Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 09:41 PM GMT

PDB ID	:	4V8S
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

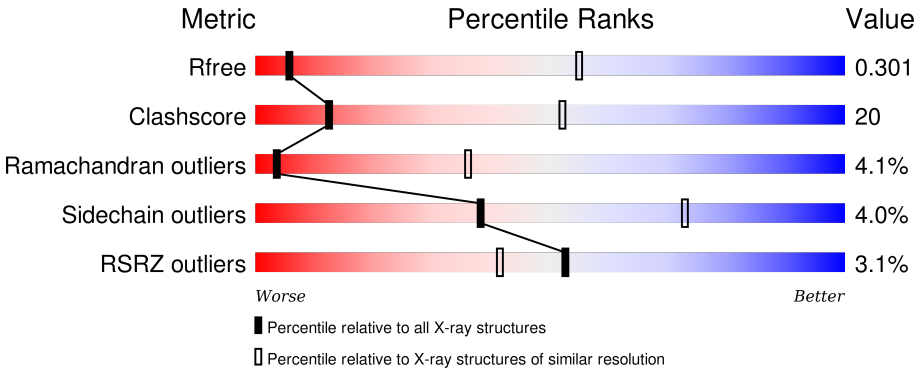
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 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}	91344	1062 (5.04-3.60)
Clashscore	102246	1169 (5.04-3.60)
Ramachandran outliers	100387	1108 (5.04-3.60)
Sidechain outliers	100360	1091 (5.04-3.60)
RSRZ outliers	91569	1065 (5.04-3.60)

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

Mol	Chain	Length	Quality of chain
1	AC	14	21% 57% 29% 7% 7%
1	BR	14	14% 50% 43% 7%
2	AD	16	19% 19% 63% 13% 6%
2	BS	16	13% 19% 75% 6%
3	AI	95	62% 23% • 12%

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Mol	Chain	Length	Quality of chain
3	BK	95	66% 19% 12%
4	AJ	104	3% 21% 19% 7% 53%
4	BQ	104	5% 20% 20% 7% 52%
5	AM	92	3% 78% 21%
5	BL	92	2% 78% 21%
6	AO	66	56% 35% 8%
6	BN	66	58% 33% 8%
7	AR	1131	2% 66% 28%
7	BB	1131	% 66% 28%
8	AS	265	6% 73% 26%
8	BD	265	3% 74% 25%
9	AT	180	10% 58% 36% 5%
9	BE	180	14% 59% 34% 5%
10	AU	113	7% 50% 36% 7% 7%
10	BF	113	8% 50% 33% 11% 7%
11	AV	132	2% 41% 40% 14%
11	BG	132	5% 39% 42% 14%
12	AW	880	3% 61% 33%
12	BA	880	2% 61% 33%
13	AX	48	50% 40% 8%
13	BP	48	50% 40% 8%
14	AY	395	2% 55% 35% 5% 5%
14	BC	395	2% 56% 33% 5% 5%
15	AZ	84	4% 62% 26% 10%
15	BH	84	2% 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

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
1	AC	13	Total	C	H	N	O	P	0	0	0
			411	127	151	38	82	13			
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
2	AD	15	Total	C	H	N	O	P	0	0	0
			485	150	170	63	87	15			
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
3	AI	84	Total	C	H	N	O	S	0	0	0
			1390	431	717	123	118	1			
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
4	AJ	49	Total	C	H	N	O	S	0	0	0
			830	264	413	70	82	1			
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			

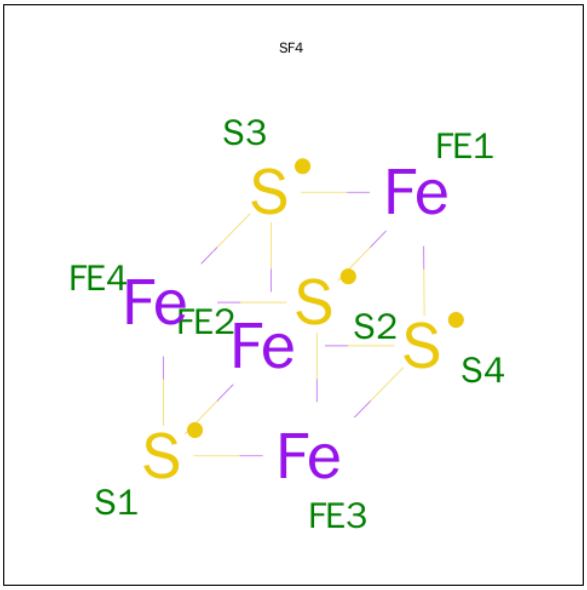
- Molecule 15 is a protein called DNA-DIRECTED RNA POLYMERASE SUBUNIT H.

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 (three-letter code: ZN) (formula: Zn).

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

- Molecule 17 is IRON/SULFUR CLUSTER (three-letter code: 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 (three-letter code: MG) (formula: Mg).

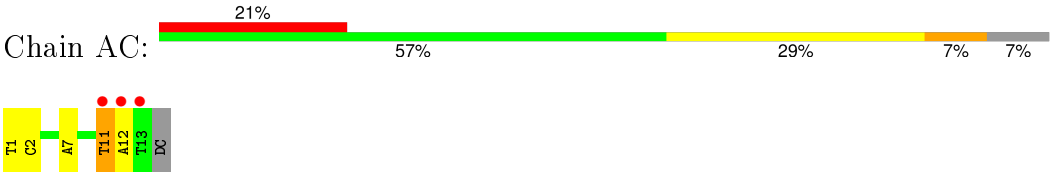
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	AW	1	Total Mg 1 1	0	0
18	BA	1	Total Mg 1 1	0	0

3 Residue-property plots (i)

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

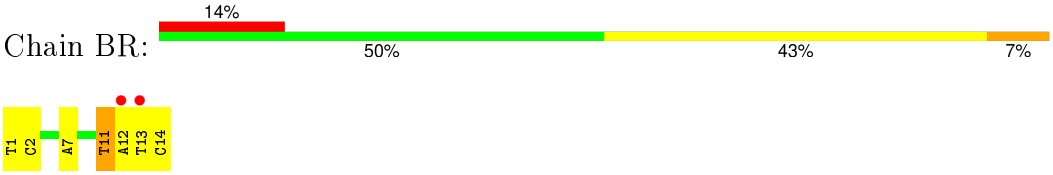
• Molecule 1: 5'-D(*TP*CP*TP*TP*AP*TP*AP*CP*TP*CP*TP*AP*TP*CP)-3'

Chain AC:



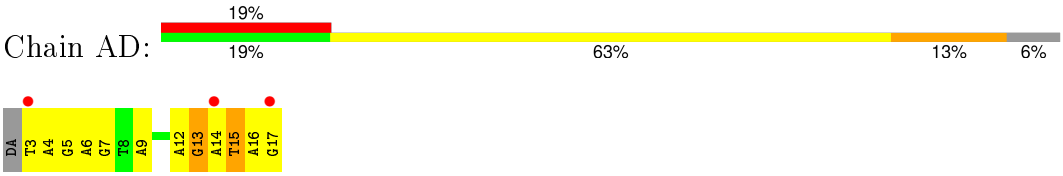
• Molecule 1: 5'-D(*TP*CP*TP*TP*AP*TP*AP*CP*TP*CP*TP*AP*TP*CP)-3'

Chain BR:



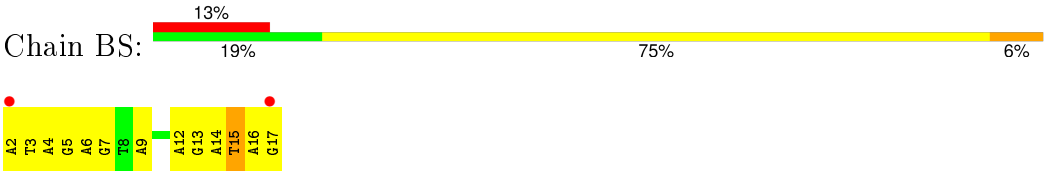
• Molecule 2: 5'-D(*AP*TP*AP*GP*AP*GP*TP*AP*TP*AP*AP*GP*AP*TP *AP*G)-3'

Chain AD:



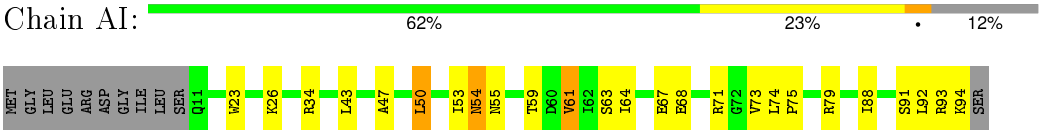
• Molecule 2: 5'-D(*AP*TP*AP*GP*AP*GP*TP*AP*TP*AP*AP*GP*AP*TP *AP*G)-3'

Chain BS:



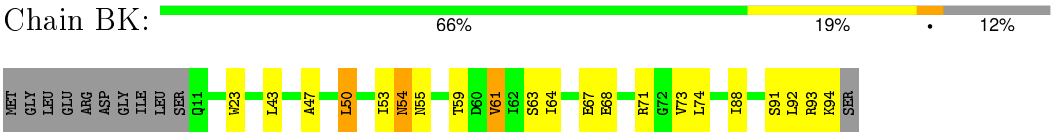
• Molecule 3: DNA-DIRECTED RNA POLYMERASE SUBUNIT K

Chain AI:



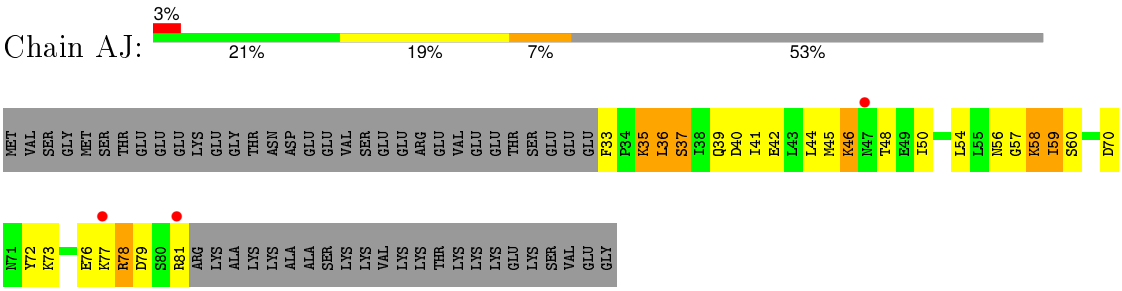
• Molecule 3: DNA-DIRECTED RNA POLYMERASE SUBUNIT K

Chain BK:



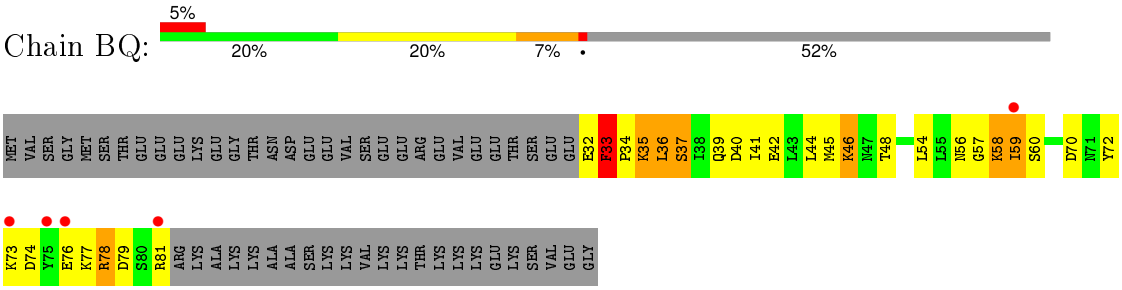
• Molecule 4: RNA POLYMERASE SUBUNIT 13

Chain AJ:



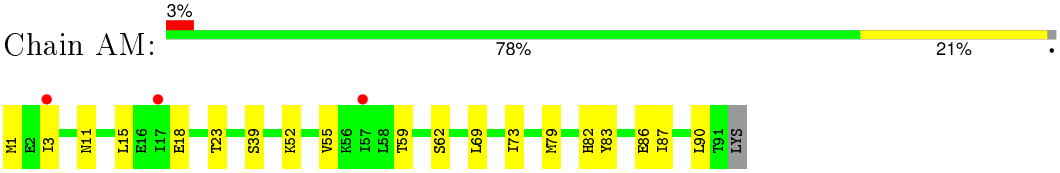
• Molecule 4: RNA POLYMERASE SUBUNIT 13

Chain BQ:



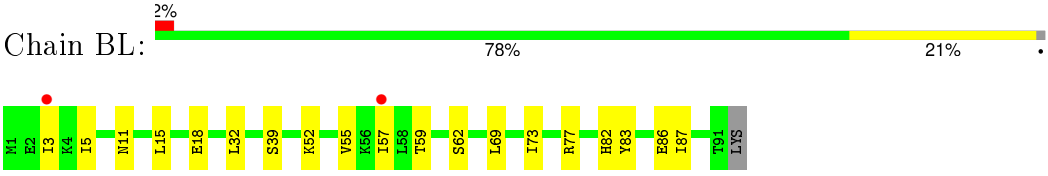
• Molecule 5: DNA-DIRECTED RNA POLYMERASE SUBUNIT L

Chain AM:



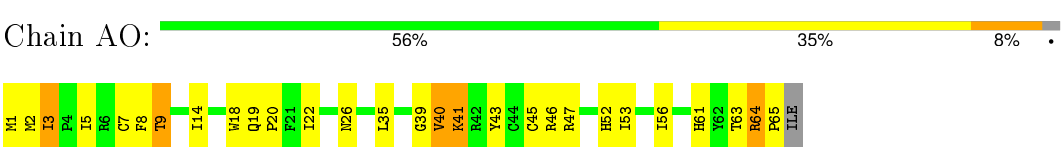
• Molecule 5: DNA-DIRECTED RNA POLYMERASE SUBUNIT L

Chain BL:



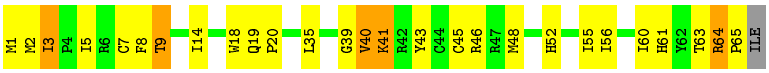
• Molecule 6: DNA-DIRECTED RNA POLYMERASE SUBUNIT N

Chain AO:



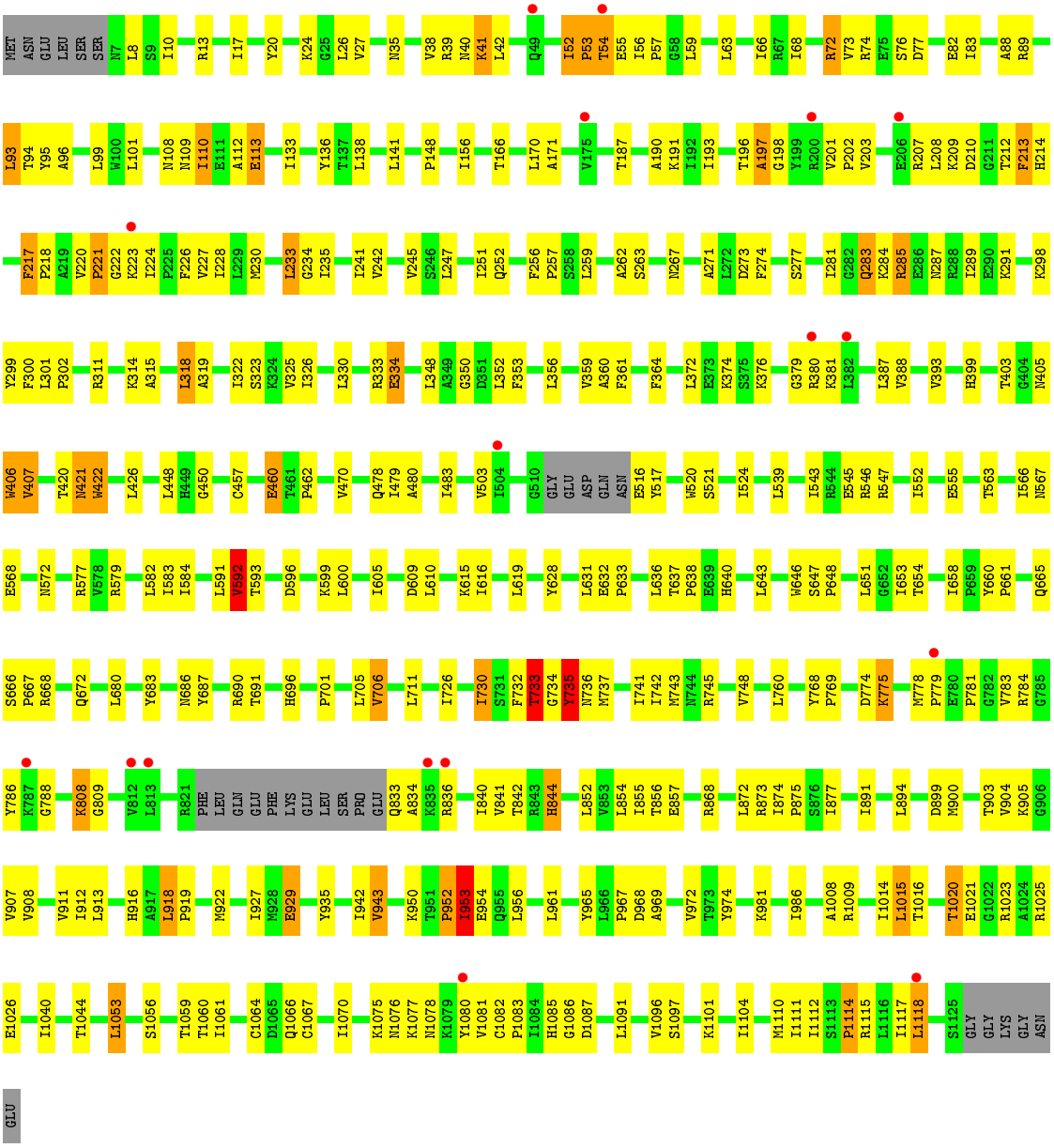
• Molecule 6: DNA-DIRECTED RNA POLYMERASE SUBUNIT N

