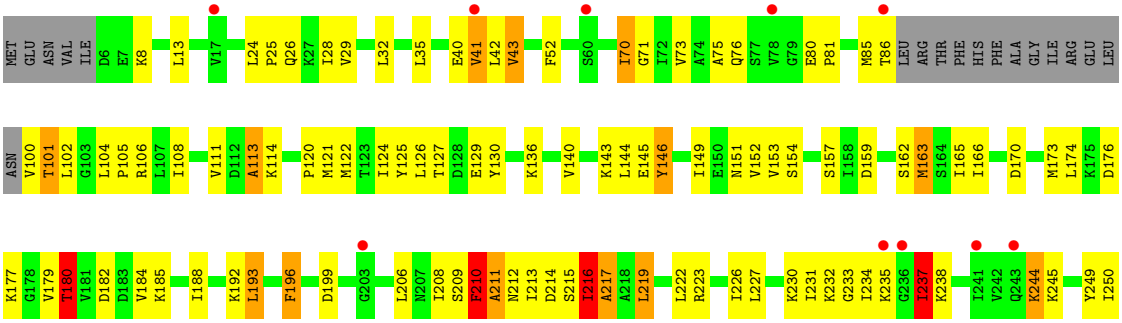


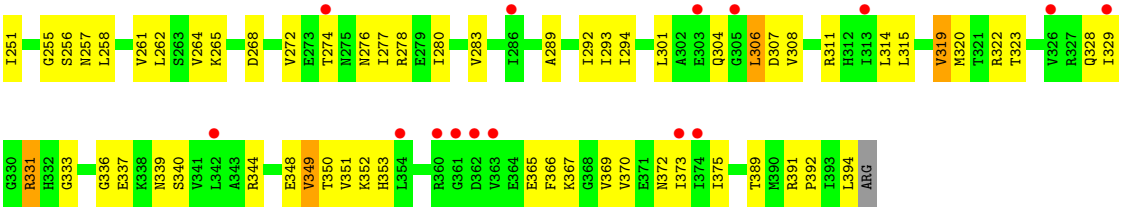


• Molecule 14: DNA-DIRECTED RNA POLYMERASE SUBUNIT A"

Chain AY:



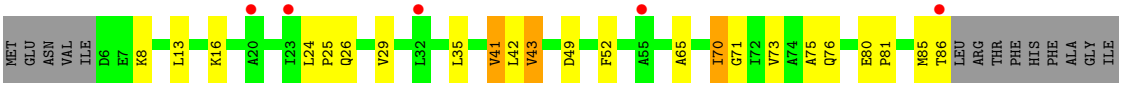


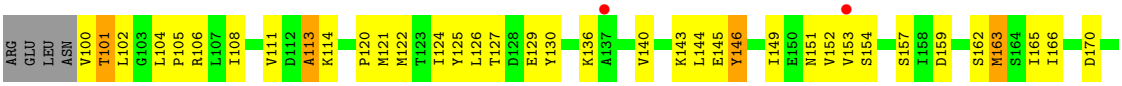


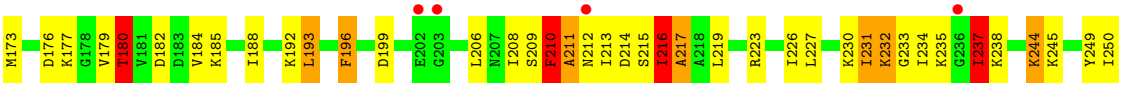
• Molecule 14: DNA-DIRECTED RNA POLYMERASE SUBUNIT A"

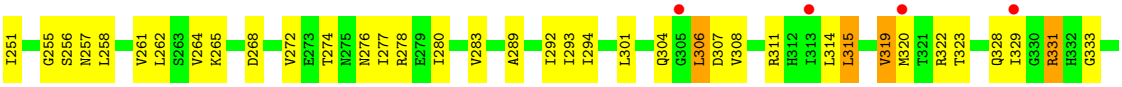
Chain BC:

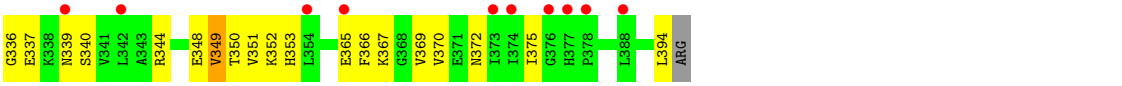








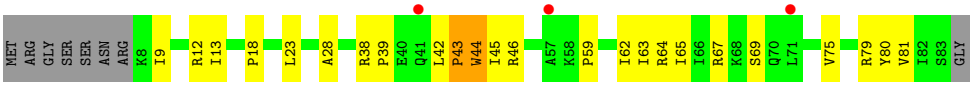




• Molecule 15: DNA-DIRECTED RNA POLYMERASE SUBUNIT H

Chain AZ:

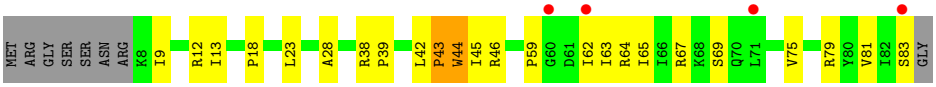




• Molecule 15: DNA-DIRECTED RNA POLYMERASE SUBUNIT H

Chain BH:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	134.13Å 199.42Å 214.25Å 90.00° 103.54° 90.00°	Depositor
Resolution (Å)	50.42 – 4.32 50.42 – 4.32	Depositor EDS
% Data completeness (in resolution range)	88.6 (50.42-4.32) 88.6 (50.42-4.32)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.42 (at 4.29Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.292 , 0.310 0.290 , 0.301	Depositor DCC
R_{free} test set	3309 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å^2)	105.4	Xtriage
Anisotropy	0.633	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 135.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.82	EDS
Total number of atoms	111598	wwPDB-VP
Average B, all atoms (Å^2)	171.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.90% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ZN, SF4

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	AC	0.10	0/288	0.56	0/441
1	BR	0.10	0/309	0.56	0/473
2	AD	0.14	0/355	0.69	0/547
2	BS	0.13	0/379	0.65	0/584
3	AI	0.30	0/682	0.69	1/921 (0.1%)
3	BK	0.27	0/682	0.67	1/921 (0.1%)
4	AJ	0.35	0/423	0.69	0/566
4	BQ	0.31	0/432	0.65	0/578
5	AM	0.27	0/717	0.64	0/968
5	BL	0.24	0/717	0.62	0/968
6	AO	0.30	0/532	0.64	0/718
6	BN	0.30	0/532	0.63	0/718
7	AR	0.27	0/8923	0.67	0/12071
7	BB	0.27	0/8923	0.67	0/12071
8	AS	0.25	0/2123	0.64	0/2870
8	BD	0.26	0/2123	0.64	0/2870
9	AT	0.25	0/1379	0.65	0/1861
9	BE	0.25	0/1379	0.65	0/1861
10	AU	0.30	0/836	0.69	0/1133
10	BF	0.29	0/836	0.68	0/1133
11	AV	0.26	0/913	0.67	0/1224
11	BG	0.25	0/913	0.67	0/1224
12	AW	0.29	0/7108	0.69	1/9618 (0.0%)
12	BA	0.29	0/7108	0.69	1/9618 (0.0%)
13	AX	0.29	0/365	0.66	0/489
13	BP	0.29	0/365	0.65	0/489
14	AY	0.28	0/2930	0.71	0/3944
14	BC	0.28	0/2930	0.71	0/3944
15	AZ	0.27	0/638	0.64	0/864
15	BH	0.26	0/638	0.63	0/864
All	All	0.27	0/56478	0.67	4/76551 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	BA	811	VAL	N-CA-C	6.32	116.43	110.30
12	AW	811	VAL	N-CA-C	6.31	116.42	110.30
3	BK	85	GLY	N-CA-C	-5.25	108.83	115.08
3	AI	85	GLY	N-CA-C	-5.23	108.86	115.08

There are no chirality outliers.

There are no planarity outliers.

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	AC	260	151	151	4	0
1	BR	279	162	162	6	0
2	AD	315	170	170	36	0
2	BS	336	181	181	25	0
3	AI	673	717	716	16	0
3	BK	673	717	716	12	0
4	AJ	417	413	413	39	0
4	BQ	426	419	419	37	0
5	AM	707	742	739	15	0
5	BL	707	742	739	13	0
6	AO	521	537	535	31	0
6	BN	521	537	535	27	0
7	AR	8756	8909	8888	307	0
7	BB	8756	8909	8888	316	0
8	AS	2087	2128	2125	56	0
8	BD	2087	2128	2125	53	0
9	AT	1359	1413	1411	64	0
9	BE	1359	1412	1411	55	0
10	AU	827	840	839	57	0
10	BF	827	840	839	56	0
11	AV	901	915	912	73	0
11	BG	901	915	912	71	0
12	AW	6957	7030	7013	343	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	BA	6957	7030	7013	338	0
13	AX	357	387	387	18	0
13	BP	357	387	387	15	0
14	AY	2906	3068	3063	172	0
14	BC	2906	3068	3063	152	0
15	AZ	624	660	658	25	0
15	BH	624	660	658	26	0
16	AO	1	0	0	0	0
16	AR	1	0	0	0	0
16	AW	3	0	0	0	0
16	AX	1	0	0	0	0
16	BA	3	0	0	0	0
16	BB	1	0	0	0	0
16	BN	1	0	0	0	0
16	BP	1	0	0	0	0
17	AS	7	0	0	2	0
17	BD	7	0	0	3	0
18	AW	1	0	0	0	0
18	BA	1	0	0	0	0
All	All	55411	56187	56068	2306	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 21.

All (2306) 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)
10:AU:93:ARG:CB	10:AU:94:THR:HA	1.85	1.06
2:AD:14:DA:OP1	14:AY:348:GLU:HG2	1.54	1.05
10:BF:93:ARG:CB	10:BF:94:THR:HA	1.85	1.05
7:AR:221:PRO:HB2	7:AR:222:GLY:HA2	1.37	1.05
7:BB:221:PRO:HB2	7:BB:222:GLY:HA2	1.38	1.01
14:AY:42:LEU:HA	14:AY:43:VAL:HB	1.47	0.96
14:BC:42:LEU:HA	14:BC:43:VAL:HB	1.47	0.93
7:BB:52:ILE:HB	7:BB:53:PRO:HD3	1.53	0.90
7:AR:52:ILE:HB	7:AR:53:PRO:HD3	1.54	0.89
14:AY:42:LEU:HA	14:AY:43:VAL:CB	2.03	0.89
14:BC:42:LEU:HA	14:BC:43:VAL:CB	2.03	0.88
10:BF:93:ARG:HB3	10:BF:94:THR:HA	1.54	0.88
10:AU:93:ARG:HB3	10:AU:94:THR:HA	1.54	0.88
10:AU:93:ARG:HB2	10:AU:94:THR:HA	1.55	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:BF:93:ARG:HB2	10:BF:94:THR:HA	1.55	0.86
12:BA:683:GLU:HA	12:BA:684:LEU:HB3	1.57	0.86
12:AW:683:GLU:HA	12:AW:684:LEU:HB3	1.57	0.86
2:AD:14:DA:H4'	12:AW:818:TYR:CZ	2.12	0.84
7:AR:833:GLN:N	7:AR:834:ALA:HB3	1.93	0.84
7:BB:833:GLN:N	7:BB:834:ALA:HB3	1.93	0.83
12:BA:36:ASP:N	12:BA:37:GLY:HA2	1.94	0.81
11:BG:65:SER:CB	11:BG:66:TYR:HA	2.10	0.81
11:AV:65:SER:CB	11:AV:66:TYR:HA	2.10	0.81
12:AW:36:ASP:N	12:AW:37:GLY:HA2	1.94	0.81
4:BQ:56:ASN:N	4:BQ:57:GLY:HA2	1.96	0.81
7:BB:53:PRO:HB2	7:BB:54:THR:HB	1.63	0.81
7:AR:53:PRO:HB2	7:AR:54:THR:HB	1.62	0.81
12:BA:131:ARG:HD3	4:BQ:36:LEU:HD11	1.63	0.80
6:AO:64:ARG:CB	6:AO:65:PRO:HD3	2.12	0.80
7:AR:1067:CYS:SG	7:AR:1085:HIS:CE1	2.74	0.80
4:AJ:56:ASN:N	4:AJ:57:GLY:HA2	1.96	0.79
12:AW:105:LYS:HZ2	12:AW:140:ALA:HB3	1.47	0.79
7:BB:53:PRO:HB2	7:BB:54:THR:CA	2.13	0.79
7:AR:53:PRO:HB2	7:AR:54:THR:CA	2.13	0.79
7:BB:53:PRO:HB2	7:BB:54:THR:HA	1.65	0.79
7:BB:406:TRP:HA	7:BB:407:VAL:HB	1.64	0.79
7:AR:406:TRP:HA	7:AR:407:VAL:HB	1.64	0.78
6:BN:64:ARG:CB	6:BN:65:PRO:HD3	2.12	0.78
7:AR:53:PRO:HB2	7:AR:54:THR:HA	1.65	0.78
12:BA:105:LYS:HZ2	12:BA:140:ALA:HB3	1.48	0.77
7:AR:833:GLN:HB2	7:AR:834:ALA:HB3	1.66	0.77
6:AO:64:ARG:HB3	6:AO:65:PRO:HD3	1.65	0.77
6:BN:64:ARG:HB3	6:BN:65:PRO:HD3	1.65	0.76
2:AD:14:DA:H4'	12:AW:818:TYR:CE1	2.21	0.76
8:AS:203:CYS:HA	17:AS:1001:SF4:S1	2.26	0.76
2:AD:14:DA:P	14:AY:348:GLU:HG2	2.25	0.75
14:AY:211:ALA:HB1	14:AY:212:ASN:C	2.12	0.75
4:BQ:32:GLU:O	4:BQ:33:PHE:HB2	1.84	0.75
7:BB:833:GLN:HB2	7:BB:834:ALA:HB3	1.66	0.75
14:BC:211:ALA:HB1	14:BC:212:ASN:C	2.12	0.75
12:BA:372:TRP:HB3	12:BA:373:PRO:HD3	1.68	0.74
11:AV:29:ILE:HB	11:AV:40:PHE:HB3	1.70	0.74
12:AW:372:TRP:HB3	12:AW:373:PRO:HD3	1.68	0.73
12:AW:541:ALA:HB3	12:AW:542:PRO:CD	2.17	0.73
11:BG:29:ILE:HB	11:BG:40:PHE:HB3	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:AV:64:LEU:HG	11:AV:114:LYS:HG3	1.69	0.73
11:BG:64:LEU:HG	11:BG:114:LYS:HG3	1.69	0.73
12:BA:541:ALA:HB3	12:BA:542:PRO:CD	2.18	0.72
11:AV:79:THR:HB	11:AV:80:GLU:HB2	1.69	0.72
10:AU:93:ARG:CB	10:AU:94:THR:CA	2.67	0.72
10:BF:91:SER:HB2	10:BF:92:ASN:HA	1.72	0.72
14:AY:42:LEU:HA	14:AY:43:VAL:CG2	2.19	0.72
7:BB:52:ILE:CB	7:BB:53:PRO:HD3	2.20	0.72
11:BG:79:THR:HB	11:BG:80:GLU:HB2	1.70	0.72
12:BA:283:GLY:HA3	12:BA:284:LEU:CG	2.20	0.72
14:BC:42:LEU:HA	14:BC:43:VAL:CG2	2.19	0.72
10:BF:93:ARG:CB	10:BF:94:THR:CA	2.67	0.71
12:AW:283:GLY:HA3	12:AW:284:LEU:CG	2.20	0.71
4:AJ:36:LEU:HD11	12:AW:131:ARG:HD3	1.73	0.70
10:AU:91:SER:HB2	10:AU:92:ASN:HA	1.72	0.70
7:BB:734:GLY:HA3	7:BB:735:TYR:CG	2.26	0.70
7:AR:52:ILE:CB	7:AR:53:PRO:HD3	2.20	0.70
9:AT:170:GLY:N	9:AT:175:ILE:HD11	2.07	0.70
7:AR:734:GLY:HA3	7:AR:735:TYR:CG	2.26	0.70
12:BA:796:PHE:CZ	7:BB:448:LEU:HD22	2.26	0.70
9:BE:170:GLY:N	9:BE:175:ILE:HD11	2.07	0.70
12:AW:283:GLY:HA3	12:AW:284:LEU:HG	1.75	0.69
7:AR:53:PRO:HB2	7:AR:54:THR:CB	2.21	0.69
14:AY:211:ALA:HA	14:AY:212:ASN:HB2	1.75	0.69
12:AW:283:GLY:HA3	12:AW:284:LEU:CB	2.22	0.69
7:BB:406:TRP:HA	7:BB:407:VAL:CB	2.22	0.69
14:BC:211:ALA:HA	14:BC:212:ASN:HB2	1.75	0.69
2:AD:17:DG:C1'	12:AW:423:PRO:HB3	2.21	0.69
12:BA:283:GLY:HA3	12:BA:284:LEU:HG	1.75	0.69
7:BB:380:ARG:HB3	7:BB:381:LYS:HA	1.75	0.68
12:BA:283:GLY:HA3	12:BA:284:LEU:CB	2.22	0.68
7:BB:53:PRO:HB2	7:BB:54:THR:CB	2.22	0.68
7:AR:406:TRP:HA	7:AR:407:VAL:CB	2.22	0.68
11:AV:65:SER:HB2	11:AV:66:TYR:HA	1.75	0.68
11:BG:65:SER:HB2	11:BG:66:TYR:HA	1.76	0.68
7:AR:380:ARG:HB3	7:AR:381:LYS:HA	1.75	0.68
2:AD:14:DA:C4'	12:AW:818:TYR:CZ	2.78	0.67
12:AW:864:LYS:HA	12:AW:865:THR:CB	2.23	0.67
12:AW:541:ALA:CB	12:AW:542:PRO:CD	2.72	0.67
12:BA:131:ARG:CD	4:BQ:36:LEU:HD11	2.24	0.67
12:BA:864:LYS:HA	12:BA:865:THR:CB	2.23	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:AR:734:GLY:HA3	7:AR:735:TYR:CB	2.23	0.67
7:BB:734:GLY:HA3	7:BB:735:TYR:CB	2.23	0.67
2:AD:3:DT:H2"	2:AD:4:DA:C5	2.29	0.67
14:BC:176:ASP:HB2	14:BC:177:LYS:HB2	1.76	0.67
2:BS:3:DT:H2"	2:BS:4:DA:C5	2.29	0.67
14:AY:176:ASP:H	14:AY:177:LYS:HB2	1.59	0.67
14:AY:211:ALA:HB3	14:AY:213:ILE:HG12	1.77	0.67
7:BB:221:PRO:HB2	7:BB:222:GLY:CA	2.21	0.67
10:AU:78:ILE:HG23	10:AU:104:ILE:HG22	1.77	0.67
14:AY:42:LEU:CA	14:AY:43:VAL:HB	2.24	0.66
14:BC:211:ALA:CA	14:BC:212:ASN:HB2	2.25	0.66
7:AR:221:PRO:HB2	7:AR:222:GLY:CA	2.21	0.66
12:BA:586:VAL:HA	12:BA:596:GLY:HA3	1.77	0.66
7:AR:406:TRP:CA	7:AR:407:VAL:HB	2.25	0.66
2:AD:17:DG:O4'	12:AW:423:PRO:HB3	1.96	0.66
14:AY:211:ALA:CA	14:AY:212:ASN:HB2	2.25	0.66
10:AU:93:ARG:HB2	10:AU:94:THR:CA	2.26	0.66
15:BH:59:PRO:HB3	4:BQ:44:LEU:HD21	1.77	0.66
12:BA:541:ALA:CB	12:BA:542:PRO:CD	2.72	0.66
7:BB:734:GLY:CA	7:BB:735:TYR:HB2	2.26	0.66
7:AR:734:GLY:CA	7:AR:735:TYR:HB2	2.26	0.66
12:AW:103:ARG:HB2	12:AW:186:LYS:HB2	1.78	0.66
14:AY:176:ASP:HB2	14:AY:177:LYS:HB2	1.76	0.66
10:BF:78:ILE:HG23	10:BF:104:ILE:HG22	1.77	0.66
7:BB:406:TRP:CA	7:BB:407:VAL:HB	2.26	0.65
7:BB:893:MET:HE2	5:BL:48:PRO:HB2	1.76	0.65
14:BC:176:ASP:H	14:BC:177:LYS:HB2	1.59	0.65
4:AJ:36:LEU:O	4:AJ:37:SER:CB	2.45	0.65
14:BC:211:ALA:HB3	14:BC:213:ILE:HG12	1.78	0.65
12:AW:33:TYR:H	12:AW:34:ASP:HB2	1.61	0.65
7:BB:356:LEU:HA	7:BB:407:VAL:HG11	1.79	0.65
7:BB:833:GLN:HB2	7:BB:834:ALA:CB	2.26	0.65
8:BD:203:CYS:HA	17:BD:1001:SF4:S1	2.37	0.65
7:AR:356:LEU:HA	7:AR:407:VAL:HG11	1.79	0.65
12:AW:586:VAL:HA	12:AW:596:GLY:HA3	1.77	0.65
12:BA:33:TYR:H	12:BA:34:ASP:HB2	1.61	0.65
12:AW:668:ALA:CB	12:AW:707:LEU:HD13	2.27	0.65
12:BA:450:CYS:HB2	12:BA:451:PRO:HD3	1.79	0.64
4:BQ:78:ARG:C	4:BQ:78:ARG:HD3	2.22	0.64
4:AJ:78:ARG:C	4:AJ:78:ARG:HD3	2.22	0.64
12:BA:346:THR:HG22	7:BB:1008:ALA:HB2	1.77	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:AU:88:ILE:HG23	10:AU:88:ILE:O	1.97	0.64
12:BA:103:ARG:HB2	12:BA:186:LYS:HB2	1.78	0.64
10:BF:88:ILE:HG23	10:BF:88:ILE:O	1.97	0.64
12:BA:131:ARG:CZ	4:BQ:36:LEU:HD21	2.27	0.64
7:AR:833:GLN:HB2	7:AR:834:ALA:CB	2.26	0.64
14:BC:211:ALA:HB1	14:BC:212:ASN:HB2	1.80	0.64
8:BD:184:PRO:HD2	17:BD:1001:SF4:S3	2.37	0.64
10:BF:79:THR:OG1	10:BF:80:PRO:HD3	1.98	0.64
2:AD:17:DG:H1'	12:AW:423:PRO:HB3	1.80	0.64
12:AW:541:ALA:CB	12:AW:542:PRO:HD3	2.28	0.64
12:AW:668:ALA:HB1	12:AW:707:LEU:HD13	1.79	0.64
14:AY:211:ALA:HB1	14:AY:212:ASN:HB2	1.80	0.64
10:BF:93:ARG:HB2	10:BF:94:THR:CA	2.26	0.64
12:BA:668:ALA:CB	12:BA:707:LEU:HD13	2.27	0.63
7:BB:1066:GLN:HG3	7:BB:1085:HIS:CE1	2.32	0.63
14:AY:211:ALA:CB	14:AY:212:ASN:HB2	2.28	0.63
12:BA:40:ILE:HG21	12:BA:47:PRO:HD3	1.80	0.63
7:AR:1014:ILE:O	7:AR:1015:LEU:CB	2.46	0.63
10:AU:79:THR:OG1	10:AU:80:PRO:HD3	1.98	0.63
7:BB:833:GLN:CB	7:BB:834:ALA:HB3	2.29	0.63
14:BC:42:LEU:CA	14:BC:43:VAL:HB	2.24	0.63
7:AR:833:GLN:CB	7:AR:834:ALA:HB3	2.29	0.63
12:AW:40:ILE:HG21	12:AW:47:PRO:HD3	1.81	0.63
12:BA:160:LYS:HB3	12:BA:161:PRO:HD2	1.81	0.63
7:AR:833:GLN:CA	7:AR:834:ALA:HB3	2.29	0.63
12:AW:450:CYS:HB2	12:AW:451:PRO:HD3	1.80	0.63
14:AY:213:ILE:H	14:AY:214:ASP:HA	1.64	0.63
7:BB:833:GLN:CA	7:BB:834:ALA:HB3	2.29	0.63
14:BC:211:ALA:CB	14:BC:212:ASN:HB2	2.28	0.63
7:AR:52:ILE:HB	7:AR:53:PRO:CD	2.28	0.63
2:AD:16:DA:O5'	12:AW:814:SER:HA	1.99	0.62
7:BB:256:PHE:N	7:BB:257:PRO:HD2	2.13	0.62
4:BQ:58:LYS:O	4:BQ:59:ILE:HB	1.97	0.62
12:BA:662:TYR:HA	12:BA:665:ILE:HG12	1.81	0.62
12:AW:662:TYR:HA	12:AW:665:ILE:HG12	1.82	0.62
12:AW:848:VAL:O	12:AW:849:ALA:HB3	1.99	0.62
12:BA:848:VAL:O	12:BA:849:ALA:HB3	1.99	0.62
14:BC:213:ILE:H	14:BC:214:ASP:HA	1.63	0.62
6:AO:64:ARG:CB	6:AO:65:PRO:CD	2.77	0.62
12:BA:668:ALA:HB1	12:BA:707:LEU:HD13	1.80	0.62
4:AJ:58:LYS:O	4:AJ:59:ILE:HB	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:BB:112:ALA:O	7:BB:113:GLU:CB	2.47	0.62
4:BQ:36:LEU:O	4:BQ:37:SER:CB	2.46	0.62
7:AR:256:PHE:N	7:AR:257:PRO:HD2	2.13	0.62
7:AR:600:LEU:HD11	7:AR:610:LEU:HD11	1.81	0.62
11:AV:65:SER:OG	11:AV:66:TYR:HA	1.99	0.62
7:BB:1014:ILE:O	7:BB:1015:LEU:CB	2.47	0.62
4:AJ:57:GLY:O	4:AJ:59:ILE:N	2.33	0.62
12:BA:33:TYR:HB3	12:BA:34:ASP:HA	1.82	0.62
7:AR:112:ALA:O	7:AR:113:GLU:CB	2.47	0.61
11:AV:106:ILE:O	11:AV:107:SER:CB	2.48	0.61
12:BA:29:THR:OG1	12:BA:30:PRO:HD3	2.00	0.61
7:BB:52:ILE:HB	7:BB:53:PRO:CD	2.28	0.61
12:AW:146:CYS:HB2	12:AW:151:GLU:HA	1.80	0.61
12:AW:160:LYS:HB3	12:AW:161:PRO:HD2	1.81	0.61
12:BA:103:ARG:CB	12:BA:186:LYS:HB2	2.30	0.61
12:BA:541:ALA:CB	12:BA:542:PRO:HD3	2.29	0.61
7:BB:112:ALA:O	7:BB:113:GLU:HB2	2.00	0.61
4:BQ:57:GLY:O	4:BQ:59:ILE:N	2.33	0.61
12:AW:29:THR:OG1	12:AW:30:PRO:HD3	2.00	0.61
14:AY:80:GLU:N	14:AY:81:PRO:CD	2.63	0.61
14:AY:348:GLU:HG3	14:AY:349:VAL:N	2.14	0.61
14:BC:176:ASP:CB	14:BC:177:LYS:HB2	2.31	0.61
14:BC:176:ASP:N	14:BC:177:LYS:O	2.34	0.61
12:AW:97:THR:HG22	12:AW:99:ARG:H	1.65	0.61
14:AY:176:ASP:N	14:AY:177:LYS:O	2.34	0.61
10:BF:76:CYS:CB	10:BF:104:ILE:HG23	2.31	0.61
11:BG:106:ILE:O	11:BG:107:SER:CB	2.48	0.61
4:AJ:36:LEU:HD11	12:AW:131:ARG:CD	2.31	0.61
7:AR:112:ALA:O	7:AR:113:GLU:HB2	2.00	0.61
7:AR:245:VAL:HA	7:AR:319:ALA:HB1	1.82	0.61
12:BA:864:LYS:HA	12:BA:865:THR:HB	1.82	0.61
15:BH:43:PRO:O	15:BH:44:TRP:CB	2.49	0.61
2:AD:14:DA:C8	2:AD:15:DT:H73	2.36	0.61
12:AW:103:ARG:CB	12:AW:186:LYS:HB2	2.30	0.61
14:AY:176:ASP:CB	14:AY:177:LYS:HB2	2.30	0.61
14:BC:80:GLU:N	14:BC:81:PRO:CD	2.63	0.61
6:BN:2:MET:O	6:BN:3:ILE:O	2.18	0.61
2:BS:2:DA:H2'	2:BS:3:DT:H5'	1.83	0.61
14:AY:76:GLN:O	14:AY:80:GLU:N	2.34	0.60
12:BA:860:SER:HB2	12:BA:864:LYS:O	2.01	0.60
4:AJ:44:LEU:HD21	15:AZ:59:PRO:HB3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:AO:2:MET:O	6:AO:3:ILE:O	2.19	0.60
8:AS:184:PRO:HD2	17:AS:1001:SF4:S2	2.40	0.60
10:AU:76:CYS:CB	10:AU:104:ILE:HG23	2.31	0.60
14:AY:162:SER:O	14:AY:163:MET:C	2.44	0.60
7:AR:786:TYR:CE2	7:AR:788:GLY:HA2	2.36	0.60
12:BA:97:THR:HG22	12:BA:99:ARG:H	1.65	0.60
7:BB:196:THR:O	7:BB:197:ALA:HB3	2.01	0.60
7:BB:786:TYR:CE2	7:BB:788:GLY:HA2	2.36	0.60
14:BC:42:LEU:HA	14:BC:43:VAL:HG23	1.83	0.60
14:BC:162:SER:O	14:BC:163:MET:C	2.44	0.60
9:AT:2:TYR:HB2	10:AU:12:ILE:HB	1.83	0.60
9:AT:85:VAL:HG11	9:AT:101:LEU:HD22	1.83	0.60
12:BA:535:GLY:O	12:BA:536:GLU:C	2.45	0.60
14:BC:24:LEU:HB3	14:BC:25:PRO:HD2	1.83	0.60
7:AR:196:THR:O	7:AR:197:ALA:HB3	2.01	0.60
8:AS:51:SER:HB2	8:AS:52:PRO:HD2	1.84	0.60
12:AW:864:LYS:HA	12:AW:865:THR:HB	1.82	0.60
14:AY:213:ILE:HB	14:AY:214:ASP:C	2.27	0.60
12:BA:146:CYS:SG	12:BA:154:PHE:CZ	2.95	0.60
14:BC:213:ILE:HB	14:BC:214:ASP:C	2.27	0.60
12:AW:33:TYR:HB3	12:AW:34:ASP:HA	1.82	0.60
12:BA:127:SER:O	12:BA:131:ARG:HD2	2.00	0.60
2:BS:14:DA:C8	2:BS:15:DT:H73	2.36	0.60
15:AZ:43:PRO:O	15:AZ:44:TRP:CB	2.49	0.60
7:BB:221:PRO:CB	7:BB:222:GLY:HA2	2.23	0.60
7:BB:245:VAL:HA	7:BB:319:ALA:HB1	1.82	0.60
14:BC:76:GLN:O	14:BC:80:GLU:N	2.35	0.60
7:AR:781:PRO:HA	7:AR:786:TYR:CE2	2.37	0.60
12:AW:860:SER:HB2	12:AW:864:LYS:O	2.02	0.60
14:AY:213:ILE:N	14:AY:214:ASP:HA	2.17	0.60
12:BA:47:PRO:HB2	12:BA:59:PRO:HG2	1.83	0.60
12:BA:683:GLU:HA	12:BA:684:LEU:CB	2.32	0.60
9:BE:85:VAL:HG11	9:BE:101:LEU:HD22	1.83	0.60
11:BG:65:SER:OG	11:BG:66:TYR:HA	2.00	0.60
7:BB:600:LEU:HD11	7:BB:610:LEU:HD11	1.82	0.59
7:AR:660:TYR:N	7:AR:661:PRO:HD3	2.17	0.59
14:BC:213:ILE:N	14:BC:214:ASP:HA	2.17	0.59
7:AR:221:PRO:CB	7:AR:222:GLY:HA2	2.22	0.59
7:AR:808:LYS:HD2	7:AR:809:GLY:N	2.17	0.59
12:AW:42:GLY:O	12:AW:43:SER:CB	2.50	0.59
6:BN:64:ARG:CB	6:BN:65:PRO:CD	2.77	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:AR:1082:CYS:HB2	7:AR:1083:PRO:HD2	1.84	0.59
12:AW:33:TYR:HB3	12:AW:34:ASP:HB2	1.84	0.59
12:BA:33:TYR:HB3	12:BA:34:ASP:HB2	1.84	0.59
7:AR:732:PHE:O	7:AR:733:THR:HG22	2.03	0.59
12:AW:98:CYS:HB2	12:AW:104:VAL:H	1.68	0.59
4:BQ:46:LYS:HA	4:BQ:46:LYS:HE2	1.85	0.59
14:AY:211:ALA:CB	14:AY:213:ILE:HG12	2.33	0.59
15:BH:43:PRO:O	15:BH:44:TRP:CG	2.56	0.59
12:AW:47:PRO:HB2	12:AW:59:PRO:HG2	1.83	0.59
12:AW:103:ARG:CG	12:AW:187:VAL:HG13	2.33	0.59
12:BA:42:GLY:O	12:BA:43:SER:CB	2.50	0.59
7:BB:781:PRO:HA	7:BB:786:TYR:CE2	2.37	0.59
8:BD:51:SER:HB2	8:BD:52:PRO:HD2	1.83	0.59
12:AW:33:TYR:HB3	12:AW:34:ASP:CA	2.33	0.58
12:BA:33:TYR:HB3	12:BA:34:ASP:CA	2.33	0.58
2:AD:14:DA:OP1	14:AY:331:ARG:NH1	2.36	0.58
15:AZ:43:PRO:O	15:AZ:44:TRP:CG	2.56	0.58
12:BA:33:TYR:CB	12:BA:34:ASP:HB2	2.33	0.58
7:BB:56:ILE:HG23	7:BB:59:LEU:HB2	1.85	0.58
14:BC:211:ALA:HB1	14:BC:212:ASN:CA	2.33	0.58
14:AY:24:LEU:HB3	14:AY:25:PRO:HD2	1.84	0.58
7:BB:808:LYS:HD2	7:BB:809:GLY:N	2.18	0.58
14:BC:144:LEU:O	14:BC:237:ILE:HD11	2.04	0.58
7:AR:56:ILE:HG23	7:AR:59:LEU:HB2	1.85	0.58
12:AW:535:GLY:O	12:AW:536:GLU:C	2.45	0.58
7:BB:660:TYR:N	7:BB:661:PRO:HD3	2.17	0.58
14:BC:213:ILE:HB	14:BC:214:ASP:O	2.04	0.58
4:AJ:36:LEU:HD11	12:AW:131:ARG:NE	2.18	0.58
14:AY:42:LEU:HA	14:AY:43:VAL:HG23	1.84	0.58
14:AY:192:LYS:HB3	14:AY:193:LEU:HB2	1.85	0.58
12:BA:98:CYS:HB2	12:BA:104:VAL:H	1.68	0.58
12:BA:103:ARG:CG	12:BA:187:VAL:HG13	2.33	0.58
2:BS:2:DA:C2'	2:BS:3:DT:H5"	2.34	0.58
7:BB:732:PHE:O	7:BB:733:THR:HG22	2.02	0.58
9:BE:5:ILE:HG23	10:BF:6:ILE:HG23	1.84	0.58
12:AW:651:VAL:HG11	12:AW:743:MET:HB3	1.86	0.58
14:AY:144:LEU:O	14:AY:237:ILE:HD11	2.04	0.58
11:BG:101:LEU:HD22	11:BG:102:LEU:N	2.18	0.58
5:AM:90:LEU:HD21	8:AS:5:LEU:HG	1.86	0.58
6:AO:14:ILE:HD11	6:AO:45:CYS:HB3	1.86	0.58
12:BA:651:VAL:HG11	12:BA:743:MET:HB3	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:BC:192:LYS:HB3	14:BC:193:LEU:HB2	1.85	0.58
6:AO:48:MET:HE2	6:AO:48:MET:HA	1.85	0.58
12:AW:372:TRP:CB	12:AW:373:PRO:HD3	2.32	0.58
14:AY:126:LEU:HB3	14:AY:130:TYR:HB2	1.86	0.58
7:BB:1111:ILE:N	7:BB:1111:ILE:HD12	2.19	0.58
4:AJ:46:LYS:HA	4:AJ:46:LYS:HE2	1.86	0.57
12:AW:541:ALA:HB3	12:AW:542:PRO:HD3	1.86	0.57
14:AY:213:ILE:HB	14:AY:214:ASP:O	2.04	0.57
12:AW:127:SER:O	12:AW:131:ARG:HD2	2.04	0.57
14:AY:192:LYS:CB	14:AY:193:LEU:HB2	2.34	0.57
12:AW:33:TYR:CB	12:AW:34:ASP:HB2	2.33	0.57
6:BN:48:MET:HE2	6:BN:48:MET:HA	1.85	0.57
11:AV:72:CYS:O	12:AW:541:ALA:HB2	2.03	0.57
14:AY:211:ALA:HB1	14:AY:212:ASN:CA	2.33	0.57
12:AW:108:GLU:HA	12:AW:147:PRO:HG2	1.86	0.57
12:AW:220:ARG:HD3	12:AW:235:LEU:HB3	1.86	0.57
12:BA:417:VAL:HG11	12:BA:464:LEU:HD21	1.85	0.57
11:BG:64:LEU:HG	11:BG:114:LYS:CG	2.34	0.57
7:AR:1111:ILE:HD12	7:AR:1111:ILE:N	2.19	0.57
12:AW:838:VAL:HB	12:AW:847:GLN:HB2	1.87	0.57
13:AX:17:GLN:HG3	13:AX:18:LEU:H	1.68	0.57
12:BA:108:GLU:HA	12:BA:147:PRO:HG2	1.87	0.57
12:AW:683:GLU:CA	12:AW:684:LEU:HB3	2.33	0.57
14:BC:192:LYS:CB	14:BC:193:LEU:HB2	2.34	0.57
14:BC:211:ALA:CB	14:BC:213:ILE:HG12	2.34	0.57
6:BN:14:ILE:HD11	6:BN:45:CYS:HB3	1.86	0.57
13:BP:17:GLN:HG3	13:BP:18:LEU:H	1.69	0.57
7:AR:1014:ILE:O	7:AR:1015:LEU:HB3	2.05	0.57
14:AY:277:ILE:O	14:AY:278:ARG:HB3	2.04	0.57
7:BB:323:SER:HA	7:BB:326:ILE:HD11	1.86	0.57
10:BF:91:SER:CB	10:BF:92:ASN:HA	2.35	0.57
7:AR:196:THR:O	7:AR:197:ALA:CB	2.53	0.57
11:AV:20:ARG:HA	11:AV:27:SER:HA	1.87	0.57
12:BA:838:VAL:HB	12:BA:847:GLN:HB2	1.87	0.57
6:BN:64:ARG:HB2	6:BN:65:PRO:HD3	1.85	0.57
6:AO:64:ARG:HB2	6:AO:65:PRO:HD3	1.85	0.57
7:AR:406:TRP:HA	7:AR:407:VAL:CG2	2.35	0.57
11:AV:101:LEU:HD22	11:AV:102:LEU:N	2.19	0.57
12:AW:417:VAL:HG11	12:AW:464:LEU:HD21	1.85	0.56
12:BA:79:ARG:HB3	12:BA:266:TRP:CZ3	2.40	0.56
7:BB:734:GLY:CA	7:BB:735:TYR:CB	2.83	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:BB:1082:CYS:HB2	7:BB:1083:PRO:HD2	1.86	0.56
4:AJ:48:THR:HG21	12:AW:125:TRP:CZ2	2.40	0.56
7:AR:1067:CYS:SG	7:AR:1085:HIS:HE1	2.21	0.56
12:BA:70:GLY:O	12:BA:71:HIS:HB2	2.05	0.56
12:BA:372:TRP:CB	12:BA:373:PRO:HD3	2.32	0.56
12:BA:683:GLU:CA	12:BA:684:LEU:HB3	2.34	0.56
10:AU:58:GLU:HB3	10:AU:103:ILE:HG21	1.86	0.56
11:AV:79:THR:HB	11:AV:80:GLU:CB	2.36	0.56
14:AY:149:ILE:HD13	14:AY:230:LYS:HB2	1.87	0.56
14:BC:211:ALA:HB1	14:BC:212:ASN:CB	2.35	0.56
14:BC:277:ILE:O	14:BC:278:ARG:HB3	2.04	0.56
10:BF:58:GLU:HB3	10:BF:103:ILE:HG21	1.86	0.56
10:AU:91:SER:CB	10:AU:92:ASN:CA	2.83	0.56
12:BA:28:ILE:HD12	12:BA:44:VAL:HA	1.88	0.56
9:BE:113:ILE:HG22	9:BE:114:THR:HG23	1.86	0.56
6:BN:3:ILE:HG22	6:BN:52:HIS:CG	2.41	0.56
2:BS:2:DA:H2'	2:BS:3:DT:C5'	2.36	0.56
9:AT:113:ILE:HG22	9:AT:114:THR:HG23	1.86	0.56
11:AV:64:LEU:HG	11:AV:114:LYS:CG	2.35	0.56
12:AW:99:ARG:O	12:AW:100:ARG:HB3	2.05	0.56
7:BB:406:TRP:HA	7:BB:407:VAL:CG2	2.35	0.56
7:AR:1046:MET:HE2	7:AR:1046:MET:HA	1.88	0.56
9:AT:82:GLN:O	10:AU:87:LEU:HG	2.05	0.56
12:AW:28:ILE:HD12	12:AW:44:VAL:HA	1.87	0.56
12:AW:525:LEU:HD21	12:AW:551:VAL:HG23	1.86	0.56
12:BA:687:ILE:HG21	12:BA:690:ARG:HB2	1.87	0.56
10:AU:91:SER:CB	10:AU:92:ASN:HA	2.35	0.56
12:AW:683:GLU:HA	12:AW:684:LEU:CB	2.32	0.56
12:BA:541:ALA:HB3	12:BA:542:PRO:HD3	1.88	0.56
12:BA:220:ARG:HD3	12:BA:235:LEU:HB3	1.86	0.56
7:BB:227:VAL:CG1	7:BB:262:ALA:HB3	2.36	0.56
11:BG:20:ARG:HA	11:BG:27:SER:HA	1.87	0.56
6:BN:8:PHE:O	6:BN:9:THR:HB	2.05	0.56
6:AO:8:PHE:O	6:AO:9:THR:HB	2.05	0.56
7:AR:227:VAL:CG1	7:AR:262:ALA:HB3	2.36	0.56
14:AY:211:ALA:HB1	14:AY:212:ASN:CB	2.35	0.56
12:BA:33:TYR:N	12:BA:34:ASP:HB2	2.21	0.56
7:BB:833:GLN:N	7:BB:834:ALA:CB	2.69	0.56
14:BC:126:LEU:HB3	14:BC:130:TYR:HB2	1.86	0.56
8:BD:257:GLU:HB2	5:BL:73:ILE:HG21	1.88	0.56
10:BF:91:SER:CB	10:BF:92:ASN:CA	2.83	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:AW:33:TYR:N	12:AW:34:ASP:HB2	2.20	0.56
12:AW:79:ARG:HB3	12:AW:266:TRP:CZ3	2.41	0.56
12:AW:687:ILE:HG21	12:AW:690:ARG:HB2	1.87	0.56
15:AZ:43:PRO:O	15:AZ:44:TRP:HB2	2.06	0.56
12:BA:525:LEU:HD21	12:BA:551:VAL:HG23	1.86	0.56
7:BB:352:LEU:HD12	7:BB:406:TRP:NE1	2.21	0.56
7:AR:284:LYS:O	7:AR:285:ARG:C	2.49	0.55
7:AR:734:GLY:CA	7:AR:735:TYR:CB	2.83	0.55
12:BA:47:PRO:HB2	12:BA:59:PRO:CG	2.37	0.55
7:BB:41:LYS:O	7:BB:42:LEU:HB3	2.05	0.55
14:BC:146:TYR:HA	14:BC:233:GLY:HA3	1.88	0.55
11:BG:78:VAL:O	11:BG:79:THR:HG23	2.06	0.55
15:BH:43:PRO:O	15:BH:44:TRP:HB2	2.06	0.55
6:BN:8:PHE:O	6:BN:9:THR:CB	2.54	0.55
6:AO:3:ILE:HG22	6:AO:52:HIS:CG	2.41	0.55
7:AR:1053:LEU:HD23	7:AR:1053:LEU:C	2.31	0.55
7:BB:39:ARG:HG3	7:BB:40:ASN:N	2.22	0.55
7:BB:1053:LEU:HD23	7:BB:1053:LEU:C	2.30	0.55
2:BS:2:DA:C2'	2:BS:3:DT:C5'	2.85	0.55
4:AJ:36:LEU:O	4:AJ:37:SER:HB2	2.06	0.55
11:AV:18:ILE:HG22	11:AV:29:ILE:HG23	1.88	0.55
12:BA:99:ARG:O	12:BA:100:ARG:HB3	2.05	0.55
12:BA:146:CYS:HB2	12:BA:151:GLU:HA	1.87	0.55
12:BA:763:THR:O	12:BA:764:ARG:HB3	2.06	0.55
7:BB:596:ASP:HA	7:BB:599:LYS:HG2	1.88	0.55
7:BB:1046:MET:HE2	7:BB:1046:MET:HA	1.88	0.55
9:BE:145:ARG:NH2	10:BF:86:ILE:HD11	2.21	0.55
11:BG:79:THR:HB	11:BG:80:GLU:CB	2.36	0.55
7:BB:284:LYS:O	7:BB:285:ARG:C	2.49	0.55
14:BC:176:ASP:N	14:BC:177:LYS:HB2	2.21	0.55
9:AT:56:GLU:HG2	14:AY:391:ARG:HG2	1.88	0.55
11:AV:101:LEU:O	11:AV:105:ILE:HG12	2.06	0.55
12:AW:763:THR:O	12:AW:764:ARG:HB3	2.05	0.55
12:BA:416:VAL:HG21	12:BA:477:LYS:HB2	1.89	0.55
7:AR:323:SER:HA	7:AR:326:ILE:HD11	1.87	0.55
11:AV:78:VAL:O	11:AV:79:THR:HG23	2.06	0.55
14:AY:146:TYR:HA	14:AY:233:GLY:HA3	1.88	0.55
14:BC:149:ILE:HD13	14:BC:230:LYS:HB2	1.87	0.55
4:BQ:36:LEU:HD13	4:BQ:41:ILE:HD11	1.89	0.55
6:AO:8:PHE:O	6:AO:9:THR:CB	2.54	0.55
7:AR:596:ASP:HA	7:AR:599:LYS:HG2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:AW:423:PRO:HB2	12:AW:425:LEU:CD1	2.37	0.55
12:BA:353:ILE:HD11	12:BA:407:VAL:HG23	1.89	0.55
11:BG:18:ILE:HG22	11:BG:29:ILE:HG23	1.89	0.55
4:AJ:36:LEU:HD13	4:AJ:41:ILE:HD11	1.89	0.55
7:AR:916:HIS:CD2	12:AW:500:GLN:HB2	2.42	0.55
14:AY:176:ASP:N	14:AY:177:LYS:HB2	2.21	0.55
15:AZ:43:PRO:HB2	15:AZ:79:ARG:HG2	1.89	0.55
7:BB:734:GLY:HA3	7:BB:735:TYR:CD2	2.42	0.55
7:BB:1014:ILE:O	7:BB:1015:LEU:HB3	2.05	0.55
13:BP:5:ARG:HA	13:BP:6:CYS:SG	2.47	0.55
12:AW:106:ILE:CG2	12:AW:143:ALA:HB3	2.37	0.55
12:AW:353:ILE:HD11	12:AW:407:VAL:HG23	1.88	0.55
7:BB:196:THR:HG21	7:BB:302:PRO:HB2	1.88	0.55
7:BB:1061:ILE:HG23	7:BB:1070:ILE:HD13	1.89	0.55
10:BF:78:ILE:H	10:BF:78:ILE:HD13	1.72	0.55
15:BH:42:LEU:HB3	15:BH:43:PRO:HD2	1.88	0.55
12:AW:47:PRO:HB2	12:AW:59:PRO:CG	2.36	0.54
12:AW:70:GLY:O	12:AW:71:HIS:HB2	2.05	0.54
7:BB:874:ILE:HG23	7:BB:875:PRO:HD2	1.89	0.54
7:AR:1066:GLN:HG3	7:AR:1085:HIS:CE1	2.41	0.54
10:AU:78:ILE:HD13	10:AU:78:ILE:H	1.72	0.54
14:AY:176:ASP:HB2	14:AY:177:LYS:HD2	1.90	0.54
7:BB:196:THR:O	7:BB:197:ALA:CB	2.54	0.54
7:BB:732:PHE:CD1	7:BB:733:THR:HB	2.43	0.54
7:BB:854:LEU:HD23	7:BB:854:LEU:C	2.33	0.54
7:AR:39:ARG:HG3	7:AR:40:ASN:N	2.22	0.54
7:AR:196:THR:HG21	7:AR:302:PRO:HB2	1.88	0.54
14:AY:140:VAL:O	14:AY:144:LEU:HG	2.08	0.54
8:BD:180:ALA:HA	8:BD:188:PHE:HB2	1.89	0.54
9:BE:125:GLY:C	9:BE:126:ILE:HG23	2.32	0.54
11:BG:101:LEU:O	11:BG:105:ILE:HG12	2.07	0.54
7:AR:30:HIS:HB3	7:AR:125:MET:HE1	1.89	0.54
7:AR:41:LYS:O	7:AR:42:LEU:HB3	2.06	0.54
7:AR:935:TYR:CD2	7:AR:956:LEU:HD22	2.43	0.54
8:AS:250:ILE:O	8:AS:253:ILE:HG22	2.08	0.54
10:AU:76:CYS:HB2	10:AU:104:ILE:HG23	1.90	0.54
12:BA:441:LEU:HD22	7:BB:1004:ILE:HD13	1.89	0.54
9:BE:164:MET:HB3	9:BE:170:GLY:HA2	1.89	0.54
4:BQ:36:LEU:O	4:BQ:37:SER:HB2	2.06	0.54
11:AV:88:ASN:HB2	12:AW:538:ALA:HB1	1.88	0.54
12:BA:574:LEU:HD23	12:BA:575:CYS:N	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:BB:852:LEU:HB3	7:BB:868:ARG:HG2	1.88	0.54
7:BB:906:GLY:HA2	8:BD:163:ILE:HD11	1.88	0.54
7:BB:935:TYR:CD2	7:BB:956:LEU:HD22	2.43	0.54
9:BE:102:GLY:O	10:BF:36:ARG:HD3	2.06	0.54
12:BA:238:LYS:HE2	12:BA:275:THR:HB	1.90	0.54
14:BC:176:ASP:HB2	14:BC:177:LYS:HD2	1.90	0.54
11:BG:16:ASN:O	11:BG:17:SER:CB	2.56	0.54
7:AR:380:ARG:CB	7:AR:381:LYS:HA	2.36	0.54
7:AR:406:TRP:CA	7:AR:407:VAL:CB	2.85	0.54
8:AS:180:ALA:HA	8:AS:188:PHE:HB2	1.89	0.54
9:AT:125:GLY:C	9:AT:126:ILE:HG23	2.32	0.54
12:AW:823:LEU:CD1	14:AY:75:ALA:HB1	2.37	0.54
7:BB:566:ILE:HD13	7:BB:568:GLU:CD	2.33	0.54
14:BC:294:ILE:HD13	14:BC:314:LEU:HD23	1.90	0.54
10:BF:76:CYS:HB2	10:BF:104:ILE:HG23	1.90	0.54
2:AD:14:DA:H5'	12:AW:818:TYR:OH	2.08	0.54
5:AM:79:MET:SD	8:AS:21:PRO:HD2	2.48	0.54
7:AR:230:MET:HE2	7:AR:230:MET:HA	1.89	0.54
7:AR:1040:ILE:HD11	14:AY:373:ILE:CD1	2.38	0.54
7:AR:1061:ILE:HG23	7:AR:1070:ILE:HD13	1.90	0.54
12:AW:842:TYR:CZ	14:AY:339:ASN:O	2.61	0.54
14:AY:294:ILE:HD13	14:AY:314:LEU:HD23	1.90	0.54
12:BA:284:LEU:HD22	12:BA:285:PRO:HD2	1.90	0.54
14:BC:140:VAL:O	14:BC:144:LEU:HG	2.08	0.54
8:BD:250:ILE:O	8:BD:253:ILE:HG22	2.08	0.54
9:AT:56:GLU:HG2	14:AY:391:ARG:CG	2.38	0.54
11:AV:16:ASN:O	11:AV:17:SER:CB	2.56	0.54
12:AW:283:GLY:CA	12:AW:284:LEU:HB2	2.38	0.54
12:BA:692:LEU:N	12:BA:692:LEU:HD12	2.23	0.54
7:BB:230:MET:HE2	7:BB:230:MET:HA	1.88	0.54
7:AR:833:GLN:N	7:AR:834:ALA:CB	2.69	0.54
7:AR:953:ILE:HD13	7:AR:953:ILE:N	2.23	0.54
11:AV:34:ASN:O	11:AV:35:ASP:HB2	2.07	0.54
12:AW:547:THR:HG23	12:AW:550:GLN:HB2	1.90	0.54
14:AY:120:PRO:HG2	14:AY:255:GLY:HA2	1.89	0.54
15:AZ:42:LEU:HB3	15:AZ:43:PRO:HD2	1.88	0.54
7:BB:30:HIS:HB3	7:BB:125:MET:HE1	1.89	0.54
7:AR:734:GLY:HA3	7:AR:735:TYR:CD2	2.42	0.53
9:AT:114:THR:HG21	9:AT:134:LYS:HD3	1.91	0.53
9:AT:164:MET:HB3	9:AT:170:GLY:HA2	1.89	0.53
11:AV:72:CYS:SG	11:AV:114:LYS:HD2	2.48	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:AW:692:LEU:HD12	12:AW:692:LEU:N	2.23	0.53
14:AY:322:ARG:O	14:AY:323:THR:HB	2.08	0.53
7:BB:953:ILE:N	7:BB:953:ILE:HD13	2.24	0.53
11:BG:72:CYS:SG	11:BG:114:LYS:HD2	2.49	0.53
12:BA:105:LYS:CE	12:BA:195:LEU:HD21	2.39	0.53
12:BA:106:ILE:CG2	12:BA:143:ALA:HB3	2.37	0.53
14:BC:120:PRO:HG2	14:BC:255:GLY:HA2	1.90	0.53
7:AR:352:LEU:HD12	7:AR:406:TRP:NE1	2.22	0.53
7:AR:566:ILE:HD13	7:AR:568:GLU:CD	2.34	0.53
7:AR:854:LEU:HD23	7:AR:854:LEU:C	2.33	0.53
12:AW:102:GLY:O	12:AW:103:ARG:C	2.52	0.53
12:AW:238:LYS:HE2	12:AW:275:THR:HB	1.90	0.53
12:AW:284:LEU:HD22	12:AW:285:PRO:HD2	1.90	0.53
12:AW:451:PRO:N	12:AW:452:PRO:HD2	2.23	0.53
7:AR:732:PHE:CD1	7:AR:733:THR:HB	2.43	0.53
7:AR:1064:CYS:HB3	7:AR:1067:CYS:HB2	1.91	0.53
8:AS:197:VAL:HG11	8:AS:200:GLU:HB2	1.91	0.53
12:AW:27:ILE:HG22	12:AW:74:HIS:CE1	2.44	0.53
12:AW:146:CYS:SG	12:AW:154:PHE:CZ	3.01	0.53
12:AW:416:VAL:HG21	12:AW:477:LYS:HB2	1.89	0.53
14:BC:101:THR:C	14:BC:102:LEU:HD22	2.33	0.53
14:BC:322:ARG:O	14:BC:323:THR:HB	2.08	0.53
2:AD:15:DT:H1'	2:AD:16:DA:P	2.48	0.53
7:AR:852:LEU:HB3	7:AR:868:ARG:HG2	1.89	0.53
12:AW:574:LEU:HD23	12:AW:575:CYS:N	2.23	0.53
12:BA:27:ILE:HG22	12:BA:74:HIS:CE1	2.44	0.53
12:BA:547:THR:HG23	12:BA:550:GLN:HB2	1.90	0.53
7:AR:108:ASN:O	7:AR:109:ASN:HB2	2.09	0.53
14:AY:101:THR:C	14:AY:102:LEU:HD22	2.33	0.53
12:BA:237:HIS:O	12:BA:240:VAL:HB	2.09	0.53
12:BA:283:GLY:CA	12:BA:284:LEU:CB	2.86	0.53
8:BD:197:VAL:HG11	8:BD:200:GLU:HB2	1.91	0.53
3:BK:91:SER:O	3:BK:92:LEU:HB2	2.09	0.53
14:AY:214:ASP:HB2	14:AY:215:SER:HA	1.89	0.53
12:BA:283:GLY:CA	12:BA:284:LEU:HB2	2.39	0.53
12:BA:451:PRO:N	12:BA:452:PRO:HD2	2.23	0.53
14:BC:214:ASP:HB2	14:BC:215:SER:HA	1.89	0.53
5:BL:83:TYR:CZ	5:BL:87:ILE:HD11	2.43	0.53
7:AR:190:ALA:HB2	7:AR:325:VAL:HG22	1.91	0.53
13:AX:5:ARG:HA	13:AX:6:CYS:SG	2.48	0.53
12:BA:868:VAL:HG12	14:BC:35:LEU:CD1	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:BB:1067:CYS:SG	7:BB:1085:HIS:HE1	2.27	0.53
2:BS:15:DT:H1'	2:BS:16:DA:P	2.49	0.53
9:AT:126:ILE:CG2	9:AT:137:GLN:HG2	2.39	0.53
11:AV:57:ALA:HA	11:AV:115:ILE:HD13	1.91	0.53
12:AW:105:LYS:CE	12:AW:195:LEU:HD21	2.39	0.53
12:AW:284:LEU:HD22	12:AW:285:PRO:CD	2.39	0.53
12:BA:98:CYS:O	12:BA:101:CYS:SG	2.67	0.53
7:BB:406:TRP:CA	7:BB:407:VAL:CB	2.85	0.53
9:BE:114:THR:HG21	9:BE:134:LYS:HD3	1.91	0.53
9:BE:126:ILE:HD11	9:BE:128:PHE:CD1	2.44	0.53
15:BH:43:PRO:HB2	15:BH:79:ARG:HG2	1.90	0.53
1:BR:13:DT:H1'	1:BR:14:DC:P	2.49	0.53
7:AR:133:ILE:HD13	7:AR:136:TYR:CE2	2.44	0.53
7:AR:874:ILE:HG23	7:AR:875:PRO:HD2	1.90	0.53
14:BC:154:SER:HB3	14:BC:170:ASP:HB2	1.91	0.53
6:BN:64:ARG:HB2	6:BN:65:PRO:CD	2.39	0.53
2:BS:2:DA:H2"	2:BS:3:DT:H5"	1.89	0.53
5:AM:83:TYR:CZ	5:AM:87:ILE:HD11	2.44	0.52
6:AO:47:ARG:NH1	7:AR:726:ILE:CD1	2.72	0.52
7:AR:734:GLY:N	7:AR:735:TYR:HB2	2.24	0.52
7:AR:1064:CYS:HA	7:AR:1091:LEU:CD2	2.39	0.52
12:BA:97:THR:HA	12:BA:103:ARG:CZ	2.39	0.52
12:BA:549:LYS:HD2	12:BA:593:LEU:HD22	1.91	0.52
7:BB:1064:CYS:SG	7:BB:1067:CYS:HB2	2.48	0.52
9:BE:126:ILE:CG2	9:BE:137:GLN:HG2	2.39	0.52
7:AR:52:ILE:CB	7:AR:53:PRO:CD	2.86	0.52
12:AW:147:PRO:O	12:AW:148:HIS:HB2	2.10	0.52
12:AW:160:LYS:HB3	12:AW:161:PRO:CD	2.40	0.52
12:BA:101:CYS:SG	12:BA:152:LYS:HG3	2.49	0.52
12:BA:284:LEU:HD22	12:BA:285:PRO:CD	2.39	0.52
7:BB:108:ASN:O	7:BB:109:ASN:HB2	2.09	0.52
7:BB:918:LEU:H	7:BB:919:PRO:HD2	1.74	0.52
14:BC:70:ILE:HA	14:BC:73:VAL:HG22	1.91	0.52
4:AJ:44:LEU:HD21	15:AZ:59:PRO:CB	2.39	0.52
12:AW:237:HIS:O	12:AW:240:VAL:HB	2.10	0.52
15:AZ:45:ILE:HG13	15:AZ:79:ARG:CB	2.40	0.52