Chain BN:



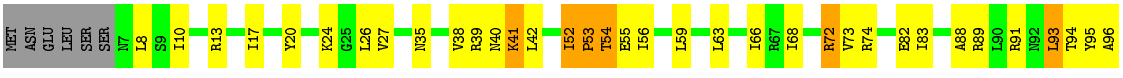
• Molecule 7: DNA-DIRECTED RNA POLYMERASE

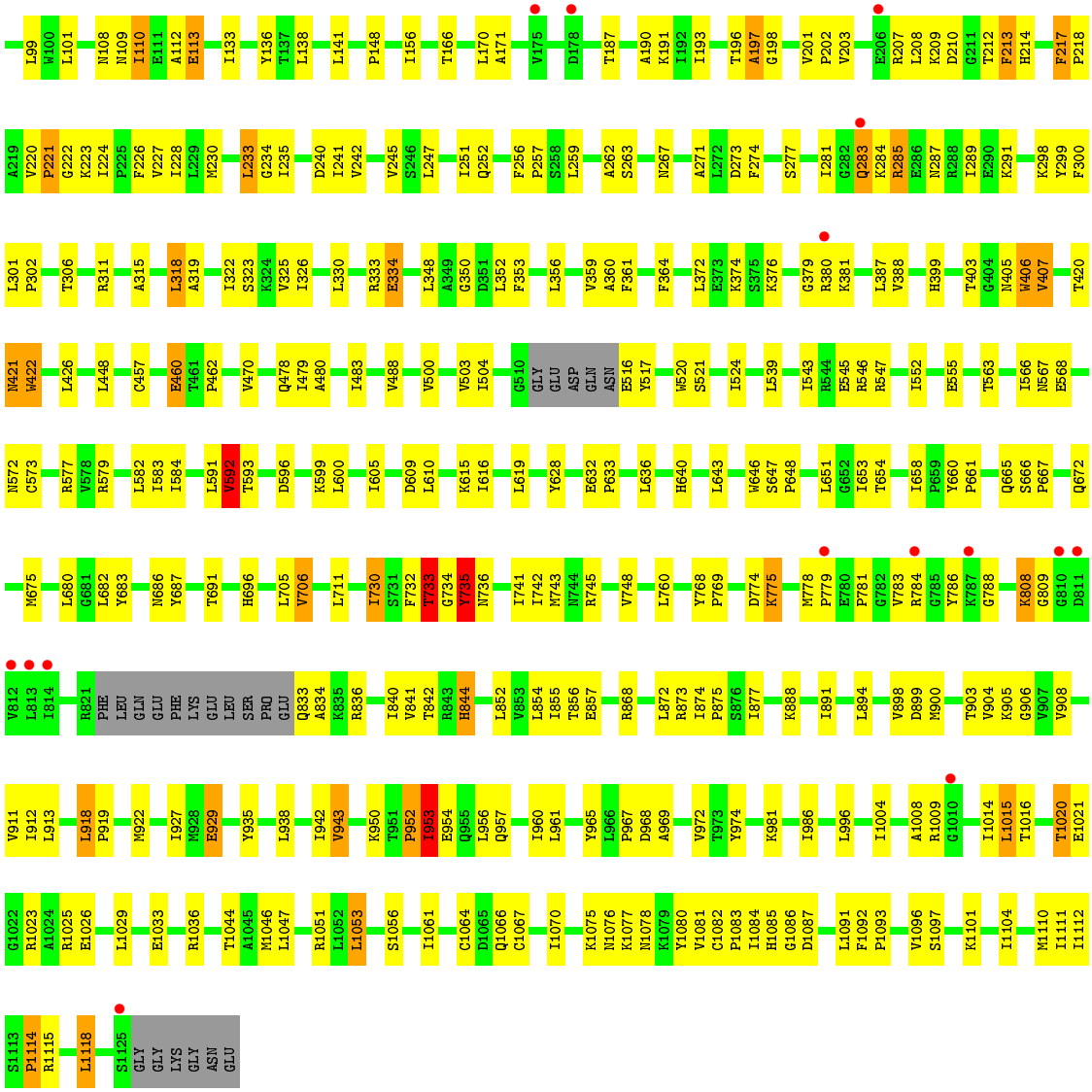
Chain AR:



• Molecule 7: DNA-DIRECTED RNA POLYMERASE

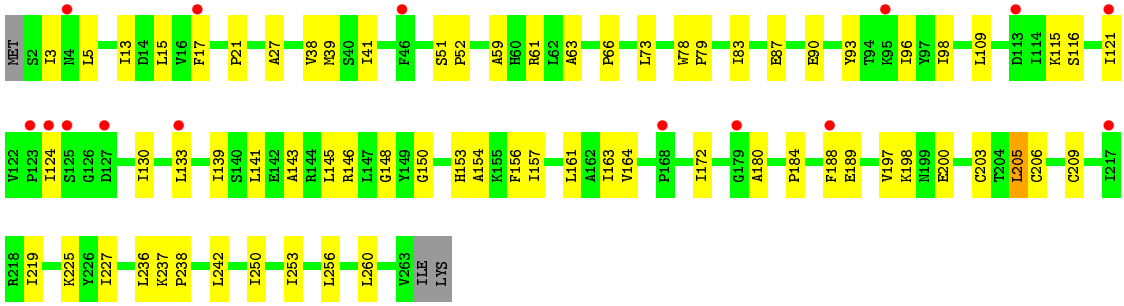
Chain BB:





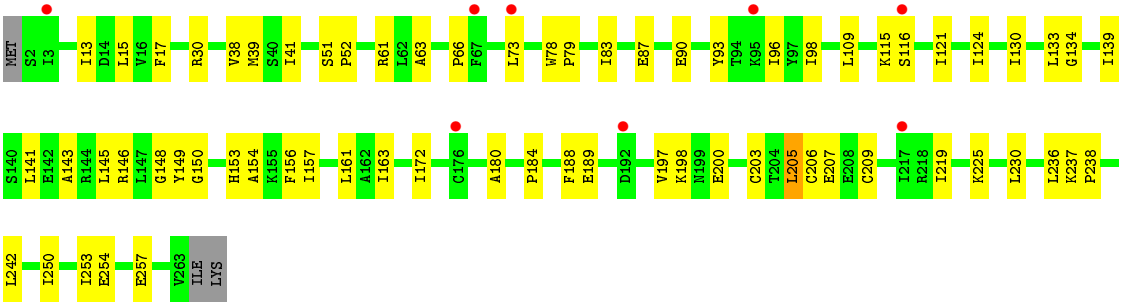
• Molecule 8: DNA-DIRECTED RNA POLYMERASE SUBUNIT D

Chain AS:

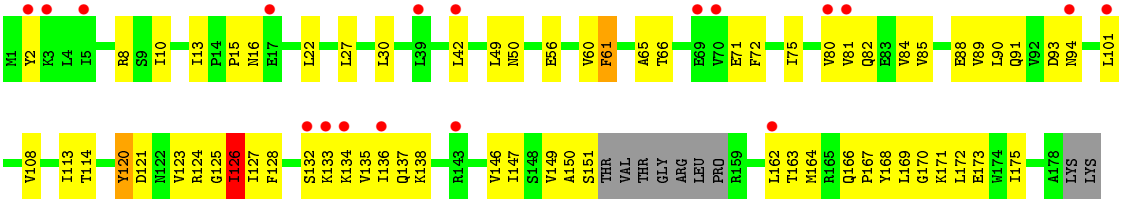


• Molecule 8: DNA-DIRECTED RNA POLYMERASE SUBUNIT D

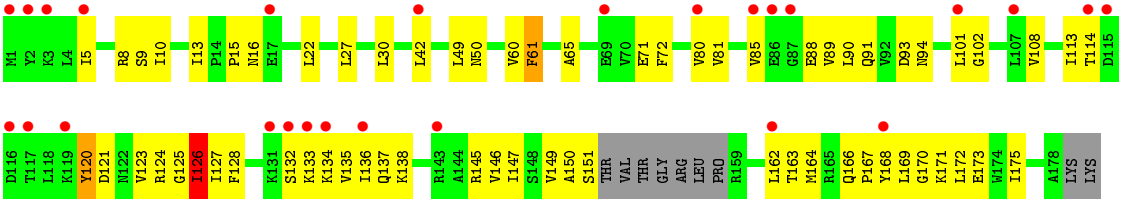
Chain BD:



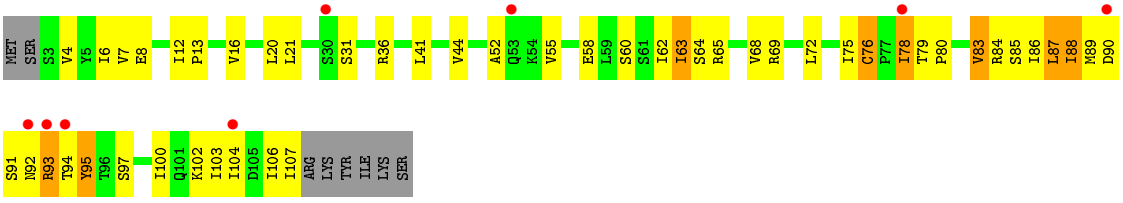
• Molecule 9: RNA POLYMERASE SUBUNIT 7



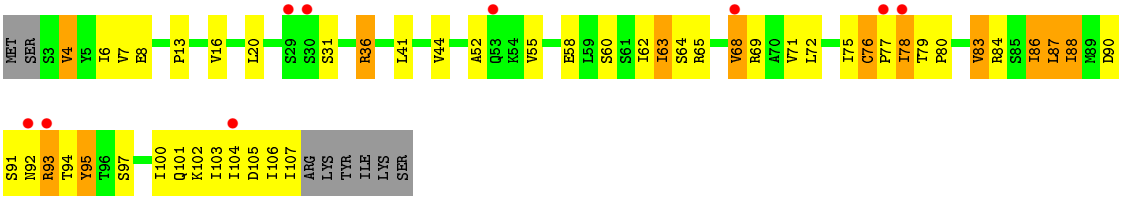
• Molecule 9: RNA POLYMERASE SUBUNIT 7



• Molecule 10: RNA POLYMERASE SUBUNIT 4

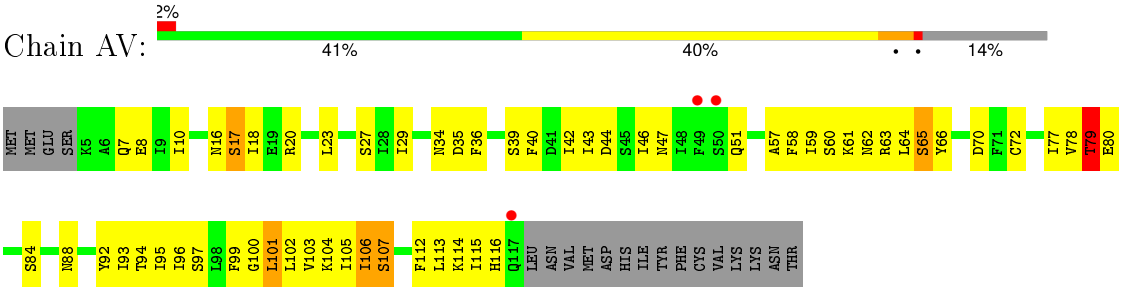


• Molecule 10: RNA POLYMERASE SUBUNIT 4



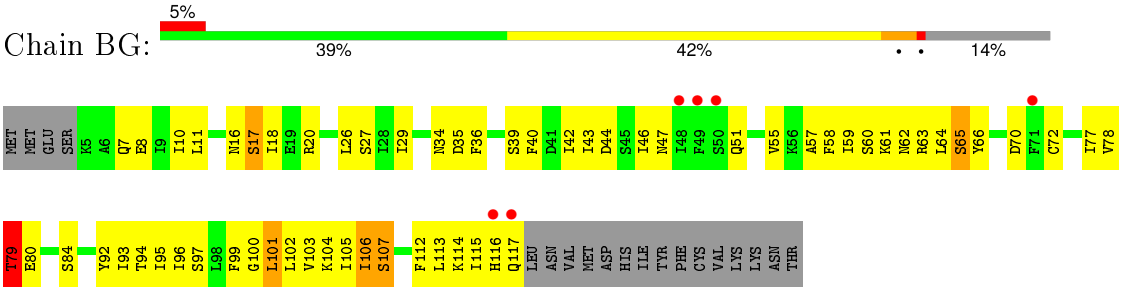
• Molecule 11: RNA POLYMERASE SUBUNIT 8

Chain AV:



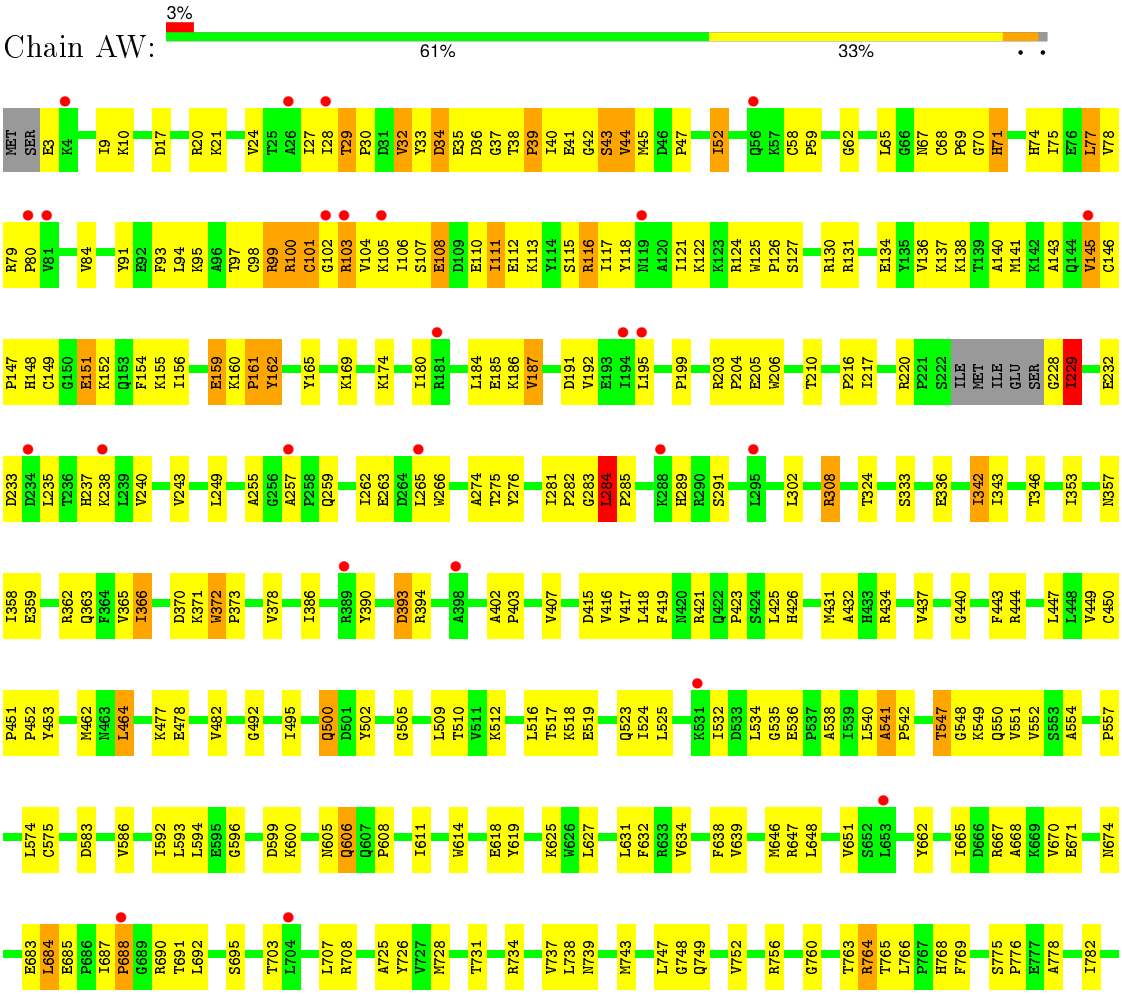
• Molecule 11: RNA POLYMERASE SUBUNIT 8

Chain BG:



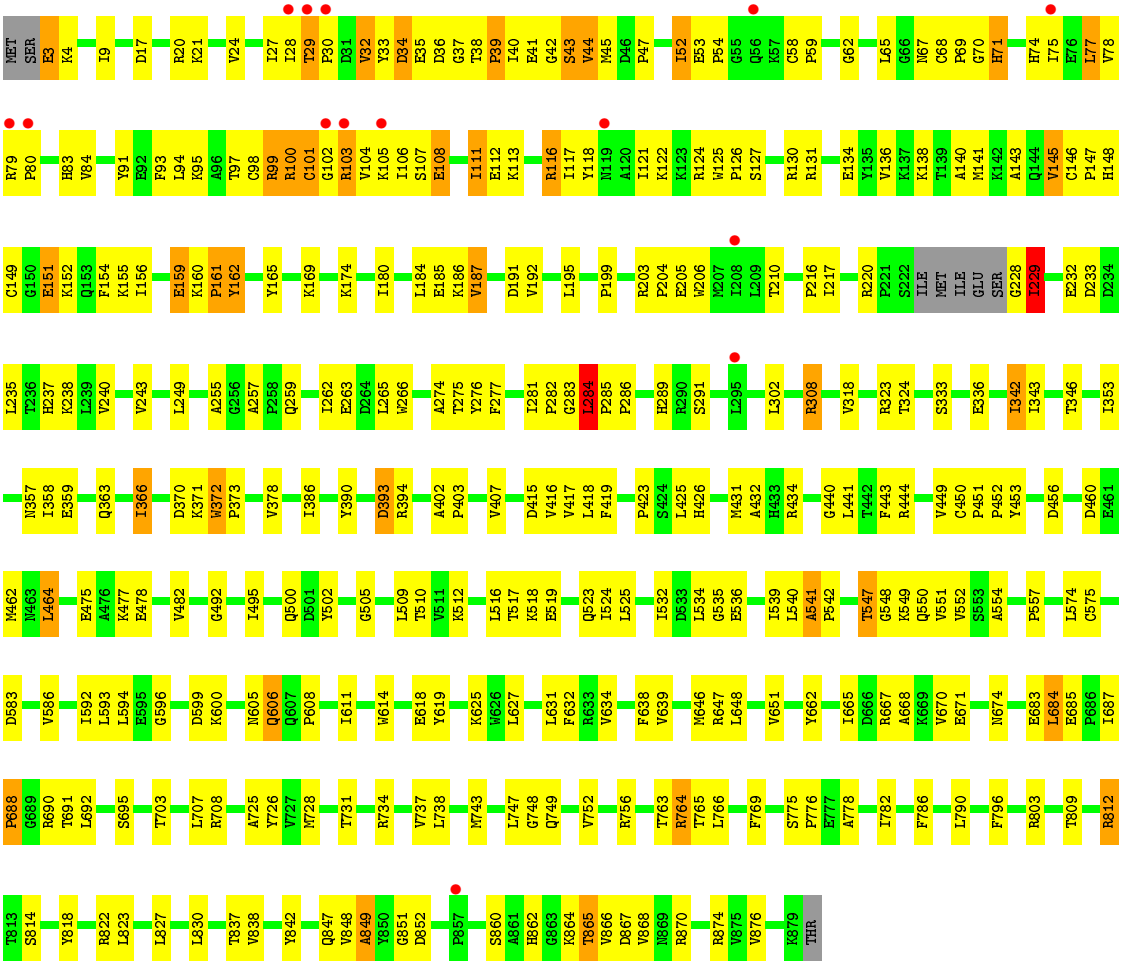
• Molecule 12: DNA-DIRECTED RNA POLYMERASE

Chain AW:



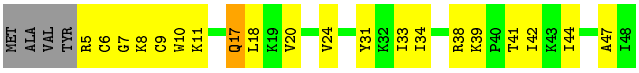
• Molecule 12: DNA-DIRECTED RNA POLYMERASE

Chain BA:



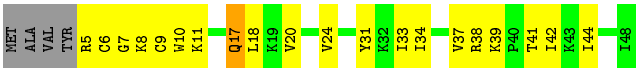
• Molecule 13: DNA-DIRECTED RNA POLYMERASE SUBUNIT P

Chain AX:



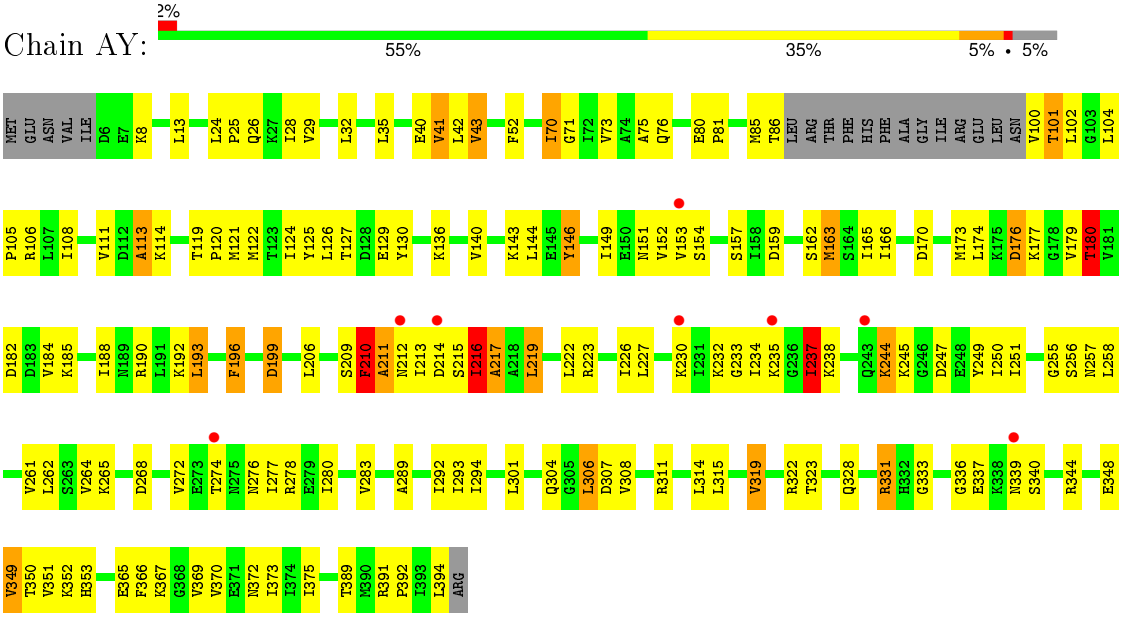
• Molecule 13: DNA-DIRECTED RNA POLYMERASE SUBUNIT P

Chain BP:



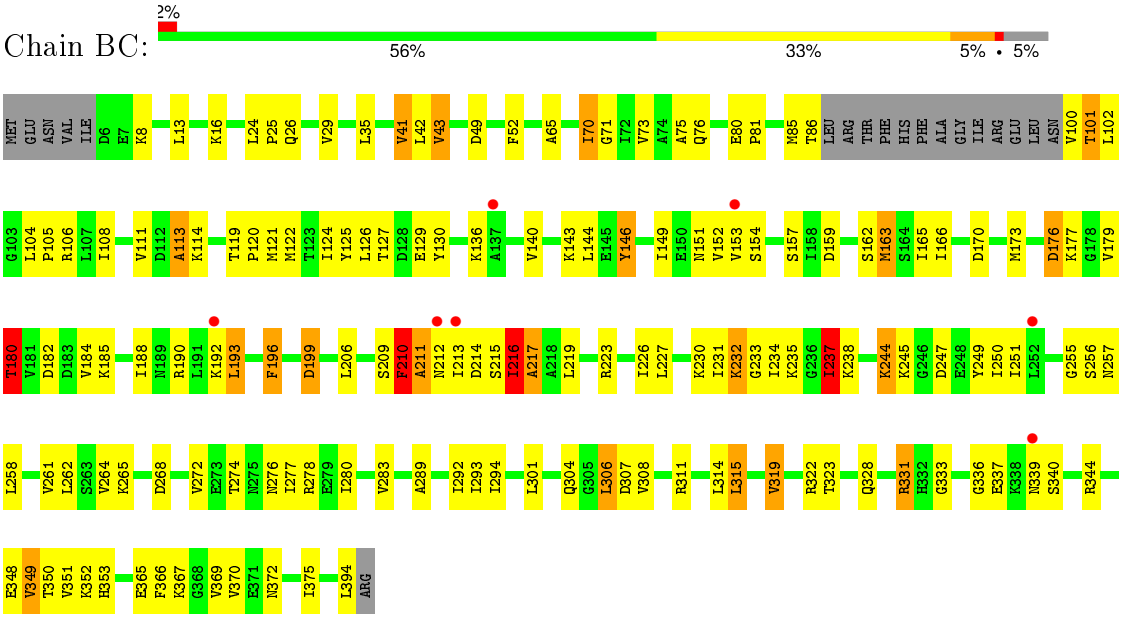
• Molecule 14: DNA-DIRECTED RNA POLYMERASE SUBUNIT A"

Chain AY:



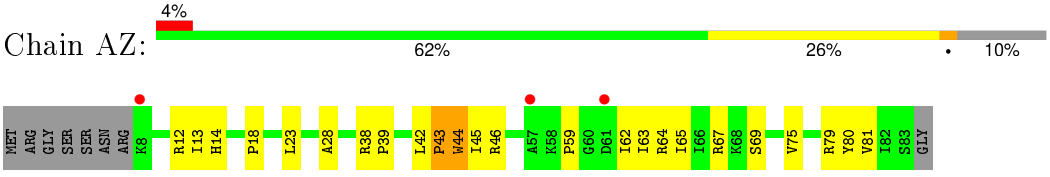
• Molecule 14: DNA-DIRECTED RNA POLYMERASE SUBUNIT A"

Chain BC:



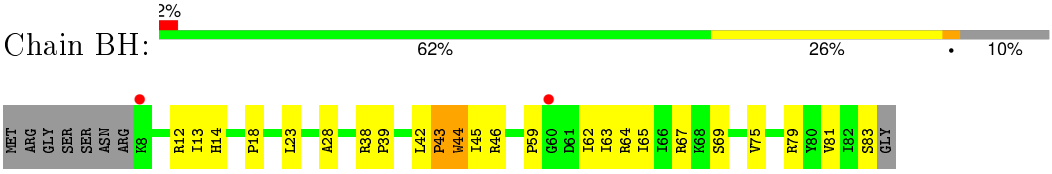
• Molecule 15: DNA-DIRECTED RNA POLYMERASE SUBUNIT H

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 0.288 , 0.301	Depositor DCC
R_{free} test set	3299 reflections (5.08%)	DCC
Wilson B-factor (Å^2)	105.4	Xtriage
Anisotropy	0.633	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 124.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Outliers	0 of 65018 reflections	Xtriage
F_o,F_c correlation	0.81	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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.42	0/288	1.18	1/441 (0.2%)
1	BR	0.43	0/309	1.16	1/473 (0.2%)
2	AD	0.47	0/355	1.18	6/547 (1.1%)
2	BS	0.46	0/379	1.14	5/584 (0.9%)
3	AI	0.21	0/682	0.40	0/921
3	BK	0.22	0/682	0.41	0/921
4	AJ	0.28	0/423	0.47	0/566
4	BQ	0.29	0/432	0.44	0/578
5	AM	0.21	0/717	0.37	0/968
5	BL	0.23	0/717	0.38	0/968
6	AO	0.22	0/532	0.42	0/718
6	BN	0.23	0/532	0.43	0/718
7	AR	0.21	0/8923	0.40	0/12071
7	BB	0.21	0/8923	0.40	0/12071
8	AS	0.21	0/2123	0.37	0/2870
8	BD	0.21	0/2123	0.37	0/2870
9	AT	0.21	0/1379	0.39	0/1861
9	BE	0.21	0/1379	0.39	0/1861
10	AU	0.21	0/836	0.41	0/1133
10	BF	0.21	0/836	0.42	0/1133
11	AV	0.22	0/913	0.40	0/1224
11	BG	0.23	0/913	0.41	0/1224
12	AW	0.23	0/7108	0.42	0/9618
12	BA	0.23	0/7108	0.42	0/9618
13	AX	0.23	0/365	0.42	0/489
13	BP	0.23	0/365	0.42	0/489
14	AY	0.22	0/2930	0.44	0/3944
14	BC	0.21	0/2930	0.44	0/3944
15	AZ	0.20	0/638	0.38	0/864
15	BH	0.21	0/638	0.39	0/864
All	All	0.23	0/56478	0.45	13/76551 (0.0%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	AD	13	DG	O4'-C1'-N9	7.03	112.92	108.00
2	BS	13	DG	O4'-C1'-N9	6.96	112.87	108.00
2	BS	15	DT	O4'-C1'-N1	6.27	112.39	108.00
2	AD	15	DT	O4'-C1'-N1	6.18	112.32	108.00
2	BS	13	DG	C1'-O4'-C4'	-5.78	104.32	110.10
2	AD	13	DG	C1'-O4'-C4'	-5.60	104.50	110.10
2	AD	13	DG	O4'-C1'-C2'	-5.51	101.50	105.90
1	AC	11	DT	C4'-C3'-C2'	-5.47	98.18	103.10
1	BR	11	DT	C4'-C3'-C2'	-5.41	98.23	103.10
2	BS	13	DG	O4'-C1'-C2'	-5.36	101.61	105.90
2	BS	12	DA	O4'-C1'-N9	5.24	111.67	108.00
2	AD	12	DA	O4'-C1'-N9	5.12	111.58	108.00
2	AD	13	DG	C3'-C2'-C1'	-5.09	96.39	102.50

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	38	0
4	BQ	426	419	419	37	0
5	AM	707	742	739	13	0
5	BL	707	742	739	12	0
6	AO	521	537	535	29	0
6	BN	521	537	535	26	0
7	AR	8756	8909	8888	285	0
7	BB	8756	8909	8888	290	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	AS	2087	2128	2125	53	0
8	BD	2087	2128	2125	49	0
9	AT	1359	1413	1411	60	0
9	BE	1359	1412	1411	53	0
10	AU	827	840	839	53	0
10	BF	827	840	839	51	0
11	AV	901	915	912	69	0
11	BG	901	915	912	68	0
12	AW	6957	7030	7013	324	0
12	BA	6957	7030	7013	316	0
13	AX	357	387	387	18	0
13	BP	357	387	387	15	0
14	AY	2906	3068	3063	168	0
14	BC	2906	3068	3063	149	0
15	AZ	624	660	658	24	0
15	BH	624	660	658	25	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	2	0
18	AW	1	0	0	0	0
18	BA	1	0	0	0	0
All	All	55411	56187	56068	2178	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 20.

All (2178) 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:OP2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
14:AY:42:LEU:HA	14:AY:43:VAL:CB	2.03	0.89
7:AR:52:ILE:HB	7:AR:53:PRO:HD3	1.54	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
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
11:BG:65:SER:CB	11:BG:66:TYR:HA	2.10	0.81
12:BA:36:ASP:N	12:BA:37:GLY:HA2	1.94	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
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
6:BN:64:ARG:CB	6:BN:65:PRO:HD3	2.12	0.78
7:AR:406:TRP:HA	7:AR:407:VAL:HB	1.64	0.78
7:AR:53:PRO:HB2	7:AR:54:THR:HA	1.65	0.78
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:541:ALA:HB3	12:AW:542:PRO:CD	2.17	0.73
12:AW:372:TRP:HB3	12:AW:373:PRO:HD3	1.68	0.73
11:BG:29:ILE:HB	11:BG:40:PHE:HB3	1.70	0.73
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
10:AU:91:SER:HB2	10:AU:92:ASN:HA	1.72	0.70
4:AJ:36:LEU:HD11	12:AW:131:ARG:HD3	1.73	0.70
14:AY:211:ALA:HB1	14:AY:212:ASN:C	2.12	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
14:BC:211:ALA:HB1	14:BC:212:ASN:C	2.12	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
9:BE:170:GLY:N	9:BE:175:ILE:HD11	2.07	0.70
12:BA:796:PHE:CZ	7:BB:448:LEU:HD22	2.26	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
7:BB:406:TRP:HA	7:BB:407:VAL:CB	2.22	0.69
12:AW:283:GLY:HA3	12:AW:284:LEU: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:BG:65:SER:HB2	11:BG:66:TYR:HA	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:AV:65:SER:HB2	11:AV:66:TYR:HA	1.75	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:BA:131:ARG:CD	4:BQ:36:LEU:HD11	2.24	0.67
12:AW:541:ALA:CB	12:AW:542:PRO:CD	2.72	0.67
12:BA:105:LYS:HZ2	12:BA:140:ALA:HB3	1.58	0.67
12:AW:105:LYS:HZ2	12:AW:140:ALA:HB3	1.59	0.67
12:BA:864:LYS:HA	12:BA:865:THR:CB	2.23	0.67
7:BB:734:GLY:HA3	7:BB:735:TYR:CB	2.23	0.67
7:AR:734:GLY:HA3	7:AR:735:TYR:CB	2.23	0.67
14:BC:176:ASP:HB2	14:BC:177:LYS:HB2	1.76	0.67
2:AD:3:DT:H2"	2:AD:4:DA:C5	2.29	0.67
2:BS:3:DT:H2"	2:BS:4:DA:C5	2.29	0.67
14:AY:211:ALA:HB3	14:AY:213:ILE:HG12	1.77	0.67
14:AY:176:ASP:H	14:AY:177:LYS:HB2	1.59	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
14:AY:176:ASP:HB2	14:AY:177:LYS:HB2	1.76	0.66
12:AW:103:ARG:HB2	12:AW:186:LYS:HB2	1.78	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
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:833:GLN:HB2	7:BB:834:ALA:CB	2.26	0.65
7:BB:356:LEU:HA	7:BB:407:VAL:HG11	1.79	0.65
8:BD:203:CYS:HA	17:BD:1001:SF4:S1	2.37	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
12:BA:346:THR:HG22	7:BB:1008:ALA:HB2	1.77	0.64
10:AU:88:ILE:HG23	10:AU:88:ILE:O	1.97	0.64
10:BF:88:ILE:O	10:BF:88:ILE:HG23	1.97	0.64
12:BA:103:ARG:HB2	12:BA:186:LYS:HB2	1.78	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
10:BF:79:THR:OG1	10:BF:80:PRO:HD3	1.98	0.64
8:BD:184:PRO:HD2	17:BD:1001:SF4:S3	2.37	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
10:BF:93:ARG:HB2	10:BF:94:THR:CA	2.26	0.64
14:AY:211:ALA:HB1	14:AY:212:ASN:HB2	1.80	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
14:BC:42:LEU:CA	14:BC:43:VAL:HB	2.24	0.63
7:BB:833:GLN:CB	7:BB:834:ALA:HB3	2.29	0.63
10:AU:79:THR:OG1	10:AU:80:PRO:HD3	1.98	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
7:BB:833:GLN:CA	7:BB:834:ALA:HB3	2.29	0.63
14:AY:213:ILE:H	14:AY:214:ASP:HA	1.64	0.63
14:BC:211:ALA:CB	14:BC:212:ASN:HB2	2.28	0.63
12:AW:450:CYS:HB2	12:AW:451:PRO:HD3	1.80	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
4:BQ:58:LYS:O	4:BQ:59:ILE:HB	1.97	0.62
7:BB:256:PHE:N	7:BB:257:PRO:HD2	2.13	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:BC:213:ILE:H	14:BC:214:ASP:HA	1.63	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
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:BQ:36:LEU:O	4:BQ:37:SER:CB	2.46	0.62
4:AJ:58:LYS:O	4:AJ:59:ILE:HB	1.98	0.62
7:BB:112:ALA:O	7:BB:113:GLU:CB	2.47	0.62
11:AV:65:SER:OG	11:AV:66:TYR:HA	1.99	0.62
7:BB:112:ALA:O	7:BB:113:GLU:HB2	2.00	0.62
7:AR:600:LEU:HD11	7:AR:610:LEU:HD11	1.81	0.62
7:AR:256:PHE:N	7:AR:257:PRO:HD2	2.13	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:BB:52:ILE:HB	7:BB:53:PRO:CD	2.28	0.61
12:BA:29:THR:OG1	12:BA:30:PRO:HD3	2.00	0.61
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
4:BQ:57:GLY:O	4:BQ:59:ILE:N	2.33	0.61
12:BA:541:ALA:CB	12:BA:542:PRO:HD3	2.29	0.61
12:BA:103:ARG:CB	12:BA:186:LYS:HB2	2.30	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
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:AY:80:GLU:N	14:AY:81:PRO:CD	2.63	0.61
12:AW:29:THR:OG1	12:AW:30:PRO:HD3	2.00	0.61
14:BC:176:ASP:N	14:BC:177:LYS:O	2.34	0.61
14:AY:176:ASP:N	14:AY:177:LYS:O	2.34	0.61
12:AW:97:THR:HG22	12:AW:99:ARG:H	1.65	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
12:BA:864:LYS:HA	12:BA:865:THR:HB	1.82	0.61
7:AR:112:ALA:O	7:AR:113:GLU:HB2	2.00	0.61
15:BH:43:PRO:O	15:BH:44:TRP:CB	2.49	0.61
7:AR:245:VAL:HA	7:AR:319:ALA:HB1	1.82	0.61
2:AD:14:DA:C8	2:AD:15:DT:H73	2.36	0.61
7:AR:196:THR:O	7:AR:197:ALA:HB3	2.01	0.61
2:BS:2:DA:H2'	2:BS:3:DT:H5'	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:AY:176:ASP:CB	14:AY:177:LYS:HB2	2.30	0.61
12:AW:103:ARG:CB	12:AW:186:LYS:HB2	2.30	0.61
6:BN:2:MET:O	6:BN:3:ILE:O	2.18	0.61
14:BC:80:GLU:N	14:BC:81:PRO:CD	2.63	0.61
12:BA:860:SER:HB2	12:BA:864:LYS:O	2.01	0.60
14:AY:76:GLN:O	14:AY:80:GLU:N	2.34	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
4:AJ:44:LEU:HD21	15:AZ:59:PRO:HB3	1.83	0.60
6:AO:2:MET:O	6:AO:3:ILE:O	2.19	0.60
14:BC:42:LEU:HA	14:BC:43:VAL:HG23	1.83	0.60
12:BA:97:THR:HG22	12:BA:99:ARG:H	1.65	0.60
7:BB:786:TYR:CE2	7:BB:788:GLY:HA2	2.36	0.60
7:BB:196:THR:O	7:BB:197:ALA:HB3	2.01	0.60
7:AR:786:TYR:CE2	7:AR:788:GLY:HA2	2.36	0.60
9:AT:2:TYR:HB2	10:AU:12:ILE:HB	1.83	0.60
14:BC:24:LEU:HB3	14:BC:25:PRO:HD2	1.83	0.60