7:BB:665:GLN:HG2	7:BB:667:PRO:HD2	1.91	0.52
7:BB:1064:CYS:HA	7:BB:1091:LEU:CD2	2.39	0.52
14:BC:104:LEU:N	14:BC:105:PRO:CD	2.73	0.52
8:AS:78:TRP:HB3	8:AS:79:PRO:HD2	1.91	0.52
11:AV:63:ARG:C	11:AV:64:LEU:HD22	2.35	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:AY:322:ARG:O	14:AY:323:THR:CB	2.57	0.52
7:BB:52:ILE:CB	7:BB:53:PRO:CD	2.86	0.52
7:BB:52:ILE:CG2	7:BB:53:PRO:HD3	2.39	0.52
7:BB:133:ILE:HD13	7:BB:136:TYR:CE2	2.45	0.52
7:BB:190:ALA:HB2	7:BB:325:VAL:HG22	1.90	0.52
7:BB:233:LEU:HD11	7:BB:311:ARG:C	2.34	0.52
11:BG:34:ASN:O	11:BG:35:ASP:HB2	2.07	0.52
12:AW:40:ILE:HG22	12:AW:41:GLU:N	2.24	0.52
14:BC:165:ILE:HD13	14:BC:223:ARG:HB2	1.92	0.52
15:BH:45:ILE:HG13	15:BH:79:ARG:CB	2.39	0.52
15:BH:59:PRO:CB	4:BQ:44:LEU:HD21	2.39	0.52
6:AO:64:ARG:HB2	6:AO:65:PRO:CD	2.39	0.52
7:AR:233:LEU:HD11	7:AR:311:ARG:C	2.35	0.52
7:AR:372:LEU:HD23	7:AR:387:LEU:HD13	1.92	0.52
12:AW:65:LEU:HD23	12:AW:65:LEU:C	2.34	0.52
12:AW:97:THR:HA	12:AW:103:ARG:CZ	2.39	0.52
14:AY:124:ILE:HB	14:AY:251:ILE:HB	1.92	0.52
12:BA:102:GLY:O	12:BA:103:ARG:C	2.52	0.52
7:BB:220:VAL:O	7:BB:221:PRO:C	2.53	0.52
7:AR:1064:CYS:SG	7:AR:1067:CYS:HB2	2.49	0.52
9:AT:126:ILE:HD11	9:AT:128:PHE:CD1	2.45	0.52
9:AT:136:ILE:HG12	9:AT:171:LYS:HB2	1.92	0.52
12:BA:65:LEU:HD23	12:BA:65:LEU:C	2.34	0.52
12:BA:108:GLU:HG3	12:BA:147:PRO:CG	2.40	0.52
12:BA:160:LYS:HB3	12:BA:161:PRO:CD	2.40	0.52
12:BA:851:GLY:O	12:BA:852:ASP:HB2	2.09	0.52
7:BB:170:LEU:HD23	7:BB:171:ALA:N	2.25	0.52
11:BG:36:PHE:CD1	11:BG:96:ILE:HD13	2.44	0.52
7:AR:72:ARG:HB3	7:AR:82:GLU:HA	1.92	0.52
7:AR:220:VAL:O	7:AR:221:PRO:C	2.53	0.52
7:AR:1080:TYR:HB3	7:AR:1091:LEU:HD12	1.92	0.52
12:AW:108:GLU:HG3	12:AW:147:PRO:CG	2.40	0.52
12:AW:851:GLY:O	12:AW:852:ASP:HB2	2.08	0.52
12:BA:532:ILE:HD13	12:BA:554:ALA:HB1	1.90	0.52
6:AO:5:ILE:HD11	8:AS:61:ARG:CZ	2.40	0.52
7:AR:52:ILE:CG2	7:AR:53:PRO:HD3	2.39	0.52
11:AV:36:PHE:CD1	11:AV:96:ILE:HD13	2.45	0.52
12:AW:283:GLY:CA	12:AW:284:LEU:CB	2.86	0.52
12:BA:282:PRO:O	12:BA:284:LEU:HG	2.10	0.52
12:BA:548:GLY:HA2	12:BA:551:VAL:HG12	1.92	0.52
8:BD:93:TYR:CE1	8:BD:146:ARG:HG2	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AI:91:SER:O	3:AI:92:LEU:HB2	2.09	0.52
7:AR:170:LEU:HD23	7:AR:171:ALA:N	2.25	0.52
12:AW:549:LYS:HD2	12:AW:593:LEU:HD22	1.92	0.52
12:AW:763:THR:O	12:AW:764:ARG:CB	2.58	0.52
14:AY:154:SER:HB3	14:AY:170:ASP:HB2	1.91	0.52
12:BA:146:CYS:SG	12:BA:154:PHE:CE2	3.03	0.52
12:BA:606:GLN:O	12:BA:608:PRO:HD3	2.10	0.52
12:BA:687:ILE:HG13	12:BA:688:PRO:HD2	1.91	0.52
12:BA:691:THR:HG22	12:BA:692:LEU:N	2.25	0.52
7:BB:406:TRP:CB	7:BB:407:VAL:HB	2.40	0.52
11:BG:57:ALA:HA	11:BG:115:ILE:HD13	1.90	0.52
3:AI:75:PRO:HB3	14:AY:394:LEU:HD11	1.92	0.51
7:AR:406:TRP:HB3	7:AR:407:VAL:C	2.35	0.51
8:AS:93:TYR:CE1	8:AS:146:ARG:HG2	2.45	0.51
12:AW:282:PRO:O	12:AW:284:LEU:HG	2.09	0.51
12:BA:36:ASP:N	12:BA:37:GLY:CA	2.71	0.51
12:BA:40:ILE:HG22	12:BA:41:GLU:N	2.24	0.51
12:BA:868:VAL:HG12	14:BC:35:LEU:HD12	1.91	0.51
7:BB:736:ASN:HB3	7:BB:742:ILE:HG13	1.92	0.51
14:BC:322:ARG:O	14:BC:323:THR:CB	2.58	0.51
10:BF:62:ILE:O	10:BF:63:ILE:HB	2.11	0.51
11:BG:63:ARG:C	11:BG:64:LEU:HD22	2.34	0.51
6:AO:43:TYR:OH	7:AR:907:VAL:HG11	2.09	0.51
7:AR:421:ASN:C	7:AR:421:ASN:OD1	2.54	0.51
7:AR:736:ASN:HB3	7:AR:742:ILE:HG13	1.92	0.51
12:AW:548:GLY:HA2	12:AW:551:VAL:HG12	1.92	0.51
14:AY:104:LEU:N	14:AY:105:PRO:CD	2.73	0.51
12:BA:830:LEU:HD11	14:BC:319:VAL:HG21	1.92	0.51
12:BA:848:VAL:O	12:BA:849:ALA:CB	2.58	0.51
12:BA:868:VAL:CG1	14:BC:35:LEU:HD12	2.41	0.51
7:BB:72:ARG:HB3	7:BB:82:GLU:HA	1.91	0.51
7:BB:406:TRP:HB3	7:BB:407:VAL:C	2.35	0.51
7:BB:974:TYR:CE2	7:BB:981:LYS:HB3	2.46	0.51
7:AR:406:TRP:CB	7:AR:407:VAL:HB	2.40	0.51
7:AR:665:GLN:HG2	7:AR:667:PRO:HD2	1.91	0.51
12:BA:524:ILE:CG2	12:BA:634:VAL:HG13	2.41	0.51
7:BB:421:ASN:C	7:BB:421:ASN:OD1	2.54	0.51
7:BB:628:TYR:CE2	7:BB:640:HIS:CE1	2.98	0.51
7:BB:636:LEU:HD21	7:BB:643:LEU:HD12	1.92	0.51
9:BE:88:GLU:HG2	9:BE:89:VAL:N	2.26	0.51
9:BE:136:ILE:HG12	9:BE:171:LYS:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:BG:79:THR:O	11:BG:84:SER:HB2	2.11	0.51
7:AR:52:ILE:HG22	7:AR:53:PRO:N	2.26	0.51
7:AR:66:ILE:HG13	7:AR:101:LEU:HD23	1.92	0.51
7:AR:545:GLU:HG3	7:AR:546:ARG:N	2.24	0.51
12:BA:665:ILE:O	12:BA:668:ALA:HB3	2.11	0.51
7:BB:235:ILE:HD12	7:BB:235:ILE:N	2.26	0.51
11:BG:64:LEU:HD22	11:BG:64:LEU:N	2.25	0.51
7:AR:918:LEU:H	7:AR:919:PRO:HD2	1.74	0.51
9:AT:91:GLN:HA	9:AT:138:LYS:HE2	1.93	0.51
14:AY:348:GLU:CG	14:AY:349:VAL:N	2.74	0.51
12:BA:763:THR:O	12:BA:764:ARG:CB	2.58	0.51
10:BF:6:ILE:HD12	10:BF:6:ILE:N	2.25	0.51
7:AR:235:ILE:N	7:AR:235:ILE:HD12	2.26	0.51
7:AR:628:TYR:CE2	7:AR:640:HIS:CE1	2.98	0.51
7:AR:974:TYR:CE2	7:AR:981:LYS:HB3	2.46	0.51
10:AU:65:ARG:O	10:AU:69:ARG:HG3	2.11	0.51
11:AV:16:ASN:O	11:AV:17:SER:HB3	2.10	0.51
12:AW:502:TYR:CD1	12:AW:632:PHE:HB3	2.46	0.51
14:AY:70:ILE:HA	14:AY:73:VAL:HG22	1.91	0.51
14:AY:301:LEU:HD13	14:AY:308:VAL:CG1	2.41	0.51
12:BA:103:ARG:HG3	12:BA:187:VAL:HG13	1.93	0.51
7:BB:52:ILE:HG22	7:BB:53:PRO:N	2.26	0.51
7:BB:372:LEU:HD23	7:BB:387:LEU:HD13	1.92	0.51
7:BB:734:GLY:N	7:BB:735:TYR:HB2	2.24	0.51
7:BB:1080:TYR:HB3	7:BB:1091:LEU:HD12	1.92	0.51
14:BC:41:VAL:O	14:BC:42:LEU:C	2.53	0.51
7:AR:242:VAL:CG1	7:AR:252:GLN:HG3	2.41	0.51
10:AU:6:ILE:HD12	10:AU:6:ILE:N	2.25	0.51
11:AV:79:THR:O	11:AV:84:SER:HB2	2.11	0.51
12:AW:606:GLN:O	12:AW:608:PRO:HD3	2.11	0.51
12:AW:687:ILE:HG13	12:AW:688:PRO:HD2	1.91	0.51
12:AW:691:THR:HG22	12:AW:692:LEU:N	2.25	0.51
12:BA:147:PRO:O	12:BA:148:HIS:HB2	2.10	0.51
12:BA:363:GLN:O	12:BA:366:ILE:HG22	2.11	0.51
8:BD:78:TRP:HB3	8:BD:79:PRO:HD2	1.91	0.51
11:BG:16:ASN:O	11:BG:17:SER:HB3	2.10	0.51
4:AJ:77:LYS:O	4:AJ:81:ARG:HG2	2.11	0.51
8:AS:219:ILE:HD12	8:AS:219:ILE:N	2.26	0.51
9:AT:88:GLU:HG2	9:AT:89:VAL:N	2.26	0.51
12:AW:21:LYS:O	12:AW:24:VAL:HG13	2.11	0.51
12:AW:185:GLU:HA	12:AW:205:GLU:CG	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:AW:363:GLN:O	12:AW:366:ILE:HG22	2.11	0.51
14:AY:165:ILE:HD13	14:AY:223:ARG:HB2	1.91	0.51
14:AY:244:LYS:HB3	14:AY:249:TYR:CD1	2.46	0.51
12:BA:185:GLU:HA	12:BA:205:GLU:CG	2.41	0.51
7:BB:242:VAL:CG1	7:BB:252:GLN:HG3	2.41	0.51
4:BQ:77:LYS:O	4:BQ:81:ARG:HG2	2.11	0.51
2:AD:14:DA:C5	2:AD:15:DT:C7	2.94	0.51
4:AJ:54:LEU:HA	4:AJ:59:ILE:HG22	1.93	0.51
7:AR:364:PHE:CE1	7:AR:388:VAL:HG13	2.46	0.51
11:AV:88:ASN:HB2	12:AW:538:ALA:CB	2.40	0.51
12:AW:524:ILE:CG2	12:AW:634:VAL:HG13	2.41	0.51
12:AW:532:ILE:HD13	12:AW:554:ALA:HB1	1.91	0.51
12:AW:703:THR:HG22	12:AW:707:LEU:CD1	2.41	0.51
12:AW:765:THR:HG22	12:AW:766:LEU:HD22	1.92	0.51
6:AO:53:ILE:HD11	7:AR:701:PRO:HG2	1.92	0.51
12:AW:378:VAL:HG22	12:AW:386:ILE:HB	1.92	0.51
12:BA:502:TYR:CD1	12:BA:632:PHE:HB3	2.46	0.51
7:BB:734:GLY:HA3	7:BB:735:TYR:HB2	1.90	0.51
8:AS:153:HIS:O	8:AS:154:ALA:HB3	2.11	0.50
11:AV:64:LEU:HD22	11:AV:64:LEU:N	2.26	0.50
12:AW:17:ASP:HA	12:AW:20:ARG:HG2	1.93	0.50
9:BE:91:GLN:HA	9:BE:138:LYS:HE2	1.93	0.50
10:BF:65:ARG:O	10:BF:69:ARG:HG3	2.10	0.50
10:BF:78:ILE:HG12	10:BF:79:THR:N	2.26	0.50
4:BQ:54:LEU:HA	4:BQ:59:ILE:HG22	1.93	0.50
7:AR:636:LEU:HD21	7:AR:643:LEU:HD12	1.93	0.50
8:AS:41:ILE:HB	8:AS:63:ALA:HA	1.93	0.50
10:AU:62:ILE:O	10:AU:63:ILE:HB	2.11	0.50
10:AU:78:ILE:HG12	10:AU:79:THR:N	2.27	0.50
12:AW:84:VAL:HG11	12:AW:274:ALA:HB1	1.93	0.50
12:AW:104:VAL:HA	12:AW:191:ASP:OD2	2.12	0.50
12:AW:665:ILE:O	12:AW:668:ALA:HB3	2.11	0.50
12:AW:823:LEU:HD13	14:AY:75:ALA:HA	1.93	0.50
12:BA:106:ILE:HG12	12:BA:154:PHE:CZ	2.47	0.50
7:BB:66:ILE:HG13	7:BB:101:LEU:HD23	1.93	0.50
7:AR:631:LEU:CD2	12:AW:768:HIS:CD2	2.95	0.50
12:AW:70:GLY:O	12:AW:71:HIS:CB	2.59	0.50
12:BA:17:ASP:HA	12:BA:20:ARG:HG2	1.93	0.50
12:BA:104:VAL:HA	12:BA:191:ASP:OD2	2.12	0.50
12:BA:378:VAL:HG22	12:BA:386:ILE:HB	1.92	0.50
14:BC:124:ILE:HB	14:BC:251:ILE:HB	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AM:49:LEU:HD21	7:AR:893:MET:HE1	1.93	0.50
6:AO:35:LEU:HD13	6:AO:46:ARG:HG3	1.93	0.50
10:AU:60:SER:HA	10:AU:69:ARG:CZ	2.41	0.50
11:AV:94:THR:HG22	11:AV:96:ILE:HD11	1.93	0.50
11:AV:95:ILE:C	11:AV:96:ILE:HG13	2.37	0.50
12:AW:600:LYS:HG2	12:AW:600:LYS:O	2.11	0.50
12:AW:848:VAL:O	12:AW:849:ALA:CB	2.58	0.50
12:BA:703:THR:HG22	12:BA:707:LEU:CD1	2.41	0.50
12:BA:765:THR:HG22	12:BA:766:LEU:HD22	1.93	0.50
8:BD:219:ILE:HD12	8:BD:219:ILE:N	2.26	0.50
11:BG:99:PHE:CD2	11:BG:99:PHE:O	2.65	0.50
6:BN:35:LEU:HD13	6:BN:46:ARG:HG3	1.94	0.50
11:AV:79:THR:CB	11:AV:80:GLU:HB2	2.37	0.50
11:AV:106:ILE:O	11:AV:107:SER:HB2	2.12	0.50
12:BA:21:LYS:O	12:BA:24:VAL:HG13	2.11	0.50
12:BA:84:VAL:HG11	12:BA:274:ALA:HB1	1.93	0.50
7:BB:545:GLU:HG3	7:BB:546:ARG:N	2.24	0.50
15:BH:23:LEU:HD21	15:BH:64:ARG:HD2	1.93	0.50
7:AR:209:LYS:O	7:AR:210:ASP:CB	2.60	0.50
7:AR:658:ILE:HG12	7:AR:672:GLN:HG2	1.94	0.50
7:AR:774:ASP:O	7:AR:775:LYS:HB3	2.11	0.50
14:BC:13:LEU:HD23	14:BC:13:LEU:C	2.37	0.50
8:BD:41:ILE:HB	8:BD:63:ALA:HA	1.93	0.50
9:BE:121:ASP:C	9:BE:125:GLY:HA2	2.37	0.50
11:BG:106:ILE:O	11:BG:107:SER:HB2	2.11	0.50
2:AD:13:DG:OP1	14:AY:352:LYS:HE3	2.12	0.50
7:AR:406:TRP:HA	7:AR:407:VAL:HG23	1.94	0.50
7:AR:592:VAL:HG23	7:AR:615:LYS:HD3	1.93	0.50
10:AU:60:SER:HA	10:AU:69:ARG:NE	2.27	0.50
12:AW:101:CYS:SG	12:AW:152:LYS:HG3	2.52	0.50
12:BA:75:ILE:HD12	12:BA:243:VAL:HG22	1.94	0.50
7:BB:364:PHE:CE1	7:BB:388:VAL:HG13	2.46	0.50
7:BB:406:TRP:CG	7:BB:407:VAL:HB	2.47	0.50
7:BB:743:MET:HE3	7:BB:748:VAL:CG2	2.41	0.50
7:BB:900:MET:SD	7:BB:912:ILE:HD11	2.52	0.50
11:BG:95:ILE:C	11:BG:96:ILE:HG13	2.37	0.50
15:BH:45:ILE:HG13	15:BH:79:ARG:HB3	1.94	0.50
7:AR:228:ILE:HG23	7:AR:271:ALA:HB1	1.93	0.50
12:AW:91:TYR:CE1	12:AW:95:LYS:HD2	2.47	0.50
12:BA:402:ALA:HB1	12:BA:403:PRO:HD2	1.93	0.50
7:BB:54:THR:OG1	7:BB:55:GLU:N	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:BB:348:LEU:O	7:BB:352:LEU:HD23	2.12	0.50
14:BC:101:THR:HG22	14:BC:121:MET:HE1	1.94	0.50
11:BG:65:SER:CB	11:BG:66:TYR:CA	2.87	0.50
2:BS:14:DA:C5	2:BS:15:DT:C7	2.94	0.50
2:AD:16:DA:OP2	12:AW:814:SER:HB3	2.12	0.50
5:AM:23:THR:HG23	8:AS:27:ALA:HA	1.94	0.50
7:AR:406:TRP:CG	7:AR:407:VAL:HB	2.47	0.50
7:AR:448:LEU:HD22	12:AW:796:PHE:CZ	2.46	0.50
12:BA:70:GLY:O	12:BA:71:HIS:CB	2.59	0.50
7:BB:226:PHE:CZ	7:BB:230:MET:HG3	2.47	0.50
14:BC:81:PRO:CB	14:BC:306:LEU:HG	2.42	0.50
14:BC:244:LYS:HB3	14:BC:249:TYR:CD1	2.46	0.50
8:BD:153:HIS:O	8:BD:154:ALA:HB3	2.11	0.50
9:AT:82:GLN:OE1	10:AU:89:MET:SD	2.70	0.49
11:AV:96:ILE:HD12	11:AV:99:PHE:HB2	1.94	0.49
12:AW:106:ILE:HG12	12:AW:154:PHE:CZ	2.47	0.49
14:AY:13:LEU:C	14:AY:13:LEU:HD23	2.37	0.49
15:AZ:38:ARG:HB3	15:AZ:39:PRO:HD2	1.93	0.49
15:AZ:45:ILE:HG13	15:AZ:79:ARG:HB3	1.93	0.49
12:BA:33:TYR:H	12:BA:34:ASP:CB	2.25	0.49
12:BA:830:LEU:HD13	14:BC:315:LEU:HD21	1.94	0.49
7:BB:774:ASP:O	7:BB:775:LYS:HB3	2.12	0.49
14:BC:80:GLU:N	14:BC:81:PRO:HD3	2.27	0.49
10:BF:60:SER:HA	10:BF:69:ARG:NE	2.27	0.49
7:AR:348:LEU:O	7:AR:352:LEU:HD23	2.12	0.49
11:AV:77:ILE:CD1	11:AV:106:ILE:HG21	2.42	0.49
12:AW:747:LEU:HD22	12:AW:786:PHE:CE2	2.48	0.49
7:BB:730:ILE:HG23	7:BB:986:ILE:HD12	1.94	0.49
14:BC:301:LEU:HD13	14:BC:308:VAL:CG1	2.41	0.49
11:BG:94:THR:HG22	11:BG:96:ILE:HD11	1.93	0.49
3:AI:88:ILE:HD12	3:AI:88:ILE:N	2.27	0.49
7:AR:743:MET:HE3	7:AR:748:VAL:CG2	2.41	0.49
7:AR:900:MET:SD	7:AR:912:ILE:HD11	2.52	0.49
9:AT:166:GLN:HB3	9:AT:167:PRO:HD2	1.94	0.49
11:AV:99:PHE:CD2	11:AV:99:PHE:O	2.65	0.49
12:AW:75:ILE:HD12	12:AW:243:VAL:HG22	1.94	0.49
12:AW:402:ALA:HB1	12:AW:403:PRO:HD2	1.93	0.49
12:AW:440:GLY:HA3	12:AW:444:ARG:NH2	2.27	0.49
12:AW:450:CYS:C	12:AW:452:PRO:HD2	2.37	0.49
14:AY:80:GLU:N	14:AY:81:PRO:HD3	2.26	0.49
12:BA:450:CYS:C	12:BA:452:PRO:HD2	2.37	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:BB:1081:VAL:C	7:BB:1091:LEU:HD11	2.36	0.49
13:BP:7:GLY:HA3	13:BP:34:ILE:HD11	1.94	0.49
7:AR:138:LEU:HG	7:AR:148:PRO:HB3	1.94	0.49
9:AT:15:PRO:HD3	9:AT:65:ALA:HB2	1.94	0.49
9:AT:121:ASP:C	9:AT:125:GLY:HA2	2.37	0.49
12:AW:517:THR:O	12:AW:518:LYS:C	2.56	0.49
12:AW:868:VAL:HG13	14:AY:32:LEU:HD23	1.94	0.49
14:AY:102:LEU:HB2	14:AY:106:ARG:HB2	1.94	0.49
12:BA:105:LYS:HE2	12:BA:136:VAL:HG12	1.94	0.49
12:BA:600:LYS:O	12:BA:600:LYS:HG2	2.11	0.49
7:BB:592:VAL:HG23	7:BB:615:LYS:HD3	1.94	0.49
7:BB:968:ASP:O	7:BB:969:ALA:HB3	2.12	0.49
9:BE:8:ARG:HG2	9:BE:71:GLU:HG2	1.93	0.49
9:BE:15:PRO:HD3	9:BE:65:ALA:HB2	1.94	0.49
10:BF:60:SER:HA	10:BF:69:ARG:CZ	2.42	0.49
15:BH:38:ARG:HB3	15:BH:39:PRO:HD2	1.94	0.49
7:AR:733:THR:HG23	7:AR:735:TYR:HD2	1.76	0.49
7:AR:1081:VAL:C	7:AR:1091:LEU:HD11	2.37	0.49
13:AX:7:GLY:HA3	13:AX:34:ILE:HD11	1.95	0.49
15:AZ:23:LEU:HD21	15:AZ:64:ARG:HD2	1.93	0.49
7:BB:201:VAL:HG23	7:BB:218:PRO:HG2	1.94	0.49
7:BB:658:ILE:HG12	7:BB:672:GLN:HG2	1.94	0.49
11:BG:93:ILE:HG22	11:BG:94:THR:N	2.27	0.49
12:AW:118:TYR:O	12:AW:121:ILE:HG22	2.13	0.49
14:AY:349:VAL:HB	14:AY:353:HIS:CE1	2.47	0.49
12:BA:77:LEU:CD2	12:BA:77:LEU:N	2.76	0.49
12:BA:440:GLY:HA3	12:BA:444:ARG:NH2	2.27	0.49
12:BA:703:THR:HG22	12:BA:707:LEU:HD12	1.95	0.49
7:BB:138:LEU:HG	7:BB:148:PRO:HB3	1.94	0.49
7:BB:228:ILE:HG23	7:BB:271:ALA:HB1	1.94	0.49
7:BB:647:SER:N	7:BB:648:PRO:CD	2.75	0.49
11:BG:96:ILE:CD1	11:BG:99:PHE:HB2	2.42	0.49
7:AR:201:VAL:HG23	7:AR:218:PRO:HG2	1.94	0.49
7:AR:226:PHE:CZ	7:AR:230:MET:HG3	2.48	0.49
10:AU:88:ILE:O	10:AU:88:ILE:CG2	2.60	0.49
12:AW:103:ARG:HG3	12:AW:187:VAL:HG13	1.93	0.49
12:AW:105:LYS:HE2	12:AW:136:VAL:HG12	1.93	0.49
14:AY:101:THR:HG22	14:AY:121:MET:HE1	1.93	0.49
14:AY:176:ASP:CA	14:AY:177:LYS:HB2	2.42	0.49
14:AY:348:GLU:O	14:AY:349:VAL:HB	2.12	0.49
12:BA:118:TYR:O	12:BA:121:ILE:HG22	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:BA:131:ARG:NH1	4:BQ:36:LEU:HD21	2.26	0.49
14:BC:349:VAL:HB	14:BC:353:HIS:CE1	2.47	0.49
14:AY:209:SER:O	14:AY:210:PHE:CB	2.61	0.49
14:AY:366:PHE:O	14:AY:367:LYS:HB2	2.12	0.49
7:BB:380:ARG:CB	7:BB:381:LYS:HA	2.36	0.49
7:BB:733:THR:HG23	7:BB:735:TYR:HD2	1.77	0.49
14:BC:210:PHE:CE1	14:BC:214:ASP:O	2.66	0.49
14:BC:216:ILE:O	14:BC:217:ALA:HB2	2.12	0.49
1:AC:1:DT:H2"	1:AC:2:DC:C6	2.48	0.49
5:AM:82:HIS:CE1	5:AM:86:GLU:OE2	2.66	0.49
7:AR:647:SER:N	7:AR:648:PRO:CD	2.76	0.49
14:AY:41:VAL:O	14:AY:42:LEU:C	2.53	0.49
14:AY:85:MET:SD	14:AY:304:GLN:HG3	2.53	0.49
14:AY:210:PHE:CE1	14:AY:214:ASP:O	2.66	0.49
12:BA:91:TYR:CE1	12:BA:95:LYS:HD2	2.47	0.49
12:BA:393:ASP:O	12:BA:394:ARG:HB3	2.13	0.49
7:BB:904:VAL:HG23	7:BB:972:VAL:HG13	1.95	0.49
7:BB:952:PRO:O	7:BB:953:ILE:C	2.56	0.49
14:BC:176:ASP:CA	14:BC:177:LYS:HB2	2.42	0.49
14:BC:185:LYS:HA	14:BC:188:ILE:HD12	1.95	0.49
1:BR:1:DT:H2"	1:BR:2:DC:C6	2.48	0.49
4:AJ:37:SER:OG	4:AJ:39:GLN:HG2	2.13	0.49
5:AM:49:LEU:CD2	7:AR:893:MET:HE1	2.43	0.49
12:AW:703:THR:HG22	12:AW:707:LEU:HD12	1.95	0.49
14:AY:104:LEU:HD23	14:AY:104:LEU:C	2.38	0.49
12:BA:418:LEU:HD21	7:BB:1047:LEU:HD21	1.95	0.49
12:BA:842:TYR:CZ	14:BC:339:ASN:O	2.66	0.49
7:BB:874:ILE:CG2	7:BB:875:PRO:HD2	2.43	0.49
10:BF:88:ILE:O	10:BF:88:ILE:CG2	2.60	0.49
7:AR:53:PRO:CB	7:AR:54:THR:HB	2.39	0.48
7:AR:242:VAL:HG13	7:AR:252:GLN:HG3	1.95	0.48
7:AR:666:SER:N	7:AR:667:PRO:HD2	2.28	0.48
7:AR:730:ILE:HG23	7:AR:986:ILE:HD12	1.95	0.48
7:AR:748:VAL:HG13	7:AR:875:PRO:HG2	1.95	0.48
7:AR:874:ILE:CG2	7:AR:875:PRO:HD2	2.43	0.48
7:AR:952:PRO:O	7:AR:953:ILE:C	2.56	0.48
9:AT:30:LEU:HD22	9:AT:72:PHE:CE2	2.47	0.48
10:AU:100:ILE:O	10:AU:104:ILE:HG13	2.13	0.48
11:AV:43:ILE:HG22	11:AV:44:ASP:N	2.28	0.48
11:AV:93:ILE:HG22	11:AV:94:THR:N	2.27	0.48
12:AW:67:ASN:C	12:AW:69:PRO:HD3	2.38	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:AW:393:ASP:O	12:AW:394:ARG:HB3	2.13	0.48
12:AW:557:PRO:HG2	12:AW:619:TYR:CZ	2.48	0.48
7:BB:209:LYS:O	7:BB:210:ASP:CB	2.60	0.48
7:BB:406:TRP:HA	7:BB:407:VAL:HG23	1.94	0.48
7:BB:406:TRP:HB3	7:BB:407:VAL:O	2.13	0.48
7:BB:748:VAL:HG13	7:BB:875:PRO:HG2	1.95	0.48
9:BE:166:GLN:HB3	9:BE:167:PRO:HD2	1.94	0.48
11:BG:39:SER:HB3	11:BG:93:ILE:HB	1.94	0.48
11:BG:77:ILE:CD1	11:BG:106:ILE:HG21	2.42	0.48
11:BG:79:THR:CB	11:BG:80:GLU:HB2	2.38	0.48
7:AR:54:THR:OG1	7:AR:55:GLU:N	2.45	0.48
8:AS:96:ILE:HG12	8:AS:145:LEU:HD11	1.95	0.48
9:AT:56:GLU:CG	14:AY:391:ARG:HG2	2.42	0.48
12:AW:505:GLY:CA	12:AW:639:VAL:CG2	2.91	0.48
12:BA:281:ILE:CD1	12:BA:284:LEU:HD12	2.43	0.48
12:BA:281:ILE:HG13	12:BA:284:LEU:HD12	1.94	0.48
12:BA:743:MET:SD	7:BB:922:MET:HG2	2.53	0.48
12:BA:747:LEU:HD22	12:BA:786:PHE:CE2	2.48	0.48
7:BB:666:SER:N	7:BB:667:PRO:HD2	2.27	0.48
14:BC:348:GLU:O	14:BC:349:VAL:HB	2.13	0.48
14:BC:366:PHE:O	14:BC:367:LYS:HB2	2.12	0.48
11:BG:43:ILE:HG22	11:BG:44:ASP:N	2.28	0.48
5:BL:82:HIS:CE1	5:BL:86:GLU:OE2	2.66	0.48
7:AR:52:ILE:HG22	7:AR:53:PRO:CD	2.43	0.48
7:AR:136:TYR:HB2	7:AR:141:LEU:CD1	2.43	0.48
7:AR:323:SER:HA	7:AR:326:ILE:CG1	2.44	0.48
9:AT:66:THR:HG21	14:AY:392:PRO:HG3	1.95	0.48
12:AW:130:ARG:O	12:AW:134:GLU:HG2	2.13	0.48
12:AW:203:ARG:HB2	12:AW:206:TRP:CD2	2.48	0.48
14:AY:151:ASN:O	14:AY:173:MET:HG2	2.13	0.48
8:BD:96:ILE:HG12	8:BD:145:LEU:HD11	1.95	0.48
9:BE:30:LEU:HD22	9:BE:72:PHE:CE2	2.47	0.48
3:BK:88:ILE:HD12	3:BK:88:ILE:N	2.28	0.48
7:AR:35:ASN:O	7:AR:38:VAL:HG12	2.13	0.48
7:AR:1112:ILE:O	7:AR:1114:PRO:HD3	2.13	0.48
11:AV:96:ILE:CD1	11:AV:99:PHE:HB2	2.42	0.48
12:AW:33:TYR:H	12:AW:34:ASP:CB	2.25	0.48
12:AW:58:CYS:HB3	12:AW:62:GLY:H	1.79	0.48
13:AX:44:ILE:HD12	13:AX:44:ILE:N	2.28	0.48
14:AY:146:TYR:HB2	14:AY:234:ILE:O	2.13	0.48
7:BB:35:ASN:O	7:BB:38:VAL:HG12	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:BB:733:THR:CG2	7:BB:734:GLY:N	2.76	0.48
14:BC:85:MET:SD	14:BC:304:GLN:HG3	2.54	0.48
15:BH:63:ILE:HD13	15:BH:81:VAL:CG2	2.42	0.48
7:AR:1096:VAL:HG12	7:AR:1097:SER:N	2.28	0.48
12:AW:40:ILE:HD13	12:AW:47:PRO:CG	2.43	0.48
10:BF:106:ILE:O	10:BF:107:ILE:C	2.56	0.48
3:AI:79:ARG:HD2	14:AY:389:THR:CG2	2.44	0.48
7:AR:68:ILE:HD12	7:AR:68:ILE:N	2.29	0.48
7:AR:406:TRP:HB3	7:AR:407:VAL:O	2.13	0.48
7:AR:733:THR:CG2	7:AR:734:GLY:N	2.76	0.48
7:AR:904:VAL:HG23	7:AR:972:VAL:HG13	1.94	0.48
7:AR:968:ASP:O	7:AR:969:ALA:HB3	2.13	0.48
9:AT:8:ARG:HG2	9:AT:71:GLU:HG2	1.94	0.48
9:AT:134:LYS:HE3	9:AT:171:LYS:HB3	1.95	0.48
10:AU:106:ILE:O	10:AU:107:ILE:C	2.56	0.48
12:AW:868:VAL:HG12	14:AY:35:LEU:HD12	1.95	0.48
12:BA:203:ARG:HB2	12:BA:206:TRP:CD2	2.48	0.48
12:BA:505:GLY:CA	12:BA:639:VAL:CG2	2.91	0.48
12:BA:517:THR:O	12:BA:518:LYS:C	2.55	0.48
12:BA:557:PRO:HG2	12:BA:619:TYR:CZ	2.49	0.48
7:BB:584:ILE:HB	7:BB:591:LEU:HD12	1.96	0.48
7:BB:1112:ILE:O	7:BB:1114:PRO:HD3	2.14	0.48
14:BC:104:LEU:C	14:BC:104:LEU:HD23	2.39	0.48
14:BC:348:GLU:HG3	14:BC:349:VAL:N	2.28	0.48
10:BF:62:ILE:CD1	10:BF:100:ILE:HG12	2.44	0.48
11:BG:96:ILE:HD12	11:BG:99:PHE:HB2	1.94	0.48
1:AC:11:DT:H2"	1:AC:12:DA:C5'	2.44	0.48
9:AT:75:ILE:HG21	10:AU:21:LEU:HD11	1.93	0.48
12:AW:191:ASP:O	12:AW:195:LEU:HG	2.14	0.48
12:AW:738:LEU:C	12:AW:738:LEU:HD12	2.38	0.48
14:AY:185:LYS:HA	14:AY:188:ILE:HD12	1.95	0.48
15:AZ:63:ILE:HD13	15:AZ:81:VAL:CG2	2.43	0.48
7:BB:242:VAL:HG13	7:BB:252:GLN:HG3	1.95	0.48
7:BB:1096:VAL:HG12	7:BB:1097:SER:N	2.28	0.48
14:BC:209:SER:O	14:BC:210:PHE:CB	2.61	0.48
9:BE:126:ILE:HG13	9:BE:127:ILE:N	2.26	0.48
9:BE:134:LYS:HE3	9:BE:171:LYS:HB3	1.96	0.48
3:BK:53:ILE:O	3:BK:54:ASN:C	2.56	0.48
2:AD:14:DA:C5	2:AD:15:DT:H73	2.49	0.48
3:AI:53:ILE:O	3:AI:54:ASN:C	2.57	0.48
7:AR:760:LEU:C	7:AR:760:LEU:HD23	2.39	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:AW:33:TYR:CA	12:AW:34:ASP:HB2	2.44	0.48
12:AW:764:ARG:HD2	12:AW:769:PHE:O	2.14	0.48
14:AY:81:PRO:CB	14:AY:306:LEU:HG	2.42	0.48
14:AY:188:ILE:HG12	14:AY:230:LYS:NZ	2.29	0.48
14:AY:237:ILE:HG12	14:AY:238:LYS:N	2.29	0.48
7:BB:605:ILE:HG22	7:BB:609:ASP:HB2	1.96	0.48
7:BB:781:PRO:HA	7:BB:786:TYR:CZ	2.49	0.48
14:BC:151:ASN:O	14:BC:173:MET:HG2	2.13	0.48
5:BL:11:ASN:HB3	5:BL:59:THR:HG23	1.96	0.48
7:AR:191:LYS:HE2	7:AR:193:ILE:HD11	1.96	0.48
9:AT:126:ILE:HG12	9:AT:128:PHE:CE2	2.49	0.48
11:AV:39:SER:HB3	11:AV:93:ILE:HB	1.94	0.48
11:AV:102:LEU:HA	11:AV:105:ILE:HG12	1.96	0.48
12:AW:77:LEU:N	12:AW:77:LEU:CD2	2.76	0.48
12:AW:865:THR:HG22	14:AY:28:ILE:HD11	1.96	0.48
14:AY:216:ILE:O	14:AY:217:ALA:HB2	2.12	0.48
12:BA:738:LEU:C	12:BA:738:LEU:HD12	2.38	0.48
7:BB:422:TRP:CZ3	7:BB:426:LEU:HD11	2.49	0.48
4:BQ:37:SER:OG	4:BQ:39:GLN:HG2	2.13	0.48
8:AS:161:LEU:HD12	8:AS:163:ILE:HD13	1.95	0.48
10:AU:62:ILE:CD1	10:AU:100:ILE:HG12	2.44	0.48
12:AW:281:ILE:HG13	12:AW:284:LEU:HD12	1.95	0.48
14:AY:277:ILE:O	14:AY:278:ARG:CB	2.62	0.48
12:BA:47:PRO:O	12:BA:59:PRO:HD2	2.14	0.48
12:BA:541:ALA:HB3	12:BA:542:PRO:HD2	1.96	0.48
14:BC:277:ILE:O	14:BC:278:ARG:CB	2.62	0.48
7:AR:422:TRP:CZ3	7:AR:426:LEU:HD11	2.49	0.47
7:AR:605:ILE:HG22	7:AR:609:ASP:HB2	1.96	0.47
7:AR:781:PRO:HA	7:AR:786:TYR:CZ	2.49	0.47
8:AS:237:LYS:HE2	8:AS:237:LYS:HA	1.96	0.47
12:AW:185:GLU:HA	12:AW:205:GLU:HG2	1.95	0.47
12:AW:667:ARG:O	12:AW:670:VAL:HG22	2.14	0.47
12:BA:130:ARG:O	12:BA:134:GLU:HG2	2.14	0.47
7:BB:53:PRO:CB	7:BB:54:THR:HB	2.39	0.47
7:BB:403:THR:HG23	7:BB:405:ASN:N	2.29	0.47
14:BC:102:LEU:HB2	14:BC:106:ARG:HB2	1.94	0.47
8:BD:141:LEU:C	8:BD:141:LEU:HD12	2.39	0.47
10:BF:100:ILE:O	10:BF:104:ILE:HG13	2.14	0.47
12:AW:32:VAL:O	12:AW:44:VAL:HG21	2.14	0.47
14:AY:143:LYS:O	14:AY:234:ILE:HB	2.14	0.47
14:AY:157:SER:HB3	14:AY:166:ILE:HB	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:BA:33:TYR:HB3	12:BA:34:ASP:CB	2.44	0.47
12:BA:67:ASN:C	12:BA:69:PRO:HD3	2.38	0.47
12:BA:78:VAL:HG21	12:BA:249:LEU:HB3	1.96	0.47
12:BA:185:GLU:HA	12:BA:205:GLU:HG2	1.95	0.47
12:BA:864:LYS:HB3	12:BA:865:THR:C	2.39	0.47
7:BB:52:ILE:HG22	7:BB:53:PRO:CD	2.43	0.47
7:BB:68:ILE:N	7:BB:68:ILE:HD12	2.29	0.47
7:BB:918:LEU:HD13	7:BB:927:ILE:HD11	1.96	0.47
7:BB:1064:CYS:HB3	7:BB:1067:CYS:HB2	1.95	0.47
8:BD:237:LYS:HE2	8:BD:237:LYS:HA	1.96	0.47
9:BE:126:ILE:HG12	9:BE:128:PHE:CE2	2.49	0.47
13:BP:44:ILE:N	13:BP:44:ILE:HD12	2.29	0.47
5:AM:3:ILE:HD12	5:AM:3:ILE:N	2.29	0.47
9:AT:42:LEU:N	9:AT:42:LEU:HD12	2.30	0.47
12:AW:70:GLY:HA2	12:AW:216:PRO:CB	2.45	0.47
12:AW:78:VAL:HG21	12:AW:249:LEU:HB3	1.96	0.47
12:AW:122:LYS:HZ3	12:AW:125:TRP:CD1	2.32	0.47
12:AW:864:LYS:HB3	12:AW:865:THR:C	2.39	0.47
14:AY:245:LYS:HE2	14:AY:250:ILE:HD11	1.97	0.47
12:BA:40:ILE:HD13	12:BA:47:PRO:CG	2.43	0.47
12:BA:764:ARG:HD2	12:BA:769:PHE:O	2.14	0.47
12:BA:818:TYR:CD1	12:BA:818:TYR:C	2.92	0.47
7:BB:323:SER:HA	7:BB:326:ILE:CG1	2.44	0.47
7:BB:760:LEU:HD23	7:BB:760:LEU:C	2.39	0.47
14:BC:188:ILE:HG12	14:BC:230:LYS:NZ	2.29	0.47
14:BC:237:ILE:HG12	14:BC:238:LYS:N	2.29	0.47
11:BG:78:VAL:C	11:BG:79:THR:HG1	2.21	0.47
2:BS:14:DA:H1'	2:BS:15:DT:H5'	1.96	0.47
2:BS:14:DA:N7	2:BS:15:DT:H73	2.30	0.47
7:AR:356:LEU:HA	7:AR:407:VAL:CG1	2.44	0.47
9:AT:134:LYS:CE	9:AT:171:LYS:HB3	2.44	0.47
12:AW:238:LYS:HG2	12:AW:276:TYR:HA	1.97	0.47
12:BA:32:VAL:O	12:BA:44:VAL:HG21	2.14	0.47
12:BA:33:TYR:N	12:BA:34:ASP:CB	2.78	0.47
12:BA:191:ASP:O	12:BA:195:LEU:HG	2.14	0.47
7:BB:196:THR:HG22	7:BB:302:PRO:C	2.39	0.47
2:AD:5:DG:C2	2:AD:6:DA:C2	3.03	0.47
2:AD:14:DA:H1'	2:AD:15:DT:H5'	1.96	0.47
2:AD:14:DA:OP2	14:AY:348:GLU:CD	2.57	0.47
7:AR:1104:ILE:HG23	7:AR:1114:PRO:HG2	1.96	0.47
10:AU:95:TYR:CE1	10:AU:97:SER:HB2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:AW:107:SER:HB3	12:AW:140:ALA:HA	1.96	0.47
12:AW:281:ILE:CD1	12:AW:284:LEU:HD12	2.44	0.47
14:AY:331:ARG:O	14:AY:336:GLY:HA3	2.14	0.47
12:BA:33:TYR:CA	12:BA:34:ASP:HB2	2.44	0.47
12:BA:618:GLU:CD	12:BA:874:ARG:HD3	2.40	0.47
7:BB:53:PRO:CB	7:BB:54:THR:CA	2.89	0.47
8:BD:109:LEU:C	8:BD:109:LEU:HD23	2.40	0.47
11:BG:72:CYS:HB3	11:BG:114:LYS:HD2	1.96	0.47
4:AJ:39:GLN:OE1	4:AJ:78:ARG:CZ	2.63	0.47
7:AR:287:ASN:O	7:AR:291:LYS:N	2.48	0.47
7:AR:457:CYS:HB3	7:AR:460:GLU:HB2	1.96	0.47
9:AT:113:ILE:CG2	9:AT:136:ILE:HD12	2.45	0.47
14:AY:130:TYR:CD2	14:AY:136:LYS:HB3	2.50	0.47
14:AY:209:SER:O	14:AY:210:PHE:HB2	2.14	0.47
12:BA:456:ASP:OD1	12:BA:460:ASP:CG	2.48	0.47
12:BA:667:ARG:O	12:BA:670:VAL:HG22	2.14	0.47
7:BB:136:TYR:HB2	7:BB:141:LEU:CD1	2.44	0.47
14:BC:331:ARG:O	14:BC:336:GLY:HA3	2.14	0.47
7:AR:403:THR:HG23	7:AR:405:ASN:N	2.29	0.47
7:AR:734:GLY:HA3	7:AR:735:TYR:HB2	1.91	0.47
8:AS:141:LEU:C	8:AS:141:LEU:HD12	2.39	0.47
11:AV:61:LYS:O	11:AV:62:ASN:HB2	2.15	0.47
11:AV:101:LEU:HD22	11:AV:101:LEU:C	2.40	0.47
12:AW:33:TYR:HB3	12:AW:34:ASP:CB	2.44	0.47
12:AW:33:TYR:N	12:AW:34:ASP:CB	2.78	0.47
12:AW:47:PRO:O	12:AW:59:PRO:HD2	2.14	0.47
12:AW:146:CYS:HB3	12:AW:149:CYS:HB2	1.81	0.47
13:AX:24:VAL:O	13:AX:24:VAL:HG13	2.15	0.47
15:AZ:18:PRO:HB3	15:AZ:67:ARG:HB3	1.97	0.47
12:BA:70:GLY:HA2	12:BA:216:PRO:CB	2.44	0.47
12:BA:302:LEU:HD23	12:BA:308:ARG:HG3	1.95	0.47
12:BA:671:GLU:O	12:BA:674:ASN:OD1	2.33	0.47
7:BB:476:MET:HE2	7:BB:649:ALA:CB	2.45	0.47
14:BC:81:PRO:HB3	14:BC:306:LEU:HG	1.97	0.47
14:BC:130:TYR:CD2	14:BC:136:LYS:HB3	2.50	0.47
14:BC:143:LYS:O	14:BC:234:ILE:HB	2.14	0.47
14:BC:146:TYR:HB2	14:BC:234:ILE:O	2.14	0.47
14:BC:209:SER:O	14:BC:210:PHE:HB2	2.14	0.47
8:BD:150:GLY:HA2	8:BD:156:PHE:HB2	1.96	0.47
9:BE:42:LEU:N	9:BE:42:LEU:HD12	2.30	0.47
9:BE:113:ILE:CG2	9:BE:136:ILE:HD12	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:BF:75:ILE:C	10:BF:76:CYS:SG	2.98	0.47
11:BG:102:LEU:HA	11:BG:105:ILE:HG12	1.95	0.47
6:BN:19:GLN:HB3	6:BN:20:PRO:HD3	1.97	0.47
1:BR:11:DT:H2"	1:BR:12:DA:C5'	2.44	0.47
5:AM:11:ASN:HB3	5:AM:59:THR:HG23	1.96	0.47
12:AW:27:ILE:CG2	12:AW:74:HIS:CE1	2.98	0.47
12:AW:38:THR:N	12:AW:39:PRO:CD	2.78	0.47
12:AW:38:THR:N	12:AW:39:PRO:HD2	2.30	0.47
12:AW:145:VAL:HG13	12:AW:146:CYS:N	2.30	0.47
12:AW:618:GLU:CD	12:AW:874:ARG:HD3	2.40	0.47
7:BB:356:LEU:HA	7:BB:407:VAL:CG1	2.43	0.47
14:BC:245:LYS:HE2	14:BC:250:ILE:HD11	1.96	0.47
9:BE:169:LEU:C	9:BE:175:ILE:HD11	2.40	0.47
4:BQ:39:GLN:OE1	4:BQ:78:ARG:CZ	2.63	0.47
2:BS:14:DA:C5	2:BS:15:DT:H73	2.49	0.47
2:AD:14:DA:N7	2:AD:15:DT:H73	2.29	0.47
7:AR:476:MET:HE2	7:AR:649:ALA:CB	2.45	0.47
7:AR:953:ILE:HG12	7:AR:954:GLU:H	1.80	0.47
8:AS:133:LEU:HD21	8:AS:139:ILE:HG12	1.96	0.47
9:AT:126:ILE:HG13	9:AT:127:ILE:N	2.26	0.47
12:AW:492:GLY:HA3	12:AW:862:HIS:HA	1.97	0.47
12:BA:277:PHE:CZ	7:BB:1111:ILE:HD13	2.50	0.47
12:BA:627:LEU:HD11	12:BA:631:LEU:HD22	1.96	0.47
7:BB:905:LYS:HG3	7:BB:965:TYR:CE2	2.50	0.47
5:BL:3:ILE:HD12	5:BL:3:ILE:N	2.30	0.47
7:AR:208:LEU:HD11	7:AR:214:HIS:CD2	2.50	0.47
7:AR:584:ILE:HB	7:AR:591:LEU:HD12	1.95	0.47
7:AR:855:ILE:O	13:AX:34:ILE:HG22	2.14	0.47
12:AW:302:LEU:HD23	12:AW:308:ARG:HG3	1.95	0.47
12:AW:627:LEU:HD11	12:AW:631:LEU:HD22	1.95	0.47
12:BA:58:CYS:HB3	12:BA:62:GLY:H	1.78	0.47
12:BA:111:ILE:HG22	12:BA:112:GLU:N	2.30	0.47
12:BA:475:GLU:OE1	7:BB:1046:MET:HB2	2.15	0.47
12:BA:864:LYS:CD	12:BA:867:ASP:HA	2.45	0.47
2:AD:14:DA:OP2	14:AY:348:GLU:OE2	2.34	0.46
4:AJ:57:GLY:O	4:AJ:58:LYS:C	2.58	0.46
7:AR:196:THR:HG22	7:AR:302:PRO:C	2.39	0.46
7:AR:1096:VAL:CG1	7:AR:1097:SER:N	2.78	0.46
9:AT:82:GLN:NE2	10:AU:89:MET:HE1	2.30	0.46
12:AW:541:ALA:HB3	12:AW:542:PRO:HD2	1.96	0.46
14:AY:184:VAL:HG12	14:AY:188:ILE:HD11	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:BA:125:TRP:CZ2	4:BQ:48:THR:HG21	2.50	0.46
14:BC:184:VAL:HG12	14:BC:188:ILE:HD11	1.97	0.46
14:BC:394:LEU:HD22	14:BC:394:LEU:N	2.31	0.46
11:BG:101:LEU:HD22	11:BG:101:LEU:C	2.40	0.46
1:BR:11:DT:H2"	1:BR:12:DA:O5'	2.15	0.46
4:AJ:39:GLN:HG2	4:AJ:40:ASP:H	1.80	0.46
4:AJ:45:MET:HB2	12:AW:122:LYS:HE2	1.98	0.46
7:AR:8:LEU:N	7:AR:8:LEU:HD22	2.31	0.46
7:AR:592:VAL:CG2	7:AR:596:ASP:CG	2.88	0.46
7:AR:905:LYS:HG3	7:AR:965:TYR:CE2	2.50	0.46
9:AT:169:LEU:C	9:AT:175:ILE:HD11	2.40	0.46
12:AW:36:ASP:N	12:AW:37:GLY:CA	2.72	0.46
12:AW:127:SER:O	12:AW:131:ARG:HG3	2.15	0.46
12:AW:818:TYR:CE1	12:AW:822:ARG:HG3	2.50	0.46
12:BA:9:ILE:HA	7:BB:1115:ARG:O	2.14	0.46
12:BA:38:THR:N	12:BA:39:PRO:HD2	2.30	0.46
7:BB:88:ALA:HA	7:BB:93:LEU:HB2	1.97	0.46
7:BB:961:LEU:HG	7:BB:967:PRO:HD3	1.97	0.46
7:BB:1096:VAL:CG1	7:BB:1097:SER:N	2.78	0.46
7:BB:1104:ILE:HG23	7:BB:1114:PRO:HG2	1.96	0.46
11:BG:78:VAL:HG12	11:BG:79:THR:OG1	2.15	0.46
11:BG:101:LEU:HD13	11:BG:102:LEU:H	1.80	0.46
7:AR:300:PHE:O	7:AR:301:LEU:C	2.58	0.46
7:AR:379:GLY:O	7:AR:380:ARG:HB2	2.16	0.46
7:AR:844:HIS:CD2	7:AR:1026:GLU:HG2	2.50	0.46
7:AR:918:LEU:HD13	7:AR:927:ILE:HD11	1.97	0.46
10:AU:64:SER:HB2	10:AU:69:ARG:CZ	2.46	0.46
12:AW:775:SER:HB2	12:AW:776:PRO:HD2	1.97	0.46
12:BA:372:TRP:C	12:BA:372:TRP:CD1	2.93	0.46
7:BB:208:LEU:HD11	7:BB:214:HIS:CD2	2.50	0.46
7:BB:287:ASN:O	7:BB:291:LYS:N	2.48	0.46
7:BB:420:THR:O	7:BB:421:ASN:CG	2.59	0.46
7:BB:457:CYS:HB3	7:BB:460:GLU:HB2	1.96	0.46
9:BE:134:LYS:CE	9:BE:171:LYS:HB3	2.44	0.46
7:AR:483:ILE:HG13	7:AR:555:GLU:HB2	1.97	0.46
12:AW:691:THR:HG22	12:AW:692:LEU:H	1.80	0.46
12:AW:864:LYS:CD	12:AW:867:ASP:HA	2.45	0.46
12:BA:94:LEU:HD21	12:BA:180:ILE:HG23	1.98	0.46
12:BA:827:LEU:O	14:BC:71:GLY:HA3	2.14	0.46
7:BB:17:ILE:O	7:BB:20:TYR:HB3	2.15	0.46
7:BB:300:PHE:O	7:BB:301:LEU:C	2.59	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:BF:76:CYS:HB2	10:BF:104:ILE:CG2	2.45	0.46
15:BH:83:SER:HB3	4:BQ:44:LEU:HD11	1.97	0.46
13:BP:24:VAL:HG13	13:BP:24:VAL:O	2.15	0.46
1:BR:7:DA:C2	2:BS:9:DA:C2	3.03	0.46
6:AO:19:GLN:HB3	6:AO:20:PRO:HD3	1.97	0.46
7:AR:873:ARG:HB3	7:AR:999:MET:HE1	1.98	0.46
8:AS:145:LEU:N	8:AS:145:LEU:HD12	2.31	0.46
8:AS:150:GLY:HA2	8:AS:156:PHE:HB2	1.97	0.46
11:AV:101:LEU:HD13	11:AV:102:LEU:H	1.80	0.46
12:AW:155:LYS:O	12:AW:156:ILE:C	2.59	0.46
12:AW:687:ILE:CG1	12:AW:688:PRO:HD2	2.46	0.46
12:BA:122:LYS:HZ3	12:BA:125:TRP:CD1	2.33	0.46
12:BA:145:VAL:HG13	12:BA:146:CYS:N	2.29	0.46
7:BB:8:LEU:HD22	7:BB:8:LEU:N	2.30	0.46
7:BB:844:HIS:CD2	7:BB:1026:GLU:HG2	2.51	0.46
7:BB:953:ILE:HG12	7:BB:954:GLU:H	1.80	0.46
4:BQ:39:GLN:HG2	4:BQ:40:ASP:H	1.81	0.46
7:AR:420:THR:O	7:AR:421:ASN:CG	2.58	0.46
7:AR:922:MET:SD	12:AW:739:ASN:HB2	2.55	0.46
7:AR:1044:THR:O	7:AR:1044:THR:HG23	2.16	0.46
12:AW:671:GLU:O	12:AW:674:ASN:OD1	2.33	0.46
14:AY:394:LEU:HD22	14:AY:394:LEU:N	2.31	0.46
7:BB:191:LYS:HE2	7:BB:193:ILE:HD11	1.96	0.46
7:BB:256:PHE:N	7:BB:257:PRO:CD	2.78	0.46
7:BB:483:ILE:HG13	7:BB:555:GLU:HB2	1.97	0.46
7:BB:873:ARG:HB3	7:BB:999:MET:HE1	1.98	0.46
8:BD:133:LEU:HD21	8:BD:139:ILE:HG12	1.97	0.46
2:BS:5:DG:C2	2:BS:6:DA:C2	3.03	0.46
7:AR:17:ILE:O	7:AR:20:TYR:HB3	2.16	0.46
8:AS:109:LEU:C	8:AS:109:LEU:HD23	2.40	0.46
9:AT:150:ALA:O	9:AT:151:SER:C	2.59	0.46
9:AT:166:GLN:HB2	9:AT:169:LEU:HD12	1.97	0.46
10:AU:75:ILE:C	10:AU:76:CYS:SG	2.98	0.46
10:AU:76:CYS:HB2	10:AU:104:ILE:CG2	2.45	0.46
12:AW:105:LYS:CE	12:AW:136:VAL:HG12	2.45	0.46
14:AY:41:VAL:O	14:AY:41:VAL:HG22	2.15	0.46
12:BA:27:ILE:CG2	12:BA:74:HIS:CE1	2.99	0.46
12:BA:38:THR:N	12:BA:39:PRO:CD	2.78	0.46
12:BA:372:TRP:CB	12:BA:373:PRO:CD	2.94	0.46
7:BB:1044:THR:HG23	7:BB:1044:THR:O	2.16	0.46
8:BD:98:ILE:HB	8:BD:141:LEU:HG	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:AJ:44:LEU:O	4:AJ:48:THR:HG23	2.16	0.46
7:AR:233:LEU:HD11	7:AR:311:ARG:O	2.16	0.46
12:AW:111:ILE:HG22	12:AW:112:GLU:N	2.30	0.46
14:AY:192:LYS:CA	14:AY:193:LEU:HB2	2.46	0.46
14:AY:214:ASP:N	14:AY:215:SER:HA	2.31	0.46
12:BA:105:LYS:HZ2	12:BA:140:ALA:CB	2.23	0.46
12:BA:747:LEU:HB2	12:BA:782:ILE:HB	1.97	0.46
7:BB:379:GLY:O	7:BB:380:ARG:HB2	2.16	0.46
7:BB:653:ILE:HG23	7:BB:654:THR:N	2.31	0.46
7:BB:680:LEU:HD22	7:BB:696:HIS:CB	2.46	0.46
7:BB:895:ILE:HB	7:BB:900:MET:HE2	1.97	0.46
15:BH:28:ALA:HB1	15:BH:62:ILE:HD11	1.98	0.46
1:AC:7:DA:C2	2:AD:9:DA:C2	3.03	0.46
8:AS:154:ALA:HA	8:AS:157:ILE:HG13	1.98	0.46
11:AV:65:SER:CB	11:AV:66:TYR:CA	2.87	0.46
12:AW:372:TRP:CB	12:AW:373:PRO:CD	2.94	0.46
12:AW:614:TRP:O	12:AW:618:GLU:HG2	2.16	0.46
15:AZ:28:ALA:HB1	15:AZ:62:ILE:HD11	1.98	0.46
12:BA:105:LYS:CE	12:BA:136:VAL:HG12	2.46	0.46
12:BA:107:SER:HB3	12:BA:140:ALA:HA	1.97	0.46
12:BA:431:MET:HB2	12:BA:453:TYR:OH	2.16	0.46
12:BA:775:SER:HB2	12:BA:776:PRO:HD2	1.97	0.46
14:BC:104:LEU:HB3	14:BC:105:PRO:HD3	1.98	0.46
10:BF:95:TYR:CE1	10:BF:97:SER:HB2	2.50	0.46
1:AC:11:DT:H2"	1:AC:12:DA:O5'	2.15	0.46
7:AR:88:ALA:HA	7:AR:93:LEU:HB2	1.97	0.46
9:AT:168:TYR:CG	10:AU:83:VAL:HG11	2.50	0.46
10:AU:13:PRO:HG2	10:AU:16:VAL:HG12	1.98	0.46
11:AV:10:ILE:C	11:AV:11:LEU:HD12	2.41	0.46
11:AV:78:VAL:HG12	11:AV:79:THR:OG1	2.15	0.46
12:AW:512:LYS:HE3	12:AW:583:ASP:HB2	1.98	0.46
12:BA:29:THR:OG1	12:BA:30:PRO:CD	2.63	0.46
14:BC:41:VAL:O	14:BC:41:VAL:HG22	2.15	0.46
10:BF:64:SER:HB2	10:BF:69:ARG:CZ	2.45	0.46
7:AR:73:VAL:HG11	7:AR:93:LEU:HD23	1.98	0.45
7:AR:778:MET:HE3	7:AR:779:PRO:HD2	1.98	0.45
8:AS:98:ILE:HB	8:AS:141:LEU:HG	1.97	0.45
10:AU:84:ARG:O	10:AU:85:SER:C	2.59	0.45
11:AV:72:CYS:HB3	11:AV:114:LYS:HD2	1.98	0.45
12:AW:94:LEU:HD21	12:AW:180:ILE:HG23	1.98	0.45
12:AW:162:TYR:O	12:AW:162:TYR:CD1	2.69	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:AW:187:VAL:HG21	12:AW:204:PRO:HG3	1.98	0.45
12:AW:431:MET:HB2	12:AW:453:TYR:OH	2.16	0.45
12:AW:747:LEU:HB2	12:AW:782:ILE:HB	1.98	0.45
14:AY:214:ASP:HB2	14:AY:215:SER:CA	2.46	0.45
12:BA:155:LYS:O	12:BA:156:ILE:C	2.59	0.45
9:BE:10:ILE:HD12	9:BE:10:ILE:N	2.32	0.45
11:BG:61:LYS:O	11:BG:62:ASN:HB2	2.15	0.45
6:BN:3:ILE:CG2	6:BN:52:HIS:CD2	3.00	0.45
13:BP:10:TRP:CE3	13:BP:11:LYS:HB3	2.51	0.45
4:BQ:35:LYS:HD3	4:BQ:35:LYS:HA	1.71	0.45
4:BQ:57:GLY:O	4:BQ:58:LYS:C	2.58	0.45
7:AR:256:PHE:N	7:AR:257:PRO:CD	2.79	0.45
7:AR:680:LEU:HD22	7:AR:696:HIS:CB	2.46	0.45
7:AR:1115:ARG:HB2	12:AW:10:LYS:HB2	1.98	0.45
12:AW:372:TRP:HB3	12:AW:373:PRO:CD	2.42	0.45
14:AY:81:PRO:HB3	14:AY:306:LEU:HG	1.96	0.45
12:BA:127:SER:O	12:BA:131:ARG:HG3	2.16	0.45
12:BA:691:THR:HG22	12:BA:692:LEU:H	1.80	0.45
14:BC:125:TYR:CE1	14:BC:250:ILE:HD13	2.51	0.45
14:BC:214:ASP:HB2	14:BC:215:SER:CA	2.46	0.45
9:BE:168:TYR:CD2	10:BF:83:VAL:HG11	2.51	0.45
11:BG:96:ILE:HG22	11:BG:97:SER:N	2.32	0.45
15:BH:83:SER:CB	4:BQ:44:LEU:HD11	2.46	0.45
6:BN:19:GLN:HB3	6:BN:20:PRO:CD	2.47	0.45
5:AM:69:LEU:HD23	8:AS:260:LEU:HD11	1.99	0.45
7:AR:1015:LEU:HD12	7:AR:1016:THR:HG23	1.99	0.45
8:AS:41:ILE:HA	8:AS:145:LEU:HG	1.98	0.45
10:AU:88:ILE:C	10:AU:90:ASP:N	2.74	0.45
13:AX:10:TRP:CE3	13:AX:11:LYS:HB3	2.51	0.45
12:BA:77:LEU:N	12:BA:77:LEU:HD23	2.32	0.45
12:BA:864:LYS:CA	12:BA:865:THR:CB	2.93	0.45
14:BC:348:GLU:HG2	2:BS:14:DA:H5"	1.98	0.45
8:BD:79:PRO:HG3	8:BD:148:GLY:HA2	1.98	0.45
8:BD:145:LEU:N	8:BD:145:LEU:HD12	2.31	0.45
6:AO:3:ILE:CG2	6:AO:52:HIS:CD2	3.00	0.45
7:AR:893:MET:HE3	7:AR:894:LEU:O	2.17	0.45
7:AR:961:LEU:HG	7:AR:967:PRO:HD3	1.98	0.45
9:AT:84:VAL:HG21	10:AU:84:ARG:NH1	2.31	0.45
9:AT:147:ILE:HD11	9:AT:163:THR:HG21	1.99	0.45
14:AY:26:GLN:O	14:AY:29:VAL:HG12	2.16	0.45
14:AY:125:TYR:CE1	14:AY:250:ILE:HD13	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:BA:238:LYS:HG2	12:BA:276:TYR:HA	1.97	0.45
7:BB:333:ARG:O	7:BB:334:GLU:HB3	2.17	0.45
7:BB:592:VAL:CG2	7:BB:596:ASP:CG	2.89	0.45
7:BB:1015:LEU:HD12	7:BB:1016:THR:HG23	1.98	0.45
14:BC:182:ASP:HA	14:BC:185:LYS:HB2	1.99	0.45
14:BC:192:LYS:CA	14:BC:193:LEU:HB2	2.46	0.45
4:AJ:45:MET:CB	12:AW:122:LYS:HE2	2.46	0.45
8:AS:153:HIS:O	8:AS:153:HIS:CG	2.70	0.45
12:AW:105:LYS:HE3	12:AW:140:ALA:HB2	1.99	0.45
15:AZ:65:ILE:HD12	15:AZ:65:ILE:N	2.31	0.45
12:BA:95:LYS:HD3	12:BA:141:MET:HE3	1.99	0.45
12:BA:97:THR:HG23	12:BA:103:ARG:HD3	1.98	0.45
7:BB:778:MET:HE3	7:BB:779:PRO:HD2	1.98	0.45
14:BC:100:VAL:O	14:BC:100:VAL:HG12	2.16	0.45
14:BC:235:LYS:CE	14:BC:264:VAL:HG21	2.46	0.45
14:BC:277:ILE:HG22	14:BC:278:ARG:N	2.32	0.45
9:BE:150:ALA:O	9:BE:151:SER:C	2.58	0.45
11:BG:18:ILE:CG2	11:BG:29:ILE:HG12	2.46	0.45
15:BH:69:SER:HB2	15:BH:75:VAL:HG23	1.97	0.45
7:AR:539:LEU:HD11	7:AR:543:ILE:HD11	1.99	0.45
11:AV:92:TYR:CE2	11:AV:113:LEU:HD21	2.52	0.45
12:AW:29:THR:OG1	12:AW:30:PRO:CD	2.63	0.45
12:AW:95:LYS:HD3	12:AW:141:MET:HE3	1.99	0.45
12:AW:324:THR:HG22	12:AW:443:PHE:CE2	2.52	0.45
12:AW:419:PHE:CE2	12:AW:462:MET:CE	3.00	0.45
12:AW:541:ALA:HB1	12:AW:542:PRO:HD3	1.99	0.45
12:AW:818:TYR:C	12:AW:818:TYR:CD1	2.91	0.45
14:AY:235:LYS:CE	14:AY:264:VAL:HG21	2.47	0.45
12:BA:187:VAL:HG21	12:BA:204:PRO:HG3	1.99	0.45
14:BC:26:GLN:O	14:BC:29:VAL:HG12	2.17	0.45
8:BD:153:HIS:O	8:BD:153:HIS:CG	2.70	0.45
8:BD:183:CYS:SG	17:BD:1001:SF4:S2	3.14	0.45
9:BE:146:VAL:CG1	9:BE:149:VAL:HG23	2.47	0.45
11:BG:99:PHE:O	11:BG:103:VAL:HG12	2.17	0.45
15:BH:18:PRO:HB3	15:BH:67:ARG:HB3	1.98	0.45
4:BQ:57:GLY:O	4:BQ:59:ILE:HG22	2.17	0.45
4:BQ:78:ARG:HD3	4:BQ:79:ASP:N	2.32	0.45
6:AO:2:MET:HG2	6:AO:56:ILE:HD12	1.99	0.45
7:AR:647:SER:HB2	7:AR:648:PRO:HD3	1.99	0.45
7:AR:653:ILE:HG23	7:AR:654:THR:N	2.31	0.45
7:AR:783:VAL:HB	7:AR:784:ARG:HA	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:AS:59:ALA:HB1	13:AX:47:ALA:HB2	1.97	0.45
8:AS:236:LEU:N	8:AS:236:LEU:HD12	2.31	0.45
9:AT:49:LEU:HD12	9:AT:49:LEU:N	2.31	0.45
12:AW:342:ILE:CG2	12:AW:343:ILE:N	2.80	0.45
12:AW:393:ASP:O	12:AW:394:ARG:CB	2.65	0.45
12:AW:456:ASP:OD1	12:AW:460:ASP:CG	2.50	0.45
12:BA:131:ARG:NE	4:BQ:36:LEU:HD11	2.32	0.45
12:BA:393:ASP:O	12:BA:394:ARG:CB	2.65	0.45
12:BA:492:GLY:HA3	12:BA:862:HIS:HA	1.98	0.45
7:BB:233:LEU:HD11	7:BB:311:ARG:O	2.16	0.45
7:BB:893:MET:HE3	7:BB:894:LEU:O	2.17	0.45
14:BC:184:VAL:O	14:BC:188:ILE:HG13	2.17	0.45
9:BE:108:VAL:HG22	9:BE:162:LEU:CB	2.47	0.45
6:BN:43:TYR:HA	6:BN:46:ARG:HB3	1.99	0.45
7:AR:251:ILE:CG2	7:AR:326:ILE:HD12	2.46	0.45
7:AR:516:GLU:O	7:AR:517:TYR:HB2	2.17	0.45
7:AR:582:LEU:HD12	7:AR:619:LEU:HD12	1.98	0.45
7:AR:895:ILE:HB	7:AR:900:MET:HE2	1.98	0.45
8:AS:79:PRO:HG3	8:AS:148:GLY:HA2	1.98	0.45
11:AV:26:LEU:HD13	11:AV:26:LEU:C	2.42	0.45
12:AW:79:ARG:HB3	12:AW:80:PRO:HD2	1.99	0.45
12:AW:708:ARG:CD	12:AW:748:GLY:HA3	2.46	0.45
12:BA:52:ILE:CG2	12:BA:217:ILE:HG22	2.47	0.45
12:BA:162:TYR:CD1	12:BA:162:TYR:O	2.69	0.45
7:BB:197:ALA:HA	7:BB:198:GLY:HA2	1.72	0.45
7:BB:226:PHE:CE1	7:BB:230:MET:CG	3.00	0.45
7:BB:322:ILE:O	7:BB:326:ILE:HG12	2.17	0.45
14:BC:104:LEU:N	14:BC:105:PRO:HD2	2.32	0.45
14:BC:157:SER:HB3	14:BC:166:ILE:HB	1.97	0.45
14:BC:173:MET:HA	14:BC:177:LYS:HD2	1.98	0.45
14:BC:214:ASP:N	14:BC:215:SER:HA	2.31	0.45
8:BD:161:LEU:HD12	8:BD:163:ILE:HD13	1.97	0.45
9:BE:147:ILE:HD11	9:BE:163:THR:HG21	1.99	0.45
11:BG:10:ILE:C	11:BG:11:LEU:HD12	2.41	0.45
11:BG:26:LEU:HD13	11:BG:26:LEU:C	2.42	0.45
3:BK:43:LEU:HD11	3:BK:68:GLU:OE2	2.17	0.45
1:BR:13:DT:C1'	1:BR:14:DC:P	3.05	0.45
7:AR:8:LEU:HD11	7:AR:593:THR:HA	1.98	0.45
7:AR:68:ILE:HG13	7:AR:99:LEU:CD2	2.47	0.45
9:AT:172:LEU:HD23	9:AT:173:GLU:N	2.32	0.45
11:AV:95:ILE:HD12	11:AV:95:ILE:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:AW:44:VAL:HG13	12:AW:45:MET:N	2.32	0.45
12:AW:97:THR:HG23	12:AW:103:ARG:HD3	1.99	0.45
12:AW:336:GLU:HA	12:AW:434:ARG:O	2.17	0.45
14:AY:122:MET:HE1	14:AY:261:VAL:HG21	1.99	0.45
14:AY:184:VAL:O	14:AY:188:ILE:HG13	2.17	0.45
14:AY:277:ILE:HG22	14:AY:278:ARG:N	2.32	0.45
7:BB:251:ILE:CG2	7:BB:326:ILE:HD12	2.46	0.45
7:BB:808:LYS:HD2	7:BB:808:LYS:C	2.42	0.45
9:BE:166:GLN:HB2	9:BE:169:LEU:HD12	1.97	0.45
7:AR:683:TYR:CZ	7:AR:687:TYR:HB2	2.52	0.45
11:AV:92:TYR:CE2	11:AV:113:LEU:CD2	3.00	0.45
12:AW:108:GLU:HG3	12:AW:147:PRO:HG3	1.99	0.45
12:BA:512:LYS:HE3	12:BA:583:ASP:HB2	1.99	0.45
12:BA:541:ALA:HB1	12:BA:542:PRO:HD3	1.99	0.45
12:BA:864:LYS:HA	12:BA:865:THR:OG1	2.17	0.45
7:BB:582:LEU:HD12	7:BB:619:LEU:HD12	1.98	0.45
7:BB:591:LEU:O	7:BB:592:VAL:HG12	2.17	0.45
7:BB:682:LEU:HD22	6:BN:55:ILE:HD12	1.99	0.45
14:BC:25:PRO:O	14:BC:26:GLN:CB	2.65	0.45
8:BD:254:GLU:OE1	5:BL:77:ARG:HD3	2.16	0.45
9:BE:49:LEU:HD12	9:BE:49:LEU:N	2.31	0.45
10:BF:84:ARG:O	10:BF:85:SER:C	2.59	0.45
5:BL:15:LEU:HB3	5:BL:55:VAL:CG2	2.47	0.45
2:BS:16:DA:C5'	2:BS:17:DG:OP1	2.65	0.45
6:AO:19:GLN:HB3	6:AO:20:PRO:CD	2.47	0.44
11:AV:18:ILE:CG2	11:AV:29:ILE:HG12	2.47	0.44
11:AV:96:ILE:HG22	11:AV:97:SER:N	2.31	0.44
13:AX:17:GLN:HG3	13:AX:18:LEU:N	2.32	0.44
14:AY:340:SER:O	14:AY:344:ARG:HD3	2.17	0.44
15:AZ:69:SER:HB2	15:AZ:75:VAL:HG23	1.97	0.44
12:BA:342:ILE:CG2	12:BA:343:ILE:N	2.80	0.44
12:BA:423:PRO:HB2	12:BA:425:LEU:CD1	2.47	0.44
7:BB:68:ILE:HG13	7:BB:99:LEU:CD2	2.47	0.44
7:BB:209:LYS:O	7:BB:210:ASP:HB2	2.18	0.44
7:BB:273:ASP:HB2	7:BB:289:ILE:HD11	1.99	0.44
7:BB:783:VAL:HB	7:BB:784:ARG:HA	1.99	0.44
7:BB:898:VAL:HG12	8:BD:30:ARG:NH2	2.32	0.44
14:BC:122:MET:HE1	14:BC:261:VAL:HG21	1.99	0.44
14:BC:351:VAL:HG23	14:BC:352:LYS:H	1.82	0.44
9:BE:172:LEU:HD23	9:BE:173:GLU:N	2.32	0.44
11:BG:92:TYR:CE2	11:BG:113:LEU:HD21	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AI:43:LEU:HD11	3:AI:68:GLU:OE2	2.17	0.44
7:AR:209:LYS:O	7:AR:210:ASP:HB2	2.17	0.44
7:AR:855:ILE:HD12	7:AR:855:ILE:N	2.33	0.44
9:AT:108:VAL:HG22	9:AT:162:LEU:CB	2.47	0.44
12:AW:417:VAL:HG11	12:AW:464:LEU:CD2	2.48	0.44
12:AW:509:LEU:HA	12:AW:638:PHE:CE2	2.53	0.44
14:AY:258:LEU:HD22	14:AY:280:ILE:HD13	1.99	0.44
12:BA:417:VAL:HG11	12:BA:464:LEU:CD2	2.48	0.44
12:BA:419:PHE:CE2	12:BA:462:MET:CE	3.00	0.44
12:BA:687:ILE:CG1	12:BA:688:PRO:HD2	2.46	0.44
7:BB:73:VAL:HG11	7:BB:93:LEU:HD23	1.99	0.44
14:BC:65:ALA:HA	3:BK:23:TRP:CZ2	2.53	0.44
14:BC:176:ASP:HB3	14:BC:177:LYS:HG3	1.99	0.44
14:BC:192:LYS:HG2	14:BC:193:LEU:HD13	1.99	0.44
6:BN:2:MET:HG2	6:BN:56:ILE:HD12	1.99	0.44
7:AR:808:LYS:HD2	7:AR:808:LYS:C	2.41	0.44
12:AW:112:GLU:O	12:AW:116:ARG:HD3	2.17	0.44
12:AW:188:PRO:HG2	12:AW:191:ASP:CG	2.43	0.44
12:BA:122:LYS:O	12:BA:122:LYS:HG2	2.17	0.44
7:BB:125:MET:HE2	7:BB:153:GLY:HA2	1.99	0.44
7:BB:683:TYR:CZ	7:BB:687:TYR:HB2	2.52	0.44
7:BB:856:THR:HG23	7:BB:857:GLU:N	2.33	0.44
10:BF:88:ILE:C	10:BF:90:ASP:N	2.74	0.44
4:BQ:70:ASP:O	4:BQ:73:LYS:HG2	2.18	0.44
2:AD:3:DT:H2"	2:AD:4:DA:N7	2.32	0.44
6:AO:43:TYR:HA	6:AO:46:ARG:HB3	1.99	0.44
7:AR:774:ASP:O	7:AR:775:LYS:CB	2.65	0.44
7:AR:1086:GLY:O	7:AR:1087:ASP:HB2	2.18	0.44
7:AR:1115:ARG:O	12:AW:9:ILE:HA	2.17	0.44
11:AV:78:VAL:C	11:AV:79:THR:OG1	2.60	0.44
12:AW:77:LEU:N	12:AW:77:LEU:HD23	2.32	0.44
12:AW:228:GLY:O	12:AW:229:ILE:HG12	2.18	0.44
12:AW:823:LEU:HD13	14:AY:75:ALA:CA	2.47	0.44
14:AY:104:LEU:N	14:AY:105:PRO:HD2	2.32	0.44
14:AY:113:ALA:O	14:AY:114:LYS:HB3	2.18	0.44
14:AY:211:ALA:HB1	14:AY:213:ILE:N	2.32	0.44
12:BA:708:ARG:CD	12:BA:748:GLY:HA3	2.48	0.44
7:BB:647:SER:HB2	7:BB:648:PRO:HD3	1.98	0.44
14:BC:311:ARG:HA	14:BC:314:LEU:HD12	1.99	0.44
8:BD:236:LEU:N	8:BD:236:LEU:HD12	2.31	0.44
11:BG:92:TYR:CE2	11:BG:113:LEU:CD2	3.01	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:AJ:36:LEU:HD21	12:AW:131:ARG:NH1	2.33	0.44
7:AR:322:ILE:O	7:AR:326:ILE:HG12	2.18	0.44
7:AR:981:LYS:HE2	8:AS:205:LEU:HD13	2.00	0.44
11:AV:99:PHE:O	11:AV:103:VAL:HG12	2.17	0.44
12:AW:98:CYS:O	12:AW:101:CYS:SG	2.75	0.44
12:AW:122:LYS:HG2	12:AW:122:LYS:O	2.17	0.44
12:AW:823:LEU:HD13	14:AY:75:ALA:HB1	1.98	0.44
12:AW:864:LYS:CA	12:AW:865:THR:CB	2.93	0.44
14:AY:192:LYS:HG2	14:AY:193:LEU:HD13	1.99	0.44
14:AY:351:VAL:HG23	14:AY:352:LYS:H	1.82	0.44
15:AZ:62:ILE:HG13	15:AZ:62:ILE:O	2.18	0.44
12:BA:42:GLY:O	12:BA:43:SER:HB3	2.17	0.44
7:BB:8:LEU:HD11	7:BB:593:THR:HA	1.98	0.44
7:BB:1110:MET:HG2	7:BB:1110:MET:O	2.17	0.44
8:BD:41:ILE:HA	8:BD:145:LEU:HG	1.99	0.44
10:BF:13:PRO:HG2	10:BF:16:VAL:HG12	1.98	0.44
15:BH:45:ILE:HG22	15:BH:46:ARG:H	1.83	0.44
2:BS:3:DT:H2"	2:BS:4:DA:N7	2.32	0.44
3:AI:61:VAL:O	3:AI:64:ILE:HB	2.17	0.44
5:AM:15:LEU:HB3	5:AM:55:VAL:CG2	2.48	0.44
7:AR:592:VAL:CG2	7:AR:615:LYS:HD3	2.48	0.44
8:AS:13:ILE:HG21	8:AS:238:PRO:HB2	2.00	0.44
9:AT:146:VAL:CG1	9:AT:149:VAL:HG23	2.47	0.44
11:AV:46:ILE:HG12	12:AW:542:PRO:HG2	2.00	0.44
14:AY:333:GLY:O	14:AY:337:GLU:HG2	2.18	0.44
15:AZ:45:ILE:HG22	15:AZ:46:ARG:H	1.83	0.44
12:BA:4:LYS:HG3	7:BB:1092:PHE:CD2	2.52	0.44
12:BA:443:PHE:CE2	12:BA:464:LEU:HB2	2.53	0.44
12:BA:614:TRP:O	12:BA:618:GLU:HG2	2.16	0.44
12:BA:818:TYR:CE1	12:BA:822:ARG:HG3	2.51	0.44
7:BB:212:THR:HG21	7:BB:214:HIS:NE2	2.33	0.44
7:BB:572:ASN:HB3	7:BB:577:ARG:HD3	2.00	0.44
7:BB:745:ARG:HB2	7:BB:894:LEU:HB3	2.00	0.44
7:BB:774:ASP:O	7:BB:775:LYS:CB	2.66	0.44
14:BC:258:LEU:HD22	14:BC:280:ILE:HD13	2.00	0.44
8:BD:96:ILE:HG13	8:BD:143:ALA:HB3	2.00	0.44
8:BD:154:ALA:HA	8:BD:157:ILE:HG13	1.98	0.44
11:BG:95:ILE:HD12	11:BG:95:ILE:N	2.33	0.44
3:BK:61:VAL:O	3:BK:64:ILE:HB	2.17	0.44
2:AD:16:DA:C5'	2:AD:17:DG:OP1	2.66	0.44
7:AR:333:ARG:O	7:AR:334:GLU:HB3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:AR:399:HIS:O	7:AR:403:THR:HG22	2.17	0.44
7:AR:525:LEU:C	7:AR:525:LEU:HD13	2.42	0.44
9:AT:10:ILE:HD12	9:AT:10:ILE:N	2.32	0.44
9:AT:30:LEU:HD22	9:AT:72:PHE:CZ	2.52	0.44
12:AW:449:VAL:O	12:AW:449:VAL:HG12	2.17	0.44
12:AW:592:ILE:O	12:AW:594:LEU:HD22	2.17	0.44
14:AY:100:VAL:O	14:AY:100:VAL:HG12	2.17	0.44
14:AY:176:ASP:HB3	14:AY:177:LYS:HG3	1.99	0.44
12:BA:30:PRO:O	12:BA:243:VAL:HG11	2.18	0.44
12:BA:188:PRO:HG2	12:BA:191:ASP:CG	2.43	0.44
12:BA:495:ILE:O	12:BA:605:ASN:HB2	2.17	0.44
12:BA:651:VAL:O	12:BA:651:VAL:HG12	2.17	0.44
12:BA:733:ALA:O	12:BA:734:ARG:C	2.61	0.44
12:BA:819:MET:HE3	12:BA:823:LEU:HD21	1.99	0.44
7:BB:399:HIS:O	7:BB:403:THR:HG22	2.17	0.44
7:BB:855:ILE:N	7:BB:855:ILE:HD12	2.33	0.44
7:BB:961:LEU:HD23	7:BB:961:LEU:O	2.17	0.44
14:BC:113:ALA:O	14:BC:114:LYS:HB3	2.18	0.44
14:BC:235:LYS:HE2	14:BC:261:VAL:HA	2.00	0.44
14:BC:372:ASN:HA	14:BC:375:ILE:HG22	2.00	0.44
8:BD:73:LEU:HD11	8:BD:236:LEU:CD2	2.48	0.44
2:AD:14:DA:C5'	12:AW:818:TYR:OH	2.66	0.44
7:AR:72:ARG:HD2	7:AR:72:ARG:C	2.43	0.44
7:AR:89:ARG:NH1	7:AR:156:ILE:HD11	2.33	0.44
7:AR:212:THR:HG21	7:AR:214:HIS:NE2	2.33	0.44
7:AR:273:ASP:HB2	7:AR:289:ILE:HD11	1.99	0.44
7:AR:520:TRP:N	7:AR:520:TRP:CD1	2.85	0.44
7:AR:591:LEU:O	7:AR:592:VAL:HG12	2.17	0.44
7:AR:742:ILE:HB	7:AR:912:ILE:HB	2.00	0.44
7:AR:1064:CYS:CB	7:AR:1067:CYS:HB2	2.47	0.44
9:AT:146:VAL:HG11	9:AT:149:VAL:CG2	2.48	0.44
12:AW:42:GLY:O	12:AW:43:SER:HB3	2.17	0.44
12:AW:818:TYR:CE1	12:AW:822:ARG:CG	3.00	0.44
12:AW:819:MET:HE3	12:AW:823:LEU:HD21	1.99	0.44
14:AY:25:PRO:O	14:AY:26:GLN:CB	2.65	0.44
14:AY:104:LEU:HB3	14:AY:105:PRO:HD3	1.99	0.44
14:AY:173:MET:HA	14:AY:177:LYS:HD2	1.99	0.44
12:BA:318:VAL:HG11	7:BB:1051:ARG:O	2.17	0.44
12:BA:449:VAL:O	12:BA:449:VAL:HG12	2.17	0.44
12:BA:511:VAL:O	12:BA:512:LYS:C	2.61	0.44
11:BG:72:CYS:CB	11:BG:114:LYS:HD2	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:AJ:57:GLY:O	4:AJ:59:ILE:HG22	2.17	0.44
7:AR:323:SER:HA	7:AR:326:ILE:CD1	2.48	0.44
7:AR:583:ILE:HD13	7:AR:616:ILE:HG12	2.00	0.44
12:AW:548:GLY:O	12:AW:551:VAL:HG12	2.18	0.44
14:AY:369:VAL:HG23	14:AY:370:VAL:N	2.33	0.44
12:BA:324:THR:HG22	12:BA:443:PHE:CE2	2.53	0.44
12:BA:548:GLY:O	12:BA:551:VAL:HG12	2.18	0.44
12:BA:592:ILE:O	12:BA:594:LEU:HD22	2.18	0.44
12:BA:723:ASN:OD1	12:BA:723:ASN:C	2.61	0.44
12:BA:818:TYR:CE1	12:BA:822:ARG:CG	3.01	0.44
7:BB:323:SER:HA	7:BB:326:ILE:CD1	2.48	0.44
14:BC:257:ASN:O	14:BC:261:VAL:HG23	2.18	0.44
9:BE:30:LEU:HD22	9:BE:72:PHE:CZ	2.52	0.44
9:BE:34:TYR:O	9:BE:35:GLN:C	2.61	0.44
9:BE:108:VAL:HG22	9:BE:162:LEU:HB2	2.00	0.44
10:BF:62:ILE:O	10:BF:62:ILE:HG22	2.17	0.44
3:BK:59:THR:CG2	3:BK:63:SER:HB3	2.48	0.44
6:AO:5:ILE:CD1	8:AS:61:ARG:CZ	2.96	0.43
7:AR:524:ILE:N	7:AR:524:ILE:HD12	2.33	0.43
7:AR:1111:ILE:HG22	7:AR:1111:ILE:O	2.18	0.43
12:AW:159:GLU:HG2	12:AW:160:LYS:O	2.18	0.43
12:AW:212:LEU:C	12:AW:212:LEU:HD23	2.43	0.43
12:AW:842:TYR:CE1	14:AY:367:LYS:HB2	2.53	0.43
14:AY:226:ILE:HG23	14:AY:230:LYS:NZ	2.33	0.43
12:BA:79:ARG:HB3	12:BA:80:PRO:HD2	1.99	0.43
12:BA:160:LYS:HD3	12:BA:165:TYR:CE2	2.53	0.43
12:BA:509:LEU:HA	12:BA:638:PHE:CE2	2.53	0.43
12:BA:516:LEU:HD12	12:BA:516:LEU:N	2.33	0.43
12:BA:541:ALA:HB2	11:BG:72:CYS:HB2	2.00	0.43
12:BA:769:PHE:CE2	12:BA:778:ALA:HA	2.52	0.43
7:BB:72:ARG:HD2	7:BB:72:ARG:C	2.43	0.43
7:BB:361:PHE:O	7:BB:364:PHE:HB3	2.18	0.43
11:BG:8:GLU:HB2	11:BG:60:SER:HB2	2.00	0.43
3:BK:68:GLU:HG3	3:BK:74:LEU:HD21	2.00	0.43
3:AI:59:THR:CG2	3:AI:63:SER:HB3	2.48	0.43
7:AR:10:ILE:HA	7:AR:13:ARG:HD3	2.00	0.43
7:AR:646:TRP:CE2	7:AR:648:PRO:HG2	2.53	0.43
7:AR:961:LEU:O	7:AR:961:LEU:HD23	2.18	0.43
11:AV:72:CYS:CB	11:AV:114:LYS:HD2	2.49	0.43
12:AW:747:LEU:HD21	12:AW:786:PHE:CD2	2.53	0.43
14:AY:182:ASP:HA	14:AY:185:LYS:HB2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:AY:196:PHE:HB2	14:AY:209:SER:OG	2.18	0.43
12:BA:3:GLU:HG3	7:BB:1093:PRO:HD2	2.00	0.43
12:BA:44:VAL:HG13	12:BA:45:MET:N	2.32	0.43
12:BA:105:LYS:HE3	12:BA:140:ALA:HB2	1.99	0.43
12:BA:112:GLU:O	12:BA:116:ARG:HD3	2.17	0.43
12:BA:336:GLU:HA	12:BA:434:ARG:O	2.17	0.43
7:BB:539:LEU:HD11	7:BB:543:ILE:HD11	1.99	0.43
7:BB:903:THR:HG22	7:BB:904:VAL:N	2.32	0.43
14:BC:108:ILE:HA	14:BC:111:VAL:HG12	1.99	0.43
14:BC:196:PHE:HB2	14:BC:209:SER:OG	2.18	0.43
9:BE:168:TYR:CG	10:BF:83:VAL:HG11	2.53	0.43
4:BQ:35:LYS:HD2	4:BQ:35:LYS:O	2.18	0.43
2:AD:14:DA:C5	2:AD:15:DT:H72	2.53	0.43
7:AR:125:MET:HE2	7:AR:153:GLY:HA2	1.99	0.43
7:AR:197:ALA:HA	7:AR:198:GLY:HA2	1.72	0.43
7:AR:255:LEU:C	7:AR:257:PRO:HD2	2.43	0.43
7:AR:857:GLU:HG3	13:AX:24:VAL:CG1	2.48	0.43
9:AT:108:VAL:HG22	9:AT:162:LEU:HB2	2.00	0.43
11:AV:8:GLU:HB2	11:AV:60:SER:HB2	2.00	0.43
12:AW:52:ILE:CG2	12:AW:217:ILE:HG22	2.47	0.43
12:AW:160:LYS:HD3	12:AW:165:TYR:CE2	2.53	0.43
12:BA:812:ARG:HG3	14:BC:86:THR:HG22	2.01	0.43
7:BB:592:VAL:CG2	7:BB:615:LYS:HD3	2.48	0.43
7:AR:226:PHE:CE1	7:AR:230:MET:CG	3.01	0.43
7:AR:833:GLN:CA	7:AR:834:ALA:CB	2.97	0.43
7:AR:1110:MET:O	7:AR:1110:MET:HG2	2.18	0.43
9:AT:13:ILE:CD1	9:AT:22:LEU:HG	2.48	0.43
9:AT:125:GLY:O	9:AT:126:ILE:HG12	2.19	0.43
10:AU:62:ILE:O	10:AU:62:ILE:HG22	2.17	0.43
11:AV:8:GLU:CB	11:AV:60:SER:HB2	2.48	0.43
12:AW:823:LEU:HD13	14:AY:75:ALA:CB	2.48	0.43
7:BB:10:ILE:HA	7:BB:13:ARG:HD3	2.00	0.43
7:BB:271:ALA:O	7:BB:274:PHE:HB3	2.18	0.43
7:BB:768:TYR:HB3	7:BB:769:PRO:HD2	2.00	0.43
7:BB:1125:SER:C	10:BF:5:TYR:CE2	2.97	0.43
14:BC:211:ALA:HB1	14:BC:213:ILE:N	2.32	0.43
14:BC:274:THR:HG22	14:BC:276:ASN:H	1.84	0.43
14:BC:340:SER:O	14:BC:344:ARG:HD3	2.18	0.43
9:BE:125:GLY:O	9:BE:126:ILE:HG12	2.19	0.43
9:BE:140:ASP:CG	9:BE:171:LYS:HE2	2.43	0.43
11:BG:8:GLU:CB	11:BG:60:SER:HB2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:BG:10:ILE:CD1	11:BG:58:PHE:CD2	3.02	0.43
13:BP:33:ILE:N	13:BP:33:ILE:HD12	2.34	0.43
4:AJ:42:GLU:O	4:AJ:45:MET:HB3	2.19	0.43
7:AR:903:THR:HG22	7:AR:904:VAL:N	2.33	0.43
12:AW:417:VAL:O	12:AW:432:ALA:HA	2.19	0.43
12:AW:486:ILE:HD13	12:AW:628:MET:HE3	1.99	0.43
12:AW:511:VAL:O	12:AW:512:LYS:C	2.61	0.43
12:AW:723:ASN:OD1	12:AW:723:ASN:C	2.61	0.43
12:AW:864:LYS:HA	12:AW:865:THR:OG1	2.17	0.43
12:BA:159:GLU:HG2	12:BA:160:LYS:O	2.18	0.43
7:BB:520:TRP:N	7:BB:520:TRP:CD1	2.85	0.43
7:BB:1086:GLY:O	7:BB:1087:ASP:HB2	2.18	0.43
9:BE:94:ASN:HB3	9:BE:120:TYR:CD2	2.54	0.43
9:BE:146:VAL:HG11	9:BE:149:VAL:CG2	2.47	0.43
10:BF:101:GLN:O	10:BF:105:ASP:N	2.52	0.43
6:AO:1:MET:O	6:AO:2:MET:HB2	2.18	0.43
9:AT:140:ASP:CG	9:AT:171:LYS:HE2	2.43	0.43
10:AU:62:ILE:O	10:AU:63:ILE:CB	2.67	0.43
10:AU:72:LEU:HG	10:AU:84:ARG:NH2	2.34	0.43
10:AU:102:LYS:O	10:AU:106:ILE:HG13	2.19	0.43
11:AV:72:CYS:H	12:AW:541:ALA:CB	2.31	0.43
12:AW:259:GLN:HA	12:AW:262:ILE:HG22	2.00	0.43
12:AW:443:PHE:CE2	12:AW:464:LEU:HB2	2.54	0.43
12:AW:516:LEU:HD12	12:AW:516:LEU:N	2.33	0.43
12:AW:769:PHE:CE2	12:AW:778:ALA:HA	2.53	0.43
14:AY:372:ASN:HA	14:AY:375:ILE:HG22	1.99	0.43
12:BA:108:GLU:HG3	12:BA:147:PRO:HG3	1.99	0.43
12:BA:259:GLN:HA	12:BA:262:ILE:HG22	2.00	0.43
12:BA:662:TYR:O	12:BA:665:ILE:HG12	2.19	0.43
7:BB:524:ILE:HD12	7:BB:524:ILE:N	2.33	0.43
7:BB:583:ILE:HD13	7:BB:616:ILE:HG12	1.99	0.43
7:BB:928:MET:HE3	7:BB:953:ILE:HG21	2.01	0.43
8:BD:41:ILE:HD13	8:BD:145:LEU:HG	2.00	0.43
2:BS:14:DA:C5	2:BS:15:DT:H72	2.53	0.43
4:AJ:78:ARG:HD3	4:AJ:79:ASP:N	2.33	0.43
7:AR:125:MET:HE2	7:AR:153:GLY:C	2.44	0.43
7:AR:856:THR:HG23	7:AR:857:GLU:N	2.33	0.43
11:AV:79:THR:CG2	11:AV:80:GLU:HB2	2.48	0.43
12:AW:165:TYR:CE1	12:AW:174:LYS:HB2	2.54	0.43
12:BA:27:ILE:HG22	12:BA:74:HIS:NE2	2.34	0.43
12:BA:165:TYR:CE1	12:BA:174:LYS:HB2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:BA:212:LEU:HD23	12:BA:212:LEU:C	2.43	0.43
12:BA:238:LYS:HD2	12:BA:238:LYS:HA	1.90	0.43
7:BB:26:LEU:HD23	7:BB:26:LEU:H	1.84	0.43
7:BB:516:GLU:O	7:BB:517:TYR:HB2	2.17	0.43
7:BB:833:GLN:N	7:BB:834:ALA:CA	2.82	0.43
14:BC:226:ILE:HG23	14:BC:230:LYS:NZ	2.33	0.43
14:BC:369:VAL:HG23	14:BC:370:VAL:N	2.34	0.43
11:BG:79:THR:CG2	11:BG:80:GLU:HB2	2.48	0.43
4:AJ:45:MET:HG3	12:AW:122:LYS:HE2	2.00	0.43
7:AR:271:ALA:O	7:AR:274:PHE:HB3	2.18	0.43
7:AR:768:TYR:HB3	7:AR:769:PRO:HD2	1.99	0.43
12:AW:30:PRO:O	12:AW:243:VAL:HG11	2.18	0.43
13:AX:38:ARG:HG2	13:AX:39:LYS:N	2.34	0.43
14:AY:237:ILE:HD13	14:AY:237:ILE:C	2.44	0.43
12:BA:228:GLY:C	12:BA:229:ILE:HG23	2.44	0.43
8:BD:13:ILE:HG21	8:BD:238:PRO:HB2	2.00	0.43
13:BP:38:ARG:HG2	13:BP:39:LYS:N	2.34	0.43
4:BQ:54:LEU:HA	4:BQ:59:ILE:CG2	2.49	0.43
4:AJ:45:MET:HB2	12:AW:122:LYS:CE	2.47	0.43
7:AR:592:VAL:HG22	7:AR:596:ASP:HB2	2.01	0.43
7:AR:942:ILE:O	7:AR:943:VAL:HB	2.19	0.43
8:AS:73:LEU:HD11	8:AS:236:LEU:CD2	2.48	0.43
8:AS:96:ILE:HG13	8:AS:143:ALA:HB3	2.00	0.43
11:AV:100:GLY:O	11:AV:104:LYS:HB2	2.19	0.43
12:AW:27:ILE:HG22	12:AW:74:HIS:NE2	2.33	0.43
12:AW:495:ILE:O	12:AW:605:ASN:HB2	2.18	0.43
12:AW:586:VAL:HG11	12:AW:611:ILE:HD11	2.01	0.43
12:AW:733:ALA:O	12:AW:734:ARG:C	2.61	0.43
13:AX:5:ARG:N	13:AX:6:CYS:HA	2.34	0.43
12:BA:417:VAL:O	12:BA:432:ALA:HA	2.19	0.43
7:BB:89:ARG:NH1	7:BB:156:ILE:HD11	2.33	0.43
7:BB:547:ARG:HA	7:BB:552:ILE:CG2	2.49	0.43
14:BC:237:ILE:C	14:BC:237:ILE:HD13	2.44	0.43
14:BC:333:GLY:O	14:BC:337:GLU:HG2	2.18	0.43
15:BH:65:ILE:HD12	15:BH:65:ILE:N	2.34	0.43
13:BP:17:GLN:HG3	13:BP:18:LEU:N	2.32	0.43
3:AI:50:LEU:HD12	3:AI:73:VAL:HG23	2.01	0.43
7:AR:73:VAL:HG13	7:AR:83:ILE:HD13	1.99	0.43
7:AR:235:ILE:HG22	7:AR:241:ILE:HG13	2.01	0.43
7:AR:298:LYS:HG3	7:AR:299:TYR:CD2	2.54	0.43
7:AR:361:PHE:O	7:AR:364:PHE:HB3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:AR:403:THR:HG23	7:AR:405:ASN:H	1.84	0.43
7:AR:733:THR:HG23	7:AR:735:TYR:CD2	2.53	0.43
8:AS:41:ILE:HD13	8:AS:145:LEU:HG	2.00	0.43
12:AW:31:ASP:C	12:AW:32:VAL:CG2	2.91	0.43
12:AW:372:TRP:CD1	12:AW:372:TRP:C	2.93	0.43
12:AW:728:MET:HA	12:AW:731:THR:HG22	2.01	0.43
12:BA:134:GLU:O	12:BA:138:LYS:HG2	2.19	0.43
12:BA:228:GLY:O	12:BA:229:ILE:HG12	2.18	0.43
12:BA:586:VAL:HG11	12:BA:611:ILE:HD11	2.01	0.43
12:BA:728:MET:HA	12:BA:731:THR:HG22	2.01	0.43
12:BA:747:LEU:HD21	12:BA:786:PHE:CD2	2.54	0.43
14:BC:145:GLU:C	14:BC:237:ILE:HD11	2.44	0.43
8:BD:260:LEU:HD23	8:BD:260:LEU:C	2.44	0.43
9:BE:13:ILE:CD1	9:BE:22:LEU:HG	2.48	0.43
9:BE:60:VAL:HG22	9:BE:61:PHE:N	2.34	0.43
10:BF:62:ILE:O	10:BF:63:ILE:CB	2.67	0.43
13:BP:20:VAL:O	13:BP:20:VAL:HG23	2.19	0.43
7:AR:572:ASN:HB3	7:AR:577:ARG:HD3	2.00	0.42
7:AR:1118:LEU:HD23	7:AR:1118:LEU:H	1.84	0.42
9:AT:123:VAL:O	9:AT:124:ARG:HB2	2.19	0.42
11:AV:64:LEU:HD21	11:AV:112:PHE:HB2	2.01	0.42
11:AV:70:ASP:OD2	11:AV:116:HIS:CD2	2.72	0.42
12:AW:505:GLY:HA3	12:AW:639:VAL:HG23	2.01	0.42
12:AW:662:TYR:O	12:AW:665:ILE:HG12	2.19	0.42
12:BA:31:ASP:C	12:BA:32:VAL:CG2	2.91	0.42
12:BA:358:ILE:HG23	12:BA:359:GLU:N	2.34	0.42
7:BB:255:LEU:C	7:BB:257:PRO:HD2	2.43	0.42
7:BB:525:LEU:HD13	7:BB:525:LEU:C	2.42	0.42
7:BB:646:TRP:CE2	7:BB:648:PRO:HG2	2.54	0.42
14:BC:348:GLU:CG	14:BC:349:VAL:N	2.82	0.42
8:BD:66:PRO:HG2	8:BD:124:ILE:HG12	2.00	0.42
2:AD:15:DT:H2"	2:AD:16:DA:OP1	2.18	0.42
3:AI:68:GLU:HG3	3:AI:74:LEU:HD21	2.01	0.42
3:AI:68:GLU:O	3:AI:73:VAL:HG22	2.19	0.42
7:AR:217:PHE:CB	7:AR:221:PRO:O	2.67	0.42
7:AR:226:PHE:CE1	7:AR:318:LEU:HD22	2.54	0.42
7:AR:745:ARG:HB2	7:AR:894:LEU:HB3	2.00	0.42
7:AR:928:MET:HE3	7:AR:953:ILE:HG21	2.01	0.42
9:AT:34:TYR:O	9:AT:35:GLN:C	2.62	0.42
14:AY:108:ILE:HA	14:AY:111:VAL:HG12	1.99	0.42
15:AZ:28:ALA:CB	15:AZ:62:ILE:HD11	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:BB:217:PHE:CB	7:BB:221:PRO:O	2.68	0.42
9:BE:9:SER:HB3	10:BF:4:VAL:HA	2.01	0.42
10:BF:72:LEU:HG	10:BF:84:ARG:NH2	2.34	0.42
10:BF:88:ILE:C	10:BF:90:ASP:H	2.27	0.42
11:BG:64:LEU:HD21	11:BG:112:PHE:HB2	2.01	0.42
11:BG:70:ASP:OD2	11:BG:116:HIS:CD2	2.72	0.42
3:AI:93:ARG:O	3:AI:94:LYS:HB2	2.18	0.42
7:AR:110:ILE:HD13	7:AR:110:ILE:N	2.34	0.42
7:AR:521:SER:HB3	7:AR:567:ASN:ND2	2.34	0.42
7:AR:841:VAL:HG12	7:AR:842:THR:N	2.34	0.42
9:AT:94:ASN:HB3	9:AT:120:TYR:CD2	2.54	0.42
12:AW:651:VAL:O	12:AW:651:VAL:HG12	2.17	0.42
12:AW:752:VAL:HG23	12:AW:752:VAL:O	2.19	0.42
14:AY:145:GLU:C	14:AY:237:ILE:HD11	2.43	0.42
14:AY:211:ALA:CA	14:AY:212:ASN:CB	2.93	0.42
14:AY:257:ASN:O	14:AY:261:VAL:HG23	2.18	0.42
14:AY:311:ARG:HA	14:AY:314:LEU:HD12	2.00	0.42
12:BA:505:GLY:HA3	12:BA:639:VAL:HG23	2.01	0.42
7:BB:298:LYS:HG3	7:BB:299:TYR:CD2	2.54	0.42
7:BB:403:THR:HG23	7:BB:405:ASN:H	1.84	0.42
7:BB:833:GLN:CA	7:BB:834:ALA:CB	2.97	0.42
7:BB:898:VAL:HG12	8:BD:30:ARG:CZ	2.50	0.42
9:BE:121:ASP:O	9:BE:125:GLY:HA2	2.20	0.42
9:BE:123:VAL:O	9:BE:124:ARG:HB2	2.19	0.42
2:AD:16:DA:OP1	2:AD:16:DA:C8	2.72	0.42
7:AR:217:PHE:HZ	7:AR:300:PHE:CA	2.32	0.42
7:AR:233:LEU:CD1	7:AR:315:ALA:HB2	2.49	0.42
7:AR:547:ARG:HA	7:AR:552:ILE:CG2	2.49	0.42
7:AR:675:MET:HE1	7:AR:888:LYS:HD3	2.00	0.42
12:AW:134:GLU:O	12:AW:138:LYS:HG2	2.19	0.42
12:AW:358:ILE:HG23	12:AW:359:GLU:N	2.33	0.42
14:AY:235:LYS:HE2	14:AY:261:VAL:HA	2.00	0.42
12:BA:40:ILE:HD13	12:BA:47:PRO:HG3	2.01	0.42
12:BA:53:GLU:HA	12:BA:54:PRO:HD3	1.93	0.42
12:BA:79:ARG:CB	12:BA:266:TRP:CZ3	3.02	0.42
12:BA:324:THR:HG22	12:BA:443:PHE:CD2	2.55	0.42
7:BB:226:PHE:CE1	7:BB:318:LEU:HD22	2.54	0.42
7:BB:233:LEU:CD1	7:BB:315:ALA:HB2	2.49	0.42
7:BB:592:VAL:HG22	7:BB:596:ASP:HB2	2.01	0.42
7:BB:942:ILE:O	7:BB:943:VAL:HB	2.19	0.42
7:BB:1020:THR:HG22	7:BB:1021:GLU:H	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:BD:172:ILE:HD11	8:BD:188:PHE:CE1	2.54	0.42
9:BE:80:VAL:HG12	9:BE:81:VAL:N	2.34	0.42
10:BF:52:ALA:O	10:BF:55:VAL:HG12	2.19	0.42
15:BH:45:ILE:HG22	15:BH:46:ARG:N	2.35	0.42
6:BN:3:ILE:HG22	6:BN:52:HIS:CD2	2.55	0.42
7:AR:76:SER:HA	7:AR:77:ASP:HA	1.73	0.42
7:AR:259:LEU:O	7:AR:263:SER:HB3	2.20	0.42
11:AV:64:LEU:N	11:AV:64:LEU:CD2	2.82	0.42
11:AV:78:VAL:C	11:AV:79:THR:HG1	2.27	0.42
11:AV:99:PHE:O	11:AV:99:PHE:CG	2.72	0.42
12:AW:92:GLU:O	12:AW:93:PHE:C	2.62	0.42
12:AW:103:ARG:HB3	12:AW:186:LYS:HB2	2.01	0.42
12:AW:228:GLY:C	12:AW:229:ILE:HG23	2.43	0.42
14:AY:274:THR:HG22	14:AY:276:ASN:H	1.83	0.42
12:BA:92:GLU:O	12:BA:93:PHE:C	2.62	0.42
12:BA:106:ILE:HD11	12:BA:154:PHE:CE1	2.54	0.42
12:BA:837:THR:HG23	12:BA:847:GLN:O	2.20	0.42
7:BB:63:LEU:HD22	7:BB:101:LEU:HD11	2.02	0.42
7:BB:742:ILE:HB	7:BB:912:ILE:HB	1.99	0.42
7:BB:841:VAL:HG12	7:BB:842:THR:N	2.34	0.42
11:BG:100:GLY:O	11:BG:104:LYS:HB2	2.20	0.42
6:BN:1:MET:O	6:BN:2:MET:HB2	2.19	0.42
2:BS:15:DT:H2"	2:BS:16:DA:OP1	2.18	0.42
4:AJ:54:LEU:HA	4:AJ:59:ILE:CG2	2.49	0.42
4:AJ:70:ASP:O	4:AJ:73:LYS:HG2	2.18	0.42
7:AR:94:THR:O	7:AR:96:ALA:N	2.53	0.42
7:AR:633:PRO:HA	7:AR:636:LEU:HD23	2.01	0.42
7:AR:918:LEU:N	7:AR:919:PRO:HD2	2.34	0.42
8:AS:93:TYR:HA	8:AS:145:LEU:O	2.20	0.42
9:AT:30:LEU:HD13	9:AT:72:PHE:CZ	2.54	0.42
9:AT:126:ILE:HG22	9:AT:137:GLN:HG2	2.02	0.42
10:AU:69:ARG:HG2	10:AU:69:ARG:NH1	2.34	0.42
11:AV:10:ILE:CD1	11:AV:58:PHE:CD2	3.02	0.42
11:AV:23:LEU:HD12	12:AW:512:LYS:HB2	2.00	0.42
12:AW:106:ILE:HD11	12:AW:154:PHE:CE1	2.54	0.42
14:AY:152:VAL:HA	14:AY:173:MET:HB3	2.02	0.42
14:AY:306:LEU:HD13	14:AY:306:LEU:H	1.84	0.42
12:BA:486:ILE:HD13	12:BA:628:MET:HE3	2.01	0.42
12:BA:683:GLU:CA	12:BA:684:LEU:CB	2.97	0.42
7:BB:125:MET:HE2	7:BB:153:GLY:C	2.44	0.42
7:BB:259:LEU:O	7:BB:263:SER:HB3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:BB:733:THR:HG23	7:BB:735:TYR:CD2	2.54	0.42
7:BB:872:LEU:HD23	7:BB:873:ARG:N	2.34	0.42
14:BC:122:MET:SD	14:BC:256:SER:HA	2.59	0.42
14:BC:152:VAL:HA	14:BC:173:MET:HB3	2.02	0.42
14:BC:173:MET:HA	14:BC:177:LYS:CD	2.50	0.42
9:BE:30:LEU:HD13	9:BE:72:PHE:CZ	2.54	0.42
10:BF:102:LYS:O	10:BF:106:ILE:HG13	2.19	0.42
11:BG:78:VAL:C	11:BG:79:THR:OG1	2.61	0.42
15:BH:28:ALA:CB	15:BH:62:ILE:HD11	2.49	0.42
3:BK:93:ARG:O	3:BK:94:LYS:HB2	2.18	0.42
2:AD:3:DT:O3'	2:AD:4:DA:C8	2.73	0.42
6:AO:5:ILE:HD13	8:AS:61:ARG:HA	2.02	0.42
7:AR:63:LEU:HD22	7:AR:101:LEU:HD11	2.02	0.42
7:AR:450:GLY:HA3	12:AW:760:GLY:HA2	2.01	0.42
7:AR:633:PRO:HA	7:AR:636:LEU:CD2	2.49	0.42
7:AR:840:ILE:N	7:AR:840:ILE:HD12	2.35	0.42
7:AR:1008:ALA:HB2	12:AW:346:THR:HG22	2.02	0.42
10:AU:88:ILE:C	10:AU:90:ASP:H	2.26	0.42
12:AW:370:ASP:O	12:AW:371:LYS:HB3	2.20	0.42
12:AW:421:ARG:HB2	12:AW:462:MET:HE3	2.02	0.42
12:AW:687:ILE:HD12	12:AW:688:PRO:HD2	2.02	0.42
13:AX:33:ILE:HD12	13:AX:33:ILE:N	2.34	0.42
12:BA:323:ARG:HB2	7:BB:1029:LEU:HD11	2.02	0.42
12:BA:752:VAL:HG23	12:BA:752:VAL:O	2.18	0.42
7:BB:94:THR:O	7:BB:96:ALA:N	2.53	0.42
8:BD:78:TRP:HB3	8:BD:79:PRO:CD	2.49	0.42
10:BF:7:VAL:HG12	10:BF:8:GLU:HG2	2.01	0.42
15:BH:9:ILE:C	15:BH:9:ILE:HD12	2.45	0.42
7:AR:56:ILE:CG2	7:AR:59:LEU:HB2	2.49	0.42
7:AR:833:GLN:N	7:AR:834:ALA:CA	2.82	0.42
7:AR:885:HIS:CE1	7:AR:925:GLY:C	2.97	0.42
9:AT:60:VAL:HG22	9:AT:61:PHE:N	2.34	0.42
9:AT:82:GLN:HE22	10:AU:89:MET:HE1	1.85	0.42
9:AT:171:LYS:HG3	9:AT:172:LEU:N	2.35	0.42
10:AU:52:ALA:O	10:AU:55:VAL:HG12	2.19	0.42
12:AW:105:LYS:HZ2	12:AW:140:ALA:CB	2.23	0.42
12:AW:418:LEU:HD23	12:AW:430:MET:HE2	2.02	0.42
14:AY:122:MET:SD	14:AY:256:SER:HA	2.59	0.42
12:BA:35:GLU:O	12:BA:39:PRO:HD2	2.20	0.42
7:BB:217:PHE:HZ	7:BB:300:PHE:CA	2.32	0.42
7:BB:521:SER:HB3	7:BB:567:ASN:ND2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:BB:706:VAL:HG11	7:BB:929:GLU:HG2	2.01	0.42
7:BB:1111:ILE:O	7:BB:1111:ILE:HG22	2.18	0.42
14:BC:268:ASP:O	14:BC:272:VAL:HG23	2.20	0.42
9:BE:132:SER:O	9:BE:133:LYS:HG2	2.20	0.42
10:BF:69:ARG:HG2	10:BF:69:ARG:HH11	1.85	0.42
10:BF:69:ARG:HG2	10:BF:69:ARG:NH1	2.34	0.42
11:BG:99:PHE:O	11:BG:99:PHE:CG	2.72	0.42
15:BH:62:ILE:HG13	15:BH:62:ILE:O	2.19	0.42
3:AI:67:GLU:O	3:AI:71:ARG:HG2	2.19	0.42
4:AJ:59:ILE:HG12	4:AJ:60:SER:N	2.35	0.42
7:AR:478:GLN:HG2	7:AR:479:ILE:N	2.34	0.42
8:AS:33:MET:HE3	8:AS:162:ALA:HB3	2.02	0.42
12:AW:21:LYS:O	12:AW:22:MET:C	2.63	0.42
12:AW:284:LEU:HD13	12:AW:285:PRO:HD2	2.02	0.42
12:AW:417:VAL:HG11	12:AW:464:LEU:HD11	2.02	0.42
14:AY:211:ALA:HA	14:AY:212:ASN:CB	2.48	0.42
12:BA:28:ILE:HG21	12:BA:243:VAL:HG21	2.02	0.42
12:BA:372:TRP:HB3	12:BA:373:PRO:CD	2.42	0.42
12:BA:422:GLN:HA	12:BA:423:PRO:C	2.45	0.42
12:BA:510:THR:CG2	12:BA:552:VAL:HG21	2.50	0.42
7:BB:478:GLN:HG2	7:BB:479:ILE:N	2.35	0.42
7:BB:633:PRO:HA	7:BB:636:LEU:CD2	2.49	0.42
7:BB:918:LEU:N	7:BB:919:PRO:HD2	2.34	0.42
8:BD:61:ARG:CZ	6:BN:5:ILE:HD11	2.49	0.42
9:BE:171:LYS:HG3	9:BE:172:LEU:N	2.35	0.42
3:BK:50:LEU:HD12	3:BK:73:VAL:HG23	2.01	0.42
3:BK:68:GLU:O	3:BK:73:VAL:HG22	2.19	0.42
2:AD:6:DA:C2	2:AD:7:DG:C2	3.08	0.42
7:AR:247:LEU:HD11	7:AR:503:VAL:HG12	2.02	0.42
7:AR:485:GLU:O	7:AR:486:LYS:C	2.63	0.42
7:AR:872:LEU:HD23	7:AR:873:ARG:N	2.35	0.42
12:AW:52:ILE:HG21	12:AW:217:ILE:HG22	2.02	0.42
12:AW:103:ARG:HB3	12:AW:186:LYS:CB	2.49	0.42
12:AW:324:THR:HG22	12:AW:443:PHE:CD2	2.54	0.42
12:AW:362:ARG:O	12:AW:365:VAL:HG12	2.20	0.42
12:AW:737:VAL:HG13	12:AW:738:LEU:N	2.35	0.42
12:AW:830:LEU:HD11	14:AY:319:VAL:HG21	2.01	0.42
13:AX:20:VAL:HG23	13:AX:20:VAL:O	2.20	0.42
14:AY:268:ASP:O	14:AY:272:VAL:HG23	2.20	0.42
12:BA:101:CYS:SG	12:BA:152:LYS:CG	3.07	0.42
12:BA:431:MET:CE	12:BA:482:VAL:HA	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:BA:646:MET:HE2	12:BA:725:ALA:HB2	2.02	0.42
7:BB:213:PHE:CZ	7:BB:326:ILE:CG2	3.03	0.42
14:BC:306:LEU:H	14:BC:306:LEU:HD13	1.83	0.42
11:BG:42:ILE:HG12	11:BG:43:ILE:N	2.35	0.42
6:BN:3:ILE:HD13	6:BN:18:TRP:CB	2.50	0.42
13:BP:5:ARG:N	13:BP:17:GLN:HA	2.35	0.42
2:BS:3:DT:O3'	2:BS:4:DA:C8	2.73	0.42
7:AR:480:ALA:HB2	7:AR:579:ARG:HD3	2.02	0.41
7:AR:632:GLU:HB3	7:AR:633:PRO:HD2	2.01	0.41
7:AR:1059:THR:HG22	7:AR:1060:THR:N	2.35	0.41
8:AS:66:PRO:HG2	8:AS:124:ILE:HG12	2.01	0.41
8:AS:260:LEU:HD23	8:AS:260:LEU:C	2.44	0.41
10:AU:69:ARG:HG2	10:AU:69:ARG:HH11	1.85	0.41
12:AW:79:ARG:CB	12:AW:266:TRP:CZ3	3.03	0.41
12:AW:106:ILE:HG22	12:AW:143:ALA:HB3	2.02	0.41
12:AW:431:MET:CE	12:AW:482:VAL:HA	2.50	0.41
12:AW:749:GLN:NE2	12:AW:756:ARG:HG2	2.35	0.41
13:AX:10:TRP:HB2	13:AX:31:TYR:CE2	2.55	0.41
15:AZ:9:ILE:C	15:AZ:9:ILE:HD12	2.44	0.41
12:BA:52:ILE:HG21	12:BA:217:ILE:HG22	2.02	0.41
12:BA:519:GLU:O	12:BA:523:GLN:HB2	2.20	0.41
7:BB:73:VAL:HG13	7:BB:83:ILE:HD13	2.00	0.41
7:BB:110:ILE:HD13	7:BB:110:ILE:N	2.34	0.41
7:BB:217:PHE:O	7:BB:221:PRO:HA	2.20	0.41
11:BG:64:LEU:N	11:BG:64:LEU:CD2	2.82	0.41
4:AJ:72:TYR:CE1	4:AJ:76:GLU:HG2	2.55	0.41
6:AO:22:ILE:HG13	6:AO:26:ASN:OD1	2.20	0.41
7:AR:691:THR:HG23	7:AR:691:THR:O	2.20	0.41
8:AS:172:ILE:HD11	8:AS:188:PHE:CE1	2.54	0.41
9:AT:121:ASP:O	9:AT:125:GLY:HA2	2.20	0.41
12:AW:113:LYS:O	12:AW:117:ILE:HG13	2.21	0.41
12:AW:388:LEU:O	12:AW:389:ARG:C	2.63	0.41
14:AY:8:LYS:N	14:AY:8:LYS:HD2	2.35	0.41
14:AY:149:ILE:O	14:AY:153:VAL:HG12	2.21	0.41
15:AZ:45:ILE:HG22	15:AZ:46:ARG:N	2.35	0.41
12:BA:103:ARG:HB3	12:BA:186:LYS:CB	2.49	0.41
12:BA:146:CYS:HB3	12:BA:149:CYS:HB2	1.72	0.41
7:BB:632:GLU:HB3	7:BB:633:PRO:HD2	2.02	0.41
7:BB:633:PRO:HA	7:BB:636:LEU:HD23	2.01	0.41
7:BB:741:ILE:HG23	7:BB:911:VAL:HG13	2.02	0.41
7:BB:1118:LEU:H	7:BB:1118:LEU:HD23	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:BC:211:ALA:CB	14:BC:213:ILE:N	2.84	0.41
8:BD:121:ILE:HD12	8:BD:121:ILE:N	2.36	0.41
4:AJ:35:LYS:O	4:AJ:35:LYS:HD3	2.21	0.41
4:AJ:48:THR:HG22	15:AZ:80:TYR:OH	2.20	0.41
10:AU:91:SER:HB2	10:AU:92:ASN:CA	2.41	0.41
12:AW:192:VAL:CG2	12:AW:199:PRO:HB3	2.50	0.41
12:AW:510:THR:CG2	12:AW:552:VAL:HG21	2.50	0.41
12:AW:684:LEU:HD12	12:AW:685:GLU:N	2.35	0.41
12:AW:802:GLY:O	12:AW:803:ARG:C	2.63	0.41
14:AY:262:LEU:HD11	14:AY:283:VAL:HG11	2.02	0.41
12:BA:32:VAL:O	12:BA:44:VAL:HG11	2.20	0.41
12:BA:421:ARG:HB2	12:BA:462:MET:HE3	2.02	0.41
12:BA:687:ILE:HD12	12:BA:688:PRO:HD2	2.02	0.41
7:BB:743:MET:HE1	7:BB:875:PRO:HB2	2.01	0.41
7:BB:877:ILE:H	7:BB:877:ILE:HD12	1.85	0.41
7:BB:1064:CYS:CB	7:BB:1067:CYS:HB2	2.50	0.41
13:BP:5:ARG:N	13:BP:6:CYS:HA	2.34	0.41
6:AO:3:ILE:HG22	6:AO:52:HIS:CD2	2.55	0.41
7:AR:213:PHE:CZ	7:AR:326:ILE:CG2	3.04	0.41
7:AR:591:LEU:O	7:AR:592:VAL:CB	2.68	0.41
7:AR:706:VAL:HG11	7:AR:929:GLU:HG2	2.02	0.41
8:AS:115:LYS:O	8:AS:116:SER:HB2	2.20	0.41
12:AW:96:ALA:HB1	12:AW:105:LYS:HZ3	1.85	0.41
12:AW:184:LEU:O	12:AW:187:VAL:CG2	2.68	0.41
12:AW:249:LEU:HD21	12:AW:265:LEU:HB2	2.02	0.41
12:AW:417:VAL:CG1	12:AW:418:LEU:N	2.84	0.41
12:AW:422:GLN:HA	12:AW:423:PRO:C	2.44	0.41
13:AX:5:ARG:N	13:AX:17:GLN:HA	2.35	0.41
14:AY:173:MET:HA	14:AY:177:LYS:CD	2.50	0.41
14:AY:234:ILE:O	14:AY:235:LYS:HB2	2.20	0.41
12:BA:285:PRO:HA	12:BA:286:PRO:HD3	1.92	0.41
14:BC:8:LYS:HD2	14:BC:8:LYS:N	2.35	0.41
14:BC:234:ILE:O	14:BC:235:LYS:HB2	2.21	0.41
3:BK:67:GLU:O	3:BK:71:ARG:HG2	2.20	0.41
4:BQ:42:GLU:O	4:BQ:45:MET:HB3	2.20	0.41
7:AR:778:MET:HE1	7:AR:792:TYR:CG	2.55	0.41
7:AR:1110:MET:C	7:AR:1111:ILE:HD12	2.46	0.41
8:AS:38:VAL:HG12	8:AS:39:MET:N	2.36	0.41
8:AS:121:ILE:HD12	8:AS:121:ILE:N	2.36	0.41
10:AU:87:LEU:CD2	10:AU:87:LEU:O	2.69	0.41
11:AV:42:ILE:HG12	11:AV:43:ILE:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:AW:33:TYR:CA	12:AW:34:ASP:CB	2.99	0.41
12:AW:162:TYR:O	12:AW:162:TYR:CG	2.73	0.41
12:AW:837:THR:HG23	12:AW:847:GLN:O	2.19	0.41
14:AY:365:GLU:O	14:AY:366:PHE:HB2	2.20	0.41
15:AZ:63:ILE:HG22	15:AZ:65:ILE:CD1	2.50	0.41
7:BB:591:LEU:O	7:BB:592:VAL:CB	2.67	0.41
14:BC:244:LYS:HB3	14:BC:249:TYR:HD1	1.85	0.41
14:BC:320:MET:HE2	14:BC:329:ILE:HD13	2.02	0.41
8:BD:189:GLU:HG2	8:BD:198:LYS:HE3	2.02	0.41
10:BF:75:ILE:C	10:BF:76:CYS:HG	2.29	0.41
10:BF:91:SER:HB3	10:BF:92:ASN:C	2.46	0.41
11:BG:96:ILE:HD12	11:BG:99:PHE:CB	2.51	0.41
15:BH:63:ILE:HG22	15:BH:65:ILE:CD1	2.50	0.41
4:BQ:34:PRO:O	4:BQ:35:LYS:CB	2.67	0.41
2:BS:4:DA:H2"	2:BS:5:DG:OP2	2.20	0.41
2:BS:6:DA:C2	2:BS:7:DG:C2	3.08	0.41
2:BS:16:DA:OP1	2:BS:16:DA:C8	2.73	0.41
6:AO:3:ILE:HD13	6:AO:18:TRP:CB	2.50	0.41
6:AO:40:VAL:O	6:AO:41:LYS:HB2	2.21	0.41
9:AT:80:VAL:HG12	9:AT:81:VAL:N	2.34	0.41
12:AW:684:LEU:O	12:AW:685:GLU:C	2.63	0.41
15:AZ:45:ILE:HG12	15:AZ:79:ARG:CD	2.50	0.41
12:BA:184:LEU:O	12:BA:187:VAL:CG2	2.68	0.41
12:BA:370:ASP:O	12:BA:371:LYS:HB3	2.20	0.41
12:BA:749:GLN:NE2	12:BA:756:ARG:HG2	2.35	0.41
7:BB:56:ILE:CG2	7:BB:59:LEU:HB2	2.49	0.41
7:BB:675:MET:HE1	7:BB:888:LYS:HD3	2.01	0.41
7:BB:691:THR:O	7:BB:691:THR:HG23	2.20	0.41
9:BE:167:PRO:O	9:BE:168:TYR:HB2	2.21	0.41
10:BF:41:LEU:HA	10:BF:44:VAL:HG12	2.03	0.41
10:BF:76:CYS:N	10:BF:77:PRO:HD3	2.36	0.41
15:BH:45:ILE:HG13	15:BH:79:ARG:HB2	2.02	0.41
2:BS:15:DT:C1'	2:BS:16:DA:P	3.08	0.41
6:AO:5:ILE:HD11	8:AS:61:ARG:CB	2.51	0.41
7:AR:877:ILE:H	7:AR:877:ILE:HD12	1.85	0.41
8:AS:15:LEU:HD11	8:AS:242:LEU:HD13	2.03	0.41
9:AT:132:SER:O	9:AT:133:LYS:HG2	2.20	0.41
10:AU:7:VAL:HG12	10:AU:8:GLU:HG2	2.02	0.41
12:AW:35:GLU:O	12:AW:39:PRO:HD2	2.20	0.41
14:AY:277:ILE:HD13	14:AY:293:ILE:HD13	2.02	0.41
12:BA:684:LEU:HD12	12:BA:685:GLU:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:BA:692:LEU:N	12:BA:692:LEU:CD1	2.83	0.41
7:BB:201:VAL:HG23	7:BB:202:PRO:HD2	2.03	0.41
7:BB:462:PRO:CG	7:BB:470:VAL:HG13	2.51	0.41
7:BB:778:MET:HE1	7:BB:792:TYR:CG	2.55	0.41
7:BB:840:ILE:N	7:BB:840:ILE:HD12	2.35	0.41
7:BB:885:HIS:CE1	7:BB:925:GLY:C	2.98	0.41
7:BB:1110:MET:C	7:BB:1111:ILE:HD12	2.45	0.41
8:BD:115:LYS:O	8:BD:116:SER:HB2	2.20	0.41
10:BF:68:VAL:O	10:BF:71:VAL:HG12	2.21	0.41
5:BL:18:GLU:HA	5:BL:52:LYS:HG2	2.03	0.41
7:AR:283:GLN:O	7:AR:283:GLN:HG3	2.21	0.41
7:AR:1117:ILE:HD11	12:AW:10:LYS:HE3	2.02	0.41
7:AR:1124:LEU:HD23	7:AR:1124:LEU:C	2.46	0.41
9:AT:126:ILE:CD1	9:AT:135:VAL:HG13	2.51	0.41
9:AT:167:PRO:O	9:AT:168:TYR:HB2	2.21	0.41
12:AW:77:LEU:HB2	12:AW:210:THR:O	2.21	0.41
12:AW:115:SER:HA	12:AW:118:TYR:HD2	1.86	0.41
12:AW:333:SER:OG	12:AW:625:LYS:HE3	2.21	0.41
12:AW:519:GLU:O	12:AW:523:GLN:HB2	2.20	0.41
14:AY:211:ALA:CB	14:AY:213:ILE:N	2.83	0.41
14:AY:226:ILE:HG23	14:AY:230:LYS:HE3	2.03	0.41
14:AY:320:MET:HE2	14:AY:329:ILE:HD13	2.02	0.41
12:BA:21:LYS:O	12:BA:22:MET:C	2.63	0.41
12:BA:33:TYR:CA	12:BA:34:ASP:CB	2.99	0.41
12:BA:33:TYR:O	12:BA:41:GLU:CB	2.68	0.41
12:BA:192:VAL:CG2	12:BA:199:PRO:HB3	2.50	0.41
12:BA:263:GLU:O	12:BA:266:TRP:HB3	2.21	0.41
7:BB:938:LEU:HD23	6:BN:43:TYR:HB3	2.02	0.41
9:BE:30:LEU:CD2	9:BE:72:PHE:CE2	3.04	0.41
9:BE:126:ILE:CD1	9:BE:135:VAL:HG13	2.51	0.41
2:AD:4:DA:H2"	2:AD:5:DG:OP2	2.20	0.41
2:AD:15:DT:C1'	2:AD:16:DA:P	3.07	0.41
3:AI:23:TRP:CZ3	3:AI:26:LYS:HE3	2.56	0.41
7:AR:26:LEU:HD23	7:AR:26:LEU:H	1.84	0.41
7:AR:539:LEU:HD13	7:AR:539:LEU:C	2.46	0.41
7:AR:741:ILE:O	7:AR:891:ILE:HA	2.20	0.41
7:AR:748:VAL:CG1	7:AR:875:PRO:HG2	2.50	0.41
7:AR:1020:THR:HG22	7:AR:1021:GLU:H	1.85	0.41
8:AS:78:TRP:HB3	8:AS:79:PRO:CD	2.49	0.41
9:AT:30:LEU:CD2	9:AT:72:PHE:CE2	3.04	0.41
10:AU:91:SER:HB3	10:AU:92:ASN:C	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:AV:96:ILE:HD12	11:AV:99:PHE:CB	2.51	0.41
12:AW:28:ILE:HG21	12:AW:243:VAL:HG21	2.02	0.41
12:AW:33:TYR:O	12:AW:41:GLU:CB	2.68	0.41
12:AW:646:MET:HE2	12:AW:725:ALA:HB2	2.01	0.41
12:AW:687:ILE:HG22	12:AW:695:SER:HB2	2.02	0.41
12:AW:812:ARG:HG3	14:AY:86:THR:HG22	2.02	0.41
12:AW:827:LEU:HB3	14:AY:71:GLY:CA	2.51	0.41
13:AX:41:THR:HG22	13:AX:42:ILE:N	2.35	0.41
14:AY:122:MET:HE2	14:AY:124:ILE:HD11	2.03	0.41
14:AY:196:PHE:CD1	14:AY:196:PHE:C	2.99	0.41
14:AY:199:ASP:HB2	14:AY:206:LEU:HD23	2.03	0.41
14:AY:265:LYS:N	14:AY:265:LYS:HD2	2.36	0.41
14:AY:289:ALA:O	14:AY:292:ILE:HG22	2.20	0.41
15:AZ:63:ILE:HD12	15:AZ:63:ILE:N	2.36	0.41
12:BA:77:LEU:HB2	12:BA:210:THR:O	2.21	0.41
12:BA:107:SER:HB2	12:BA:108:GLU:HB2	2.03	0.41
12:BA:249:LEU:HD21	12:BA:265:LEU:HB2	2.03	0.41
12:BA:684:LEU:O	12:BA:685:GLU:C	2.63	0.41
12:BA:687:ILE:HG22	12:BA:695:SER:HB2	2.02	0.41
12:BA:747:LEU:HD11	12:BA:790:LEU:HD21	2.03	0.41
12:BA:823:LEU:HD13	14:BC:75:ALA:HA	2.03	0.41
12:BA:870:ARG:HA	12:BA:870:ARG:HD2	1.91	0.41
7:BB:108:ASN:O	7:BB:110:ILE:HD13	2.21	0.41
7:BB:359:VAL:HG13	7:BB:360:ALA:N	2.36	0.41
7:BB:562:VAL:O	7:BB:563:THR:C	2.64	0.41
7:BB:741:ILE:O	7:BB:891:ILE:HA	2.20	0.41
7:BB:748:VAL:CG1	7:BB:875:PRO:HG2	2.50	0.41
14:BC:199:ASP:HB2	14:BC:206:LEU:HD23	2.03	0.41
14:BC:289:ALA:O	14:BC:292:ILE:HG22	2.20	0.41
14:BC:365:GLU:O	14:BC:366:PHE:HB2	2.20	0.41
8:BD:79:PRO:HG2	8:BD:149:TYR:CD2	2.56	0.41
10:BF:87:LEU:CD2	10:BF:87:LEU:O	2.68	0.41
11:BG:64:LEU:HD23	11:BG:114:LYS:HE3	2.03	0.41
6:BN:18:TRP:O	6:BN:19:GLN:C	2.64	0.41
4:BQ:72:TYR:CE1	4:BQ:76:GLU:HG2	2.56	0.41
2:AD:15:DT:H1'	2:AD:16:DA:OP2	2.21	0.41
3:AI:34:ARG:NE	9:AT:61:PHE:CE1	2.89	0.41
4:AJ:35:LYS:HD3	4:AJ:35:LYS:HA	1.79	0.41
7:AR:217:PHE:O	7:AR:221:PRO:HA	2.20	0.41
7:AR:737:MET:SD	12:AW:447:LEU:HD13	2.61	0.41
7:AR:743:MET:HE1	7:AR:875:PRO:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:AS:17:PHE:O	8:AS:225:LYS:HA	2.21	0.41
8:AS:189:GLU:HG2	8:AS:198:LYS:HE3	2.03	0.41
10:AU:88:ILE:CG2	10:AU:92:ASN:OD1	2.69	0.41
12:AW:32:VAL:O	12:AW:44:VAL:HG11	2.20	0.41
12:AW:40:ILE:HD13	12:AW:47:PRO:HG3	2.02	0.41
12:AW:263:GLU:O	12:AW:266:TRP:HB3	2.21	0.41
12:AW:687:ILE:CD1	12:AW:688:PRO:HD2	2.50	0.41
12:AW:769:PHE:CD2	12:AW:778:ALA:HA	2.56	0.41
12:AW:879:LYS:HE3	14:AY:40:GLU:O	2.21	0.41
12:BA:103:ARG:HB3	12:BA:186:LYS:HB2	2.01	0.41
12:BA:107:SER:OG	12:BA:140:ALA:HB2	2.20	0.41
12:BA:113:LYS:O	12:BA:117:ILE:HG13	2.21	0.41
12:BA:162:TYR:O	12:BA:162:TYR:CG	2.73	0.41
12:BA:417:VAL:CG1	12:BA:418:LEU:N	2.84	0.41
7:BB:273:ASP:O	7:BB:277:SER:N	2.54	0.41
7:BB:306:THR:O	7:BB:306:THR:HG22	2.21	0.41
7:BB:485:GLU:O	7:BB:486:LYS:C	2.64	0.41
7:BB:488:VAL:HG21	7:BB:573:CYS:SG	2.61	0.41
7:BB:705:LEU:O	7:BB:706:VAL:CG1	2.69	0.41
7:BB:1061:ILE:HD11	7:BB:1101:LYS:HD2	2.02	0.41
8:BD:33:MET:HE3	8:BD:162:ALA:HB3	2.02	0.41
8:BD:38:VAL:HG12	8:BD:39:MET:N	2.36	0.41
15:BH:45:ILE:HG12	15:BH:79:ARG:CD	2.50	0.41
5:BL:5:ILE:O	5:BL:5:ILE:HG13	2.20	0.41
13:BP:10:TRP:HB2	13:BP:31:TYR:CE2	2.56	0.41
7:AR:668:ARG:HA	7:AR:668:ARG:HD3	1.94	0.40
7:AR:1061:ILE:HD11	7:AR:1101:LYS:HD2	2.02	0.40
10:AU:75:ILE:C	10:AU:76:CYS:HG	2.29	0.40
10:AU:104:ILE:HG22	10:AU:104:ILE:O	2.21	0.40
12:AW:266:TRP:CD1	12:AW:266:TRP:C	2.99	0.40
12:AW:366:ILE:HD13	12:AW:366:ILE:C	2.46	0.40
12:AW:516:LEU:HD23	12:AW:524:ILE:HD12	2.03	0.40
13:AX:10:TRP:CB	13:AX:31:TYR:CE2	3.05	0.40
12:BA:96:ALA:HB1	12:BA:105:LYS:HZ3	1.86	0.40
12:BA:98:CYS:O	12:BA:154:PHE:CE1	2.75	0.40
12:BA:103:ARG:HB3	12:BA:186:LYS:C	2.46	0.40
12:BA:443:PHE:CZ	12:BA:464:LEU:HB2	2.56	0.40
12:BA:516:LEU:HD23	12:BA:524:ILE:HD12	2.03	0.40
12:BA:737:VAL:HG13	12:BA:738:LEU:N	2.36	0.40
7:BB:247:LEU:HD11	7:BB:503:VAL:HG12	2.02	0.40
7:BB:283:GLN:HG3	7:BB:283:GLN:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:BB:480:ALA:HB2	7:BB:579:ARG:HD3	2.03	0.40
7:BB:665:GLN:O	7:BB:666:SER:C	2.65	0.40
14:BC:149:ILE:O	14:BC:153:VAL:HG12	2.21	0.40
14:BC:226:ILE:HG23	14:BC:230:LYS:HE3	2.03	0.40
8:BD:93:TYR:HA	8:BD:145:LEU:O	2.20	0.40
5:BL:32:LEU:HD13	5:BL:57:ILE:HG12	2.04	0.40
6:BN:40:VAL:O	6:BN:41:LYS:HB2	2.21	0.40
4:BQ:44:LEU:O	4:BQ:48:THR:HG23	2.20	0.40
4:AJ:53:ASN:O	4:AJ:57:GLY:C	2.64	0.40
6:AO:18:TRP:O	6:AO:19:GLN:C	2.64	0.40
7:AR:273:ASP:O	7:AR:277:SER:N	2.54	0.40
11:AV:59:ILE:N	11:AV:59:ILE:HD12	2.36	0.40
12:AW:40:ILE:CG2	12:AW:41:GLU:N	2.84	0.40
12:AW:107:SER:OG	12:AW:140:ALA:HB2	2.20	0.40
14:AY:179:VAL:HG12	14:AY:180:THR:O	2.21	0.40
12:BA:95:LYS:HD3	12:BA:141:MET:CE	2.51	0.40
12:BA:106:ILE:HG22	12:BA:143:ALA:HB3	2.02	0.40
12:BA:541:ALA:HB2	11:BG:72:CYS:N	2.36	0.40
12:BA:687:ILE:CD1	12:BA:688:PRO:HD2	2.50	0.40
12:BA:802:GLY:O	12:BA:803:ARG:C	2.64	0.40
7:BB:235:ILE:HG22	7:BB:241:ILE:HG13	2.01	0.40
7:BB:238:ASP:CG	7:BB:259:LEU:HD11	2.46	0.40
7:BB:364:PHE:CZ	7:BB:388:VAL:HG13	2.56	0.40
7:BB:996:LEU:HD12	7:BB:996:LEU:N	2.37	0.40
14:BC:122:MET:HE2	14:BC:124:ILE:HD11	2.03	0.40
14:BC:179:VAL:HG12	14:BC:180:THR:O	2.21	0.40
14:BC:231:ILE:O	14:BC:232:LYS:HB2	2.21	0.40
14:BC:277:ILE:HD13	14:BC:293:ILE:HD13	2.03	0.40
8:BD:17:PHE:O	8:BD:225:LYS:HA	2.21	0.40
8:BD:97:TYR:C	8:BD:98:ILE:HD12	2.46	0.40
8:BD:134:GLY:N	6:BN:60:ILE:HD11	2.36	0.40
10:BF:20:LEU:N	10:BF:20:LEU:HD12	2.36	0.40
11:BG:55:VAL:HG12	11:BG:117:GLN:HA	2.03	0.40
13:BP:41:THR:HG22	13:BP:42:ILE:N	2.36	0.40
2:AD:14:DA:H2"	2:AD:15:DT:O5'	2.21	0.40
5:AM:1:MET:SD	8:AS:256:LEU:HB2	2.61	0.40
5:AM:86:GLU:OE1	8:AS:3:ILE:N	2.54	0.40
6:AO:5:ILE:HD11	8:AS:61:ARG:HB3	2.03	0.40
7:AR:56:ILE:HA	7:AR:57:PRO:HD3	1.98	0.40
8:AS:164:VAL:HA	8:AS:227:ILE:O	2.22	0.40
10:AU:41:LEU:HA	10:AU:44:VAL:HG12	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:AW:95:LYS:HD3	12:AW:141:MET:CE	2.52	0.40
12:AW:815:GLN:HB3	14:AY:108:ILE:HD11	2.03	0.40
14:AY:29:VAL:HG23	14:AY:52:PHE:HE1	1.86	0.40
14:AY:244:LYS:HB3	14:AY:249:TYR:HD1	1.85	0.40
14:AY:349:VAL:HB	14:AY:353:HIS:ND1	2.36	0.40
12:BA:83:HIS:CD2	12:BA:277:PHE:CE2	3.10	0.40
12:BA:108:GLU:HG3	12:BA:147:PRO:HG2	2.03	0.40
12:BA:417:VAL:HG11	12:BA:464:LEU:HD11	2.02	0.40
12:BA:505:GLY:CA	12:BA:639:VAL:HG23	2.51	0.40
12:BA:769:PHE:CD2	12:BA:778:ALA:HA	2.56	0.40
7:BB:235:ILE:HG23	7:BB:240:ASP:HB3	2.04	0.40
7:BB:539:LEU:HD13	7:BB:539:LEU:C	2.46	0.40
7:BB:952:PRO:O	7:BB:954:GLU:N	2.54	0.40
14:BC:265:LYS:HD2	14:BC:265:LYS:N	2.36	0.40
8:BD:15:LEU:HD11	8:BD:242:LEU:HD13	2.03	0.40
11:BG:46:ILE:HG12	11:BG:46:ILE:O	2.21	0.40
11:BG:59:ILE:HD12	11:BG:59:ILE:N	2.36	0.40
6:BN:19:GLN:N	6:BN:20:PRO:HD2	2.37	0.40
4:BQ:59:ILE:HG12	4:BQ:60:SER:N	2.36	0.40
4:BQ:73:LYS:HG3	4:BQ:74:ASP:N	2.36	0.40
7:AR:201:VAL:HG23	7:AR:202:PRO:HD2	2.04	0.40
7:AR:359:VAL:HG13	7:AR:360:ALA:N	2.36	0.40
7:AR:462:PRO:CG	7:AR:470:VAL:HG13	2.51	0.40
7:AR:705:LEU:O	7:AR:706:VAL:CG1	2.69	0.40
8:AS:162:ALA:C	8:AS:163:ILE:HD12	2.47	0.40
10:AU:20:LEU:N	10:AU:20:LEU:HD12	2.36	0.40
11:AV:46:ILE:HG12	11:AV:46:ILE:O	2.21	0.40
14:AY:219:LEU:HA	14:AY:222:LEU:HD23	2.03	0.40
12:BA:127:SER:O	12:BA:131:ARG:CD	2.69	0.40
12:BA:284:LEU:HD13	12:BA:285:PRO:HD2	2.02	0.40
12:BA:418:LEU:HD23	12:BA:430:MET:HE2	2.03	0.40
12:BA:539:ILE:HG21	11:BG:46:ILE:HD11	2.02	0.40
12:BA:541:ALA:O	12:BA:542:PRO:C	2.63	0.40
12:BA:728:MET:CE	7:BB:919:PRO:HG3	2.51	0.40
7:BB:500:VAL:O	7:BB:504:ILE:HG12	2.21	0.40
7:BB:1033:GLU:O	7:BB:1036:ARG:HB3	2.21	0.40
7:BB:1124:LEU:HD23	7:BB:1124:LEU:C	2.46	0.40
14:BC:16:LYS:HE2	14:BC:49:ASP:HA	2.04	0.40
14:BC:42:LEU:CA	14:BC:43:VAL:HG23	2.50	0.40
5:BL:69:LEU:O	5:BL:73:ILE:HG12	2.22	0.40
2:BS:14:DA:H2"	2:BS:15:DT:O5'	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AI:93:ARG:O	3:AI:94:LYS:CB	2.69	0.40
4:AJ:36:LEU:HD21	12:AW:131:ARG:CZ	2.51	0.40
4:AJ:46:LYS:O	4:AJ:50:ILE:HG13	2.21	0.40
5:AM:18:GLU:HA	5:AM:52:LYS:HG2	2.04	0.40
5:AM:69:LEU:O	5:AM:73:ILE:HG12	2.22	0.40
7:AR:72:ARG:NH1	7:AR:74:ARG:CG	2.85	0.40
7:AR:108:ASN:O	7:AR:110:ILE:HD13	2.21	0.40
7:AR:311:ARG:HA	7:AR:314:LYS:HE2	2.04	0.40
7:AR:364:PHE:HB2	7:AR:393:VAL:HG22	2.04	0.40
7:AR:637:THR:HB	7:AR:638:PRO:HD2	2.03	0.40
7:AR:741:ILE:HG23	7:AR:911:VAL:HG13	2.03	0.40
9:AT:126:ILE:HD12	9:AT:135:VAL:HG13	2.04	0.40
11:AV:61:LYS:O	11:AV:62:ASN:CB	2.70	0.40
11:AV:94:THR:CG2	11:AV:96:ILE:HD11	2.52	0.40
12:AW:110:GLU:OE2	12:AW:148:HIS:CE1	2.75	0.40
12:AW:747:LEU:HD11	12:AW:790:LEU:HD21	2.04	0.40
14:AY:170:ASP:O	14:AY:174:LEU:HD12	2.21	0.40
14:AY:223:ARG:HG2	14:AY:227:LEU:HD13	2.04	0.40
12:BA:40:ILE:CG2	12:BA:41:GLU:N	2.84	0.40
12:BA:228:GLY:C	12:BA:230:ARG:H	2.30	0.40
12:BA:333:SER:OG	12:BA:625:LYS:HE3	2.20	0.40
12:BA:357:ASN:O	12:BA:358:ILE:C	2.65	0.40
12:BA:456:ASP:CG	12:BA:458:ASP:CG	2.90	0.40
12:BA:864:LYS:HD2	12:BA:867:ASP:CA	2.52	0.40
7:BB:72:ARG:NH1	7:BB:74:ARG:CG	2.85	0.40
7:BB:91:ARG:HB2	7:BB:93:LEU:HD13	2.04	0.40
7:BB:752:MET:HE1	7:BB:910:ASP:HB3	2.04	0.40
7:BB:957:GLN:HA	7:BB:960:ILE:HG12	2.04	0.40
7:BB:1084:ILE:N	7:BB:1084:ILE:HD12	2.37	0.40
14:BC:29:VAL:HG23	14:BC:52:PHE:HE1	1.86	0.40
14:BC:223:ARG:HG2	14:BC:227:LEU:HD13	2.03	0.40
14:BC:262:LEU:HD11	14:BC:283:VAL:HG11	2.02	0.40
8:BD:205:LEU:O	8:BD:207:GLU:N	2.55	0.40
8:BD:230:LEU:HD12	8:BD:242:LEU:CD2	2.52	0.40
11:BG:31:MET:HE1	11:BG:55:VAL:HG21	2.04	0.40
5:BL:3:ILE:CG2	5:BL:15:LEU:HD11	2.52	0.40
13:BP:37:VAL:HG22	13:BP:38:ARG:N	2.37	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	
3	AI	82/95 (86%)	68 (83%)	9 (11%)	5 (6%)	1	13
3	BK	82/95 (86%)	68 (83%)	9 (11%)	5 (6%)	1	13
4	AJ	47/104 (45%)	39 (83%)	4 (8%)	4 (8%)	0	9
4	BQ	48/104 (46%)	39 (81%)	4 (8%)	5 (10%)	0	6
5	AM	89/92 (97%)	82 (92%)	5 (6%)	2 (2%)	5	29
5	BL	89/92 (97%)	81 (91%)	6 (7%)	2 (2%)	5	29
6	AO	63/66 (96%)	47 (75%)	9 (14%)	7 (11%)	0	6
6	BN	63/66 (96%)	47 (75%)	9 (14%)	7 (11%)	0	6
7	AR	1097/1131 (97%)	925 (84%)	129 (12%)	43 (4%)	2	19
7	BB	1097/1131 (97%)	925 (84%)	130 (12%)	42 (4%)	2	19
8	AS	260/265 (98%)	218 (84%)	36 (14%)	6 (2%)	5	28
8	BD	260/265 (98%)	218 (84%)	36 (14%)	6 (2%)	5	28
9	AT	167/180 (93%)	150 (90%)	15 (9%)	2 (1%)	10	42
9	BE	167/180 (93%)	150 (90%)	15 (9%)	2 (1%)	10	42
10	AU	103/113 (91%)	79 (77%)	18 (18%)	6 (6%)	1	14
10	BF	103/113 (91%)	79 (77%)	18 (18%)	6 (6%)	1	14
11	AV	111/132 (84%)	80 (72%)	25 (22%)	6 (5%)	1	15
11	BG	111/132 (84%)	80 (72%)	25 (22%)	6 (5%)	1	15
12	AW	868/880 (99%)	716 (82%)	121 (14%)	31 (4%)	2	20
12	BA	868/880 (99%)	717 (83%)	121 (14%)	30 (4%)	3	20
13	AX	42/48 (88%)	29 (69%)	10 (24%)	3 (7%)	1	11
13	BP	42/48 (88%)	29 (69%)	10 (24%)	3 (7%)	1	11
14	AY	372/395 (94%)	303 (82%)	50 (13%)	19 (5%)	1	15
14	BC	372/395 (94%)	303 (82%)	50 (13%)	19 (5%)	1	15
15	AZ	74/84 (88%)	64 (86%)	6 (8%)	4 (5%)	1	15

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
15	BH	74/84 (88%)	64 (86%)	6 (8%)	4 (5%)	1 15
All	All	6751/7170 (94%)	5600 (83%)	876 (13%)	275 (4%)	2 18

All (275) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	AI	55	ASN
4	AJ	37	SER
4	AJ	58	LYS
4	AJ	59	ILE
6	AO	3	ILE
6	AO	9	THR
6	AO	64	ARG
7	AR	52	ILE
7	AR	113	GLU
7	AR	221	PRO
7	AR	285	ARG
7	AR	953	ILE
7	AR	1015	LEU
9	AT	126	ILE
11	AV	17	SER
11	AV	107	SER
12	AW	34	ASP
12	AW	43	SER
12	AW	44	VAL
12	AW	229	ILE
12	AW	291	SER
12	AW	541	ALA
12	AW	684	LEU
12	AW	764	ARG
13	AX	17	GLN
14	AY	41	VAL
14	AY	43	VAL
15	AZ	13	ILE
15	AZ	44	TRP
12	BA	34	ASP
12	BA	43	SER
12	BA	44	VAL
12	BA	229	ILE
12	BA	291	SER
12	BA	541	ALA
12	BA	684	LEU

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Mol	Chain	Res	Type
12	BA	764	ARG
7	BB	52	ILE
7	BB	113	GLU
7	BB	221	PRO
7	BB	285	ARG
7	BB	953	ILE
7	BB	1015	LEU
14	BC	41	VAL
14	BC	43	VAL
9	BE	126	ILE
11	BG	17	SER
11	BG	107	SER
15	BH	13	ILE
15	BH	44	TRP
3	BK	55	ASN
6	BN	3	ILE
6	BN	9	THR
6	BN	64	ARG
13	BP	17	GLN
4	BQ	37	SER
4	BQ	58	LYS
4	BQ	59	ILE
3	AI	61	VAL
6	AO	39	GLY
6	AO	40	VAL
7	AR	95	TYR
7	AR	197	ALA
7	AR	407	VAL
7	AR	592	VAL
7	AR	735	TYR
7	AR	836	ARG
7	AR	943	VAL
7	AR	1009	ARG
8	AS	87	GLU
10	AU	4	VAL
12	AW	71	HIS
12	AW	372	TRP
13	AX	8	LYS
14	AY	127	THR
14	AY	163	MET
14	AY	193	LEU
14	AY	210	PHE

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Mol	Chain	Res	Type
14	AY	349	VAL
12	BA	71	HIS
12	BA	372	TRP
7	BB	95	TYR
7	BB	197	ALA
7	BB	407	VAL
7	BB	592	VAL
7	BB	735	TYR
7	BB	836	ARG
7	BB	943	VAL
7	BB	1009	ARG
14	BC	127	THR
14	BC	163	MET
14	BC	193	LEU
14	BC	210	PHE
14	BC	349	VAL
8	BD	87	GLU
10	BF	4	VAL
11	BG	79	THR
3	BK	61	VAL
6	BN	39	GLY
6	BN	40	VAL
13	BP	8	LYS
3	AI	47	ALA
3	AI	54	ASN
7	AR	41	LYS
7	AR	267	ASN
7	AR	283	GLN
7	AR	706	VAL
7	AR	844	HIS
7	AR	1056	SER
7	AR	1078	ASN
8	AS	206	CYS
11	AV	51	GLN
11	AV	79	THR
12	AW	29	THR
12	AW	161	PRO
12	AW	734	ARG
12	AW	814	SER
12	AW	849	ALA
13	AX	9	CYS
14	AY	101	THR

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Mol	Chain	Res	Type
14	AY	113	ALA
14	AY	129	GLU
14	AY	146	TYR
14	AY	180	THR
12	BA	29	THR
12	BA	161	PRO
12	BA	734	ARG
12	BA	814	SER
12	BA	849	ALA
7	BB	41	LYS
7	BB	267	ASN
7	BB	283	GLN
7	BB	706	VAL
7	BB	844	HIS
7	BB	1056	SER
7	BB	1078	ASN
14	BC	101	THR
14	BC	113	ALA
14	BC	129	GLU
14	BC	146	TYR
14	BC	180	THR
8	BD	206	CYS
11	BG	51	GLN
3	BK	47	ALA
3	BK	54	ASN
13	BP	9	CYS
4	BQ	36	LEU
4	AJ	36	LEU
7	AR	24	LYS
7	AR	53	PRO
7	AR	187	THR
7	AR	334	GLU
7	AR	460	GLU
7	AR	1076	ASN
8	AS	90	GLU
8	AS	130	ILE
8	AS	205	LEU
10	AU	63	ILE
10	AU	83	VAL
12	AW	257	ALA
12	AW	308	ARG
14	AY	211	ALA

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Mol	Chain	Res	Type
14	AY	217	ALA
14	AY	331	ARG
14	AY	350	THR
15	AZ	12	ARG
12	BA	151	GLU
12	BA	257	ALA
12	BA	308	ARG
7	BB	24	LYS
7	BB	53	PRO
7	BB	187	THR
7	BB	334	GLU
7	BB	460	GLU
7	BB	1076	ASN
14	BC	211	ALA
14	BC	217	ALA
14	BC	331	ARG
14	BC	350	THR
8	BD	90	GLU
8	BD	130	ILE
8	BD	205	LEU
10	BF	63	ILE
10	BF	83	VAL
11	BG	106	ILE
15	BH	12	ARG
3	AI	50	LEU
5	AM	39	SER
5	AM	62	SER
6	AO	41	LYS
6	AO	63	THR
7	AR	213	PHE
7	AR	223	LYS
7	AR	281	ILE
7	AR	563	THR
7	AR	733	THR
7	AR	775	LYS
7	AR	952	PRO
7	AR	1053	LEU
7	AR	1075	LYS
9	AT	50	ASN
10	AU	31	SER
10	AU	93	ARG
11	AV	47	ASN

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Mol	Chain	Res	Type
11	AV	106	ILE
12	AW	103	ARG
12	AW	108	GLU
12	AW	126	PRO
12	AW	151	GLU
12	AW	393	ASP
12	AW	599	ASP
12	AW	866	VAL
14	AY	237	ILE
12	BA	103	ARG
12	BA	108	GLU
12	BA	126	PRO
12	BA	393	ASP
12	BA	599	ASP
12	BA	866	VAL
7	BB	213	PHE
7	BB	223	LYS
7	BB	281	ILE
7	BB	563	THR
7	BB	733	THR
7	BB	775	LYS
7	BB	952	PRO
7	BB	1053	LEU
7	BB	1075	LYS
14	BC	237	ILE
9	BE	50	ASN
10	BF	31	SER
10	BF	93	ARG
11	BG	47	ASN
3	BK	50	LEU
5	BL	39	SER
5	BL	62	SER
6	BN	41	LYS
6	BN	63	THR
4	BQ	33	PHE
7	AR	690	ARG
10	AU	68	VAL
12	AW	39	PRO
12	AW	255	ALA
12	AW	812	ARG
14	AY	328	GLN
12	BA	39	PRO

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Mol	Chain	Res	Type
12	BA	255	ALA
12	BA	812	ARG
14	BC	328	GLN
10	BF	68	VAL
7	AR	27	VAL
7	AR	918	LEU
7	AR	1114	PRO
12	AW	284	LEU
12	AW	688	PRO
15	AZ	43	PRO
12	BA	284	LEU
12	BA	688	PRO
7	BB	27	VAL
7	BB	918	LEU
7	BB	1114	PRO
15	BH	43	PRO
7	AR	203	VAL
8	AS	83	ILE
7	BB	203	VAL
8	BD	83	ILE
7	AR	234	GLY
14	AY	216	ILE
7	BB	234	GLY
14	BC	216	ILE
7	AR	350	GLY
12	BA	876	VAL
7	BB	350	GLY
12	AW	437	VAL
12	AW	876	VAL

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	
3	AI	74/83 (89%)	74 (100%)	0	100	100
3	BK	74/83 (89%)	74 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	AJ	47/96 (49%)	44 (94%)	3 (6%)	16 38
4	BQ	48/96 (50%)	46 (96%)	2 (4%)	26 48
5	AM	79/80 (99%)	79 (100%)	0	100 100
5	BL	79/80 (99%)	79 (100%)	0	100 100
6	AO	59/60 (98%)	57 (97%)	2 (3%)	32 54
6	BN	59/60 (98%)	57 (97%)	2 (3%)	32 54
7	AR	951/975 (98%)	914 (96%)	37 (4%)	28 50
7	BB	951/975 (98%)	914 (96%)	37 (4%)	28 50
8	AS	235/238 (99%)	234 (100%)	1 (0%)	84 82
8	BD	235/238 (99%)	234 (100%)	1 (0%)	84 82
9	AT	150/158 (95%)	143 (95%)	7 (5%)	23 46
9	BE	150/158 (95%)	143 (95%)	7 (5%)	23 46
10	AU	99/107 (92%)	92 (93%)	7 (7%)	13 36
10	BF	99/107 (92%)	92 (93%)	7 (7%)	13 36
11	AV	106/125 (85%)	101 (95%)	5 (5%)	23 46
11	BG	106/125 (85%)	101 (95%)	5 (5%)	23 46
12	AW	758/766 (99%)	722 (95%)	36 (5%)	23 46
12	BA	758/766 (99%)	722 (95%)	36 (5%)	23 46
13	AX	40/43 (93%)	40 (100%)	0	100 100
13	BP	40/43 (93%)	40 (100%)	0	100 100
14	AY	324/341 (95%)	308 (95%)	16 (5%)	22 45
14	BC	324/341 (95%)	308 (95%)	16 (5%)	22 45
15	AZ	69/75 (92%)	69 (100%)	0	100 100
15	BH	69/75 (92%)	69 (100%)	0	100 100
All	All	5983/6294 (95%)	5756 (96%)	227 (4%)	29 51

All (227) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	AJ	33	PHE
4	AJ	35	LYS
4	AJ	46	LYS
6	AO	7	CYS
6	AO	61	HIS

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Mol	Chain	Res	Type
7	AR	54	THR
7	AR	72	ARG
7	AR	93	LEU
7	AR	101	LEU
7	AR	110	ILE
7	AR	166	THR
7	AR	217	PHE
7	AR	224	ILE
7	AR	230	MET
7	AR	233	LEU
7	AR	318	LEU
7	AR	326	ILE
7	AR	330	LEU
7	AR	345	ARG
7	AR	376	LYS
7	AR	421	ASN
7	AR	422	TRP
7	AR	470	VAL
7	AR	529	LEU
7	AR	592	VAL
7	AR	711	LEU
7	AR	730	ILE
7	AR	733	THR
7	AR	735	TYR
7	AR	872	LEU
7	AR	908	VAL
7	AR	913	LEU
7	AR	929	GLU
7	AR	950	LYS
7	AR	953	ILE
7	AR	1020	THR
7	AR	1023	ARG
7	AR	1025	ARG
7	AR	1061	ILE
7	AR	1070	ILE
7	AR	1077	LYS
7	AR	1081	VAL
8	AS	209	CYS
9	AT	16	ASN
9	AT	27	LEU
9	AT	61	PHE
9	AT	90	LEU

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Mol	Chain	Res	Type
9	AT	93	ASP
9	AT	120	TYR
9	AT	126	ILE
10	AU	36	ARG
10	AU	41	LEU
10	AU	76	CYS
10	AU	78	ILE
10	AU	86	ILE
10	AU	87	LEU
10	AU	88	ILE
11	AV	7	GLN
11	AV	65	SER
11	AV	79	THR
11	AV	101	LEU
11	AV	109	LYS
12	AW	29	THR
12	AW	32	VAL
12	AW	52	ILE
12	AW	68	CYS
12	AW	77	LEU
12	AW	99	ARG
12	AW	100	ARG
12	AW	101	CYS
12	AW	111	ILE
12	AW	124	ARG
12	AW	145	VAL
12	AW	159	GLU
12	AW	160	LYS
12	AW	162	TYR
12	AW	187	VAL
12	AW	229	ILE
12	AW	232	GLU
12	AW	233	ASP
12	AW	284	LEU
12	AW	289	HIS
12	AW	342	ILE
12	AW	366	ILE
12	AW	378	VAL
12	AW	426	HIS
12	AW	464	LEU
12	AW	478	GLU
12	AW	500	GLN

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Mol	Chain	Res	Type
12	AW	534	LEU
12	AW	540	LEU
12	AW	547	THR
12	AW	606	GLN
12	AW	647	ARG
12	AW	648	LEU
12	AW	726	TYR
12	AW	809	THR
12	AW	865	THR
14	AY	70	ILE
14	AY	159	ASP
14	AY	180	THR
14	AY	196	PHE
14	AY	208	ILE
14	AY	210	PHE
14	AY	216	ILE
14	AY	219	LEU
14	AY	231	ILE
14	AY	232	LYS
14	AY	237	ILE
14	AY	244	LYS
14	AY	306	LEU
14	AY	307	ASP
14	AY	315	LEU
14	AY	319	VAL
12	BA	29	THR
12	BA	32	VAL
12	BA	52	ILE
12	BA	68	CYS
12	BA	77	LEU
12	BA	99	ARG
12	BA	100	ARG
12	BA	101	CYS
12	BA	111	ILE
12	BA	124	ARG
12	BA	145	VAL
12	BA	159	GLU
12	BA	160	LYS
12	BA	162	TYR
12	BA	187	VAL
12	BA	229	ILE
12	BA	232	GLU

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Mol	Chain	Res	Type
12	BA	233	ASP
12	BA	284	LEU
12	BA	289	HIS
12	BA	342	ILE
12	BA	366	ILE
12	BA	378	VAL
12	BA	426	HIS
12	BA	464	LEU
12	BA	478	GLU
12	BA	500	GLN
12	BA	534	LEU
12	BA	540	LEU
12	BA	547	THR
12	BA	606	GLN
12	BA	647	ARG
12	BA	648	LEU
12	BA	726	TYR
12	BA	809	THR
12	BA	865	THR
7	BB	54	THR
7	BB	72	ARG
7	BB	93	LEU
7	BB	101	LEU
7	BB	110	ILE
7	BB	166	THR
7	BB	217	PHE
7	BB	224	ILE
7	BB	230	MET
7	BB	233	LEU
7	BB	318	LEU
7	BB	326	ILE
7	BB	330	LEU
7	BB	345	ARG
7	BB	376	LYS
7	BB	421	ASN
7	BB	422	TRP
7	BB	470	VAL
7	BB	529	LEU
7	BB	592	VAL
7	BB	711	LEU
7	BB	730	ILE
7	BB	733	THR

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Mol	Chain	Res	Type
7	BB	735	TYR
7	BB	872	LEU
7	BB	908	VAL
7	BB	913	LEU
7	BB	929	GLU
7	BB	950	LYS
7	BB	953	ILE
7	BB	1020	THR
7	BB	1023	ARG
7	BB	1025	ARG
7	BB	1061	ILE
7	BB	1070	ILE
7	BB	1077	LYS
7	BB	1081	VAL
14	BC	70	ILE
14	BC	159	ASP
14	BC	180	THR
14	BC	196	PHE
14	BC	208	ILE
14	BC	210	PHE
14	BC	216	ILE
14	BC	219	LEU
14	BC	231	ILE
14	BC	232	LYS
14	BC	237	ILE
14	BC	244	LYS
14	BC	306	LEU
14	BC	307	ASP
14	BC	315	LEU
14	BC	319	VAL
8	BD	209	CYS
9	BE	16	ASN
9	BE	27	LEU
9	BE	61	PHE
9	BE	90	LEU
9	BE	93	ASP
9	BE	120	TYR
9	BE	126	ILE
10	BF	36	ARG
10	BF	41	LEU
10	BF	76	CYS
10	BF	78	ILE

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Mol	Chain	Res	Type
10	BF	86	ILE
10	BF	87	LEU
10	BF	88	ILE
11	BG	7	GLN
11	BG	65	SER
11	BG	79	THR
11	BG	101	LEU
11	BG	109	LYS
6	BN	7	CYS
6	BN	61	HIS
4	BQ	35	LYS
4	BQ	46	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
5	AM	47	HIS
5	AM	82	HIS
7	AR	167	GLN
7	AR	613	GLN
7	AR	640	HIS
7	AR	664	ASN
7	AR	702	GLN
7	AR	885	HIS
7	AR	1005	HIS
8	AS	26	ASN
9	AT	82	GLN
9	AT	100	ASN
11	AV	25	ASN
11	AV	88	ASN
11	AV	116	HIS
12	AW	83	HIS
12	AW	148	HIS
12	AW	237	HIS
12	AW	246	ASN
12	AW	272	HIS
12	AW	357	ASN
12	AW	500	GLN
12	AW	630	ASN
12	AW	862	HIS
14	AY	339	ASN
14	AY	353	HIS

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Mol	Chain	Res	Type
12	BA	148	HIS
12	BA	237	HIS
12	BA	246	ASN
12	BA	272	HIS
12	BA	357	ASN
12	BA	500	GLN
12	BA	630	ASN
12	BA	862	HIS
7	BB	613	GLN
7	BB	626	ASN
7	BB	640	HIS
7	BB	663	HIS
7	BB	664	ASN
7	BB	885	HIS
7	BB	1005	HIS
7	BB	1018	GLN
14	BC	339	ASN
9	BE	166	GLN
11	BG	7	GLN
11	BG	25	ASN
11	BG	88	ASN
11	BG	116	HIS
5	BL	82	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 16 ligands modelled in this entry, 14 are monoatomic - leaving 2 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	$\#\|Z\| > 2$
17	SF4	BD	1001	8	0,9,12	-	-	-		
17	SF4	AS	1001	8	0,9,12	-	-	-		

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
17	SF4	BD	1001	8	-	-	0/3/3/5
17	SF4	AS	1001	8	-	-	0/3/3/5

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.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	BD	1001	SF4	3	0
17	AS	1001	SF4	2	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	AC	13/14 (92%)	0.81	0 100 100	228, 239, 256, 263	0
1	BR	14/14 (100%)	0.56	0 100 100	206, 215, 246, 250	0
2	AD	15/16 (93%)	1.17	3 (20%) 3 6	229, 238, 257, 259	0
2	BS	16/16 (100%)	1.01	1 (6%) 26 26	200, 212, 236, 244	0
3	AI	84/95 (88%)	0.47	2 (2%) 59 47	154, 162, 172, 177	0
3	BK	84/95 (88%)	0.67	3 (3%) 46 37	143, 160, 171, 176	0
4	AJ	49/104 (47%)	0.43	1 (2%) 65 50	190, 209, 231, 239	0
4	BQ	50/104 (48%)	0.46	0 100 100	190, 203, 221, 226	0
5	AM	91/92 (98%)	0.39	3 (3%) 49 39	164, 176, 184, 188	0
5	BL	91/92 (98%)	0.71	7 (7%) 19 22	154, 167, 174, 176	0
6	AO	65/66 (98%)	0.40	3 (4%) 37 33	174, 181, 194, 203	0
6	BN	65/66 (98%)	0.47	1 (1%) 72 56	153, 168, 186, 193	0
7	AR	1103/1131 (97%)	0.66	72 (6%) 25 25	147, 164, 182, 199	0
7	BB	1103/1131 (97%)	0.66	73 (6%) 24 25	135, 158, 178, 194	0
8	AS	262/265 (98%)	0.50	9 (3%) 48 38	167, 186, 200, 208	0
8	BD	262/265 (98%)	0.52	13 (4%) 34 31	153, 170, 193, 213	0
9	AT	171/180 (95%)	0.39	4 (2%) 61 48	165, 200, 235, 249	0
9	BE	171/180 (95%)	0.57	9 (5%) 32 30	164, 195, 236, 253	0
10	AU	105/113 (92%)	0.38	3 (2%) 53 41	184, 226, 255, 280	0
10	BF	105/113 (92%)	0.43	2 (1%) 66 52	177, 214, 242, 264	0
11	AV	113/132 (85%)	0.49	6 (5%) 32 30	166, 185, 206, 213	0
11	BG	113/132 (85%)	0.61	8 (7%) 22 24	153, 175, 196, 202	0
12	AW	872/880 (99%)	0.61	46 (5%) 32 30	144, 166, 201, 225	0
12	BA	872/880 (99%)	0.60	54 (6%) 26 27	135, 158, 184, 203	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	AX	44/48 (91%)	0.46	0 100 100	167, 180, 190, 193	0
13	BP	44/48 (91%)	0.82	2 (4%) 38 33	154, 177, 188, 192	0
14	AY	376/395 (95%)	0.61	25 (6%) 24 25	155, 169, 195, 211	0
14	BC	376/395 (95%)	0.60	25 (6%) 24 25	142, 162, 189, 205	0
15	AZ	76/84 (90%)	0.63	3 (3%) 43 36	164, 177, 186, 190	0
15	BH	76/84 (90%)	0.46	4 (5%) 32 30	149, 163, 172, 176	0
All	All	6881/7230 (95%)	0.59	382 (5%) 30 29	135, 167, 211, 280	0

All (382) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
15	AZ	57	ALA	6.2
12	BA	119	ASN	6.2
12	AW	808	ASP	5.2
7	AR	68	ILE	4.9
12	AW	119	ASN	4.6
7	BB	1116	LEU	4.6
7	AR	913	LEU	4.5
12	AW	28	ILE	4.5
7	AR	727	LEU	4.5
11	BG	46	ILE	4.5
7	AR	716	TYR	4.4
8	AS	168	PRO	4.4
15	BH	60	GLY	4.3
7	AR	1052	LEU	4.3
7	AR	343	ASN	4.2
12	BA	861	ALA	4.2
7	BB	911	VAL	4.2
14	BC	137	ALA	4.2
7	AR	42	LEU	4.0
7	AR	144	ILE	4.0
12	BA	530	VAL	4.0
7	BB	122	LEU	3.9
12	AW	132	LEU	3.9
7	AR	175	VAL	3.8
7	BB	127	LYS	3.8
12	BA	644	PHE	3.8
12	AW	24	VAL	3.7
14	AY	17	VAL	3.7
7	AR	423	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
5	BL	57	ILE	3.6
7	AR	911	VAL	3.6
7	BB	175	VAL	3.6
14	AY	342	LEU	3.5
7	BB	68	ILE	3.5
12	AW	530	VAL	3.5
5	AM	17	ILE	3.5
12	BA	208	ILE	3.5
11	BG	87	ASN	3.5
14	AY	326	VAL	3.5
2	BS	17	DG	3.5
11	AV	46	ILE	3.5
7	AR	653	ILE	3.5
7	BB	42	LEU	3.4
12	AW	325	VAL	3.4
5	BL	17	ILE	3.4
12	AW	159	GLU	3.4
7	BB	727	LEU	3.4
14	AY	374	ILE	3.3
14	BC	320	MET	3.3
7	BB	558	VAL	3.3
7	AR	46	ILE	3.3
7	BB	343	ASN	3.3
14	AY	363	VAL	3.3
7	BB	126	LEU	3.3
12	BA	24	VAL	3.3
11	BG	71	PHE	3.3
7	AR	476	MET	3.3
14	AY	243	GLN	3.2
12	AW	527	VAL	3.2
12	BA	672	VAL	3.2
12	BA	496	ILE	3.2
12	BA	122	LYS	3.2
7	BB	66	ILE	3.2
12	BA	28	ILE	3.2
8	AS	6	LEU	3.2
12	AW	672	VAL	3.2
7	AR	710	ALA	3.2
8	BD	62	LEU	3.2
7	AR	66	ILE	3.2
12	BA	29	THR	3.1
7	BB	46	ILE	3.1

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Mol	Chain	Res	Type	RSRZ
7	AR	1116	LEU	3.1
7	AR	130	ILE	3.1
12	BA	532	ILE	3.1
5	BL	15	LEU	3.0
7	BB	176	LEU	3.0
11	AV	87	ASN	3.0
12	BA	628	MET	3.0
12	BA	80	PRO	3.0
7	BB	945	ALA	3.0
14	AY	78	VAL	3.0
12	AW	81	VAL	3.0
11	AV	95	ILE	3.0
7	BB	1039	LEU	3.0
14	AY	236	GLY	3.0
7	AR	1106	GLU	3.0
7	BB	250	GLU	3.0
12	AW	528	ALA	3.0
12	BA	18	GLU	3.0
12	BA	103	ARG	2.9
14	AY	303	GLU	2.9
7	AR	176	LEU	2.9
12	AW	525	LEU	2.9
7	BB	1006	ALA	2.9
7	AR	63	LEU	2.9
10	AU	34	LEU	2.9
7	BB	177	VAL	2.9
7	BB	423	LEU	2.9
8	BD	127	ASP	2.9
7	BB	171	ALA	2.9
7	BB	454	GLY	2.9
7	BB	365	VAL	2.9
9	AT	60	VAL	2.9
7	AR	383	ALA	2.9
7	AR	733	THR	2.9
8	BD	81	GLU	2.9
14	BC	339	ASN	2.9
7	BB	913	LEU	2.8
12	AW	489	PRO	2.8
7	AR	558	VAL	2.8
7	AR	776	ILE	2.8
14	AY	373	ILE	2.8
12	BA	648	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
7	AR	54	THR	2.8
7	AR	1006	ALA	2.8
14	BC	388	LEU	2.8
14	BC	313	ILE	2.8
7	BB	83	ILE	2.8
12	AW	676	ILE	2.8
5	BL	70	LEU	2.8
7	BB	996	LEU	2.8
13	BP	35	PHE	2.8
7	AR	126	LEU	2.7
7	BB	330	LEU	2.7
15	AZ	71	LEU	2.7
7	BB	155	PHE	2.7
7	BB	124	ILE	2.7
14	BC	342	LEU	2.7
7	AR	714	ILE	2.7
12	BA	603	ILE	2.7
14	BC	212	ASN	2.7
8	BD	256	LEU	2.7
12	AW	653	LEU	2.7
12	AW	824	ILE	2.7
12	BA	137	LYS	2.7
11	BG	92	TYR	2.6
14	BC	86	THR	2.6
7	AR	424	SER	2.6
7	BB	144	ILE	2.6
7	BB	937	ALA	2.6
12	AW	639	VAL	2.6
7	BB	141	LEU	2.6
12	BA	192	VAL	2.6
14	BC	378	PRO	2.6
3	BK	78	ILE	2.6
12	AW	700	ILE	2.6
14	AY	360	ARG	2.6
7	AR	148	PRO	2.6
12	BA	857	PRO	2.6
12	BA	413	ASP	2.6
10	BF	104	ILE	2.6
14	BC	376	GLY	2.6
7	BB	787	LYS	2.6
14	AY	203	GLY	2.6
14	BC	203	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
7	BB	401	LEU	2.6
12	BA	612	LEU	2.6
2	AD	17	DG	2.6
7	AR	155	PHE	2.5
12	BA	395	LYS	2.5
15	BH	83	SER	2.5
7	AR	270	ASP	2.5
8	BD	249	ILE	2.5
12	AW	704	LEU	2.5
8	AS	81	GLU	2.5
14	AY	274	THR	2.5
7	BB	492	LEU	2.5
7	BB	1052	LEU	2.5
11	BG	48	ILE	2.5
8	BD	25	VAL	2.5
14	AY	305	GLY	2.5
7	AR	12	GLU	2.5
7	AR	191	LYS	2.5
5	BL	69	LEU	2.5
14	BC	55	ALA	2.5
7	BB	337	ASP	2.5
14	AY	362	ASP	2.5
7	AR	57	PRO	2.5
9	BE	14	PRO	2.5
7	BB	776	ILE	2.5
12	AW	6	ILE	2.5
5	BL	50	THR	2.5
12	AW	807	VAL	2.5
14	AY	41	VAL	2.5
14	BC	20	ALA	2.5
7	BB	1106	GLU	2.5
12	AW	694	GLU	2.5
7	AR	418	ASP	2.5
7	BB	178	ASP	2.5
12	BA	484	LYS	2.5
7	BB	653	ILE	2.5
7	BB	714	ILE	2.5
2	AD	14	DA	2.5
7	AR	978	THR	2.5
12	BA	809	THR	2.5
14	BC	365	GLU	2.5
14	AY	354	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
7	AR	812	VAL	2.5
7	BB	108	ASN	2.5
12	BA	105	LYS	2.5
11	AV	88	ASN	2.5
9	BE	151	SER	2.4
7	BB	27	VAL	2.4
12	BA	207	MET	2.4
7	AR	787	LYS	2.4
12	BA	528	ALA	2.4
12	BA	486	ILE	2.4
14	AY	86	THR	2.4
12	AW	207	MET	2.4
12	AW	413	ASP	2.4
7	BB	191	LYS	2.4
12	AW	826	ALA	2.4
7	AR	704	PRO	2.4
8	BD	116	SER	2.4
9	BE	17	GLU	2.4
14	BC	305	GLY	2.4
7	AR	141	LEU	2.4
7	AR	1031	PHE	2.4
14	BC	373	ILE	2.4
2	AD	16	DA	2.4
7	BB	1069	TYR	2.4
7	BB	215	VAL	2.4
7	BB	254	GLU	2.4
12	BA	643	GLY	2.4
9	AT	65	ALA	2.4
12	AW	105	LYS	2.4
12	AW	809	THR	2.4
7	BB	1010	GLY	2.4
11	BG	97	SER	2.4
12	AW	75	ILE	2.4
12	BA	852	ASP	2.4
12	AW	59	PRO	2.4
12	BA	790	LEU	2.4
7	AR	108	ASN	2.4
11	BG	88	ASN	2.4
7	BB	112	ALA	2.3
10	AU	100	ILE	2.3
12	AW	559	ASP	2.3
12	BA	559	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
12	AW	594	LEU	2.3
7	BB	1047	LEU	2.3
8	BD	168	PRO	2.3
3	AI	56	ILE	2.3
7	BB	328	LEU	2.3
14	BC	377	HIS	2.3
12	AW	588	ILE	2.3
12	BA	56	GLN	2.3
12	BA	523	GLN	2.3
12	AW	484	LYS	2.3
14	BC	32	LEU	2.3
8	BD	3	ILE	2.3
9	AT	103	PRO	2.3
9	BE	80	VAL	2.3
12	BA	807	VAL	2.3
7	AR	122	LEU	2.3
8	AS	243	LEU	2.3
7	BB	179	THR	2.3
15	BH	62	ILE	2.3
7	AR	99	LEU	2.3
7	AR	1118	LEU	2.3
8	AS	173	LEU	2.3
12	BA	427	ARG	2.3
12	BA	676	ILE	2.3
7	BB	530	VAL	2.3
12	BA	209	LEU	2.3
7	AR	899	ASP	2.3
7	BB	985	ARG	2.3
7	AR	49	GLN	2.3
12	BA	232	GLU	2.2
12	BA	694	GLU	2.2
15	AZ	41	GLN	2.3
7	BB	814	ILE	2.2
8	AS	206	CYS	2.2
10	AU	104	ILE	2.2
7	AR	454	GLY	2.2
8	BD	215	GLY	2.2
12	BA	43	SER	2.2
9	BE	30	LEU	2.2
12	AW	77	LEU	2.2
12	BA	808	ASP	2.2
7	AR	713	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
8	BD	209	CYS	2.2
15	BH	71	LEU	2.2
7	AR	655	ALA	2.2
7	BB	134	SER	2.2
11	AV	97	SER	2.2
5	AM	85	ASP	2.2
7	AR	657	ILE	2.2
6	AO	17	LYS	2.2
7	AR	401	LEU	2.2
7	AR	426	LEU	2.2
14	BC	354	LEU	2.2
3	BK	65	ALA	2.2
7	AR	654	THR	2.2
5	BL	73	ILE	2.2
7	AR	607	PHE	2.2
7	BB	87	GLU	2.2
10	BF	66	GLU	2.2
7	BB	99	LEU	2.2
8	AS	256	LEU	2.2
12	AW	648	LEU	2.2
12	AW	701	LEU	2.2
9	BE	12	ARG	2.2
14	AY	286	ILE	2.2
14	AY	329	ILE	2.2
7	AR	677	LYS	2.2
12	BA	7	LYS	2.2
7	AR	330	LEU	2.2
12	BA	295	LEU	2.2
9	BE	11	VAL	2.2
14	BC	153	VAL	2.2
7	AR	430	ARG	2.2
7	BB	657	ILE	2.2
12	AW	7	LYS	2.2
9	BE	55	GLU	2.2
7	AR	38	VAL	2.2
14	BC	236	GLY	2.2
5	AM	73	ILE	2.2
7	AR	275	ILE	2.2
7	AR	814	ILE	2.2
7	AR	986	ILE	2.2
12	BA	700	ILE	2.2
14	AY	235	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
14	AY	241	ILE	2.2
6	AO	21	PHE	2.1
3	AI	82	LEU	2.1
8	BD	114	ILE	2.1
9	AT	59	LEU	2.1
6	AO	43	TYR	2.1
3	BK	49	ALA	2.1
12	BA	579	ASP	2.1
7	BB	1031	PHE	2.1
7	BB	200	ARG	2.1
7	AR	138	LEU	2.1
14	BC	374	ILE	2.1
7	BB	270	ASP	2.1
7	BB	49	GLN	2.1
12	BA	828	SER	2.1
14	AY	60	SER	2.1
7	BB	956	LEU	2.1
12	AW	269	LEU	2.1
6	BN	25	VAL	2.1
7	BB	812	VAL	2.1
12	AW	523	GLN	2.1
12	AW	643	GLY	2.1
7	BB	111	GLU	2.1
14	BC	202	GLU	2.1
14	BC	329	ILE	2.1
7	AR	83	ILE	2.1
7	AR	357	PHE	2.1
11	AV	71	PHE	2.1
14	BC	23	ILE	2.1
7	BB	14	TRP	2.1
7	AR	358	ARG	2.1
7	AR	127	LYS	2.1
9	BE	172	LEU	2.1
8	AS	253	ILE	2.1
13	BP	30	GLY	2.1
14	AY	361	GLY	2.1
12	BA	64	THR	2.1
7	AR	171	ALA	2.0
7	BB	361	PHE	2.0
7	BB	422	TRP	2.0
12	AW	322	SER	2.0
7	BB	429	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
12	BA	316	LYS	2.0
11	BG	93	ILE	2.0
14	AY	313	ILE	2.0
12	AW	26	ALA	2.0
12	AW	579	ASP	2.0
12	AW	810	ALA	2.0
7	BB	123	PRO	2.0
8	AS	209	CYS	2.0
7	BB	598	GLU	2.0
12	AW	133	THR	2.0
7	AR	33	SER	2.0
8	BD	6	LEU	2.0
12	BA	824	ILE	2.0
12	BA	30	PRO	2.0
7	AR	478	GLN	2.0
12	BA	531	LYS	2.0
4	AJ	33	PHE	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 oligosaccharides 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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
18	MG	BA	904	1/1	0.48	0.25	117,117,117,117	0
18	MG	AW	904	1/1	0.79	0.16	132,132,132,132	0
16	ZN	AO	100	1/1	0.89	0.13	188,188,188,188	0
16	ZN	AW	903	1/1	0.90	0.12	134,134,134,134	0
16	ZN	BA	902	1/1	0.90	0.09	209,209,209,209	0
16	ZN	BA	903	1/1	0.92	0.14	118,118,118,118	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
16	ZN	BN	100	1/1	0.93	0.09	153,153,153,153	0
17	SF4	AS	1001	7/8	0.93	0.18	186,189,193,194	0
16	ZN	AX	101	1/1	0.94	0.06	204,204,204,204	0
17	SF4	BD	1001	7/8	0.95	0.19	149,150,154,157	0
16	ZN	AW	902	1/1	0.95	0.12	245,245,245,245	0
16	ZN	BA	901	1/1	0.95	0.06	161,161,161,161	0
16	ZN	AR	1300	1/1	0.96	0.06	193,193,193,193	0
16	ZN	AW	901	1/1	0.97	0.06	183,183,183,183	0
16	ZN	BP	101	1/1	0.97	0.05	200,200,200,200	0
16	ZN	BB	1300	1/1	0.98	0.04	177,177,177,177	0

6.5 Other polymers (i)

There are no such residues in this entry.