9:AT:85:VAL:HG11	9:AT:101:LEU:HD22	1.83	0.60
12:AW:864:LYS:HA	12:AW:865:THR:HB	1.82	0.60
12:BA:146:CYS:SG	12:BA:154:PHE:CZ	2.95	0.60
8:AS:51:SER:HB2	8:AS:52:PRO:HD2	1.84	0.60
12:BA:127:SER:O	12:BA:131:ARG:HD2	2.00	0.60
12:AW:33:TYR:HB3	12:AW:34:ASP:HA	1.82	0.60
2:BS:14:DA:C8	2:BS:15:DT:H73	2.36	0.60
7:BB:221:PRO:CB	7:BB:222:GLY:HA2	2.23	0.60
14:BC:76:GLN:O	14:BC:80:GLU:N	2.35	0.60
15:AZ:43:PRO:O	15:AZ:44:TRP:CB	2.49	0.60
7:BB:245:VAL:HA	7:BB:319:ALA:HB1	1.82	0.60
4:BQ:78:ARG:C	4:BQ:78:ARG:HD3	2.22	0.60
7:AR:781:PRO:HA	7:AR:786:TYR:CE2	2.37	0.60
12:BA:683:GLU:HA	12:BA:684:LEU:CB	2.32	0.60
11:BG:65:SER:OG	11:BG:66:TYR:HA	2.00	0.60
14:AY:213:ILE:N	14:AY:214:ASP:HA	2.17	0.60
12:AW:860:SER:HB2	12:AW:864:LYS:O	2.02	0.60
12:BA:47:PRO:HB2	12:BA:59:PRO:HG2	1.83	0.60
9:BE:85:VAL:HG11	9:BE:101:LEU:HD22	1.83	0.60
7:BB:600:LEU:HD11	7:BB:610:LEU:HD11	1.82	0.59
14:BC:213:ILE:N	14:BC:214:ASP:HA	2.17	0.59
7:AR:660:TYR:N	7:AR:661:PRO:HD3	2.17	0.59
7:AR:221:PRO:CB	7:AR:222:GLY:HA2	2.22	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)
12:AW:42:GLY:O	12:AW:43:SER:CB	2.50	0.59
7:AR:808:LYS:HD2	7:AR:809:GLY:N	2.17	0.59
4:AJ:78:ARG:HD3	4:AJ:78:ARG:C	2.22	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:1082:CYS:HB2	7:AR:1083:PRO:HD2	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:103:ARG:CG	12:AW:187:VAL:HG13	2.33	0.59
12:AW:47:PRO:HB2	12:AW:59:PRO:HG2	1.83	0.59
7:BB:781:PRO:HA	7:BB:786:TYR:CE2	2.37	0.59
12:BA:42:GLY:O	12:BA:43:SER:CB	2.50	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:OP2	14:AY:331:ARG:NH1	2.36	0.58
14:BC:211:ALA:HB1	14:BC:212:ASN:CA	2.33	0.58
12:BA:33:TYR:CB	12:BA:34:ASP:HB2	2.33	0.58
15:AZ:43:PRO:O	15:AZ:44:TRP:CG	2.56	0.58
7:BB:56:ILE:HG23	7:BB:59:LEU:HB2	1.85	0.58
14:BC:144:LEU:O	14:BC:237:ILE:HD11	2.04	0.58
7:BB:808:LYS:HD2	7:BB:809:GLY:N	2.18	0.58
14:AY:24:LEU:HB3	14:AY:25:PRO:HD2	1.84	0.58
14:BC:213:ILE:HB	14:BC:214:ASP:O	2.04	0.58
7:AR:56:ILE:HG23	7:AR:59:LEU:HB2	1.85	0.58
7:BB:660:TYR:N	7:BB:661:PRO:HD3	2.17	0.58
14:AY:42:LEU:HA	14:AY:43:VAL:HG23	1.84	0.58
4:AJ:36:LEU:HD11	12:AW:131:ARG:NE	2.18	0.58
12:BA:98:CYS:HB2	12:BA:104:VAL:H	1.68	0.58
2:BS:2:DA:C2'	2:BS:3:DT:H5"	2.34	0.58
12:BA:103:ARG:CG	12:BA:187:VAL:HG13	2.33	0.58
14:AY:192:LYS:HB3	14:AY:193:LEU:HB2	1.85	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
11:BG:101:LEU:HD22	11:BG:102:LEU:N	2.18	0.58
14:AY:144:LEU:O	14:AY:237:ILE:HD11	2.04	0.58
12:AW:651:VAL:HG11	12:AW:743:MET:HB3	1.86	0.58
5:AM:90:LEU:HD21	8:AS:5:LEU:HG	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
14:BC:192:LYS:HB3	14:BC:193:LEU:HB2	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:HD12	7:BB:1111:ILE:N	2.19	0.58
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
4:AJ:46:LYS:HE2	4:AJ:46:LYS:HA	1.86	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
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
11:BG:64:LEU:HG	11:BG:114:LYS:CG	2.34	0.57
12:AW:220:ARG:HD3	12:AW:235:LEU:HB3	1.86	0.57
12:AW:108:GLU:HA	12:AW:147:PRO:HG2	1.86	0.57
12:BA:417:VAL:HG11	12:BA:464:LEU:HD21	1.85	0.57
12:BA:108:GLU:HA	12:BA:147:PRO:HG2	1.87	0.57
13:AX:17:GLN:HG3	13:AX:18:LEU:H	1.68	0.57
12:AW:838:VAL:HB	12:AW:847:GLN:HB2	1.87	0.57
7:AR:1111:ILE:N	7:AR:1111:ILE:HD12	2.19	0.57
12:AW:683:GLU:CA	12:AW:684:LEU:HB3	2.33	0.57
14:BC:211:ALA:CB	14:BC:213:ILE:HG12	2.34	0.57
14:BC:192:LYS:CB	14:BC:193:LEU:HB2	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
10:BF:91:SER:CB	10:BF:92:ASN:HA	2.35	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
6:BN:64:ARG:HB2	6:BN:65:PRO:HD3	1.85	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: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
7:BB:734:GLY:CA	7:BB:735:TYR:CB	2.83	0.56
12:BA:79:ARG:HB3	12:BA:266:TRP:CZ3	2.40	0.56
12:AW:417:VAL:HG11	12:AW:464:LEU:HD21	1.85	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
12:BA:683:GLU:CA	12:BA:684:LEU:HB3	2.34	0.56
7:AR:1067:CYS:SG	7:AR:1085:HIS:HE1	2.21	0.56
12:BA:372:TRP:CB	12:BA:373:PRO:HD3	2.32	0.56
4:AJ:48:THR:HG21	12:AW:125:TRP:CZ2	2.40	0.56
12:BA:70:GLY:O	12:BA:71:HIS:HB2	2.05	0.56
11:AV:79:THR:HB	11:AV:80:GLU:CB	2.36	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
14:AY:149:ILE:HD13	14:AY:230:LYS:HB2	1.87	0.56
10:BF:58:GLU:HB3	10:BF:103:ILE:HG21	1.86	0.56
10:AU:58:GLU:HB3	10:AU:103:ILE:HG21	1.86	0.56
10:AU:91:SER:CB	10:AU:92:ASN:CA	2.83	0.56
2:BS:2:DA:H2'	2:BS:3:DT:C5'	2.36	0.56
12:BA:28:ILE:HD12	12:BA:44:VAL:HA	1.88	0.56
6:BN:3:ILE:HG22	6:BN:52:HIS:CG	2.41	0.56
9:BE:113:ILE:HG22	9:BE:114:THR:HG23	1.86	0.56
6:BN:48:MET:HA	6:BN:48:MET:HE2	1.86	0.56
7:BB:406:TRP:HA	7:BB:407:VAL:CG2	2.35	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
9:AT:113:ILE:HG22	9:AT:114:THR:HG23	1.86	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
9:AT:82:GLN:O	10:AU:87:LEU:HG	2.05	0.56
12:BA:687:ILE:HG21	12:BA:690:ARG:HB2	1.87	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
10:AU:91:SER:CB	10:AU:92:ASN:HA	2.35	0.56
6:BN:8:PHE:O	6:BN:9:THR:HB	2.05	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
14:AY:162:SER:O	14:AY:163:MET:C	2.44	0.56
12:BA:220:ARG:HD3	12:BA:235:LEU:HB3	1.86	0.56
7:BB:833:GLN:N	7:BB:834:ALA:CB	2.69	0.56
10:BF:91:SER:CB	10:BF:92:ASN:CA	2.83	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
14:BC:126:LEU:HB3	14:BC:130:TYR:HB2	1.86	0.56
7:AR:227:VAL:CG1	7:AR:262:ALA:HB3	2.36	0.56
6:AO:8:PHE:O	6:AO:9:THR:HB	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:BD:257:GLU:HB2	5:BL:73:ILE:HG21	1.88	0.56
7:BB:352:LEU:HD12	7:BB:406:TRP:NE1	2.21	0.56
12:AW:33:TYR:N	12:AW:34:ASP:HB2	2.20	0.56
15:AZ:43:PRO:O	15:AZ:44:TRP:HB2	2.06	0.56
12:AW:687:ILE:HG21	12:AW:690:ARG:HB2	1.87	0.56
14:BC:162:SER:O	14:BC:163:MET:C	2.44	0.56
12:BA:525:LEU:HD21	12:BA:551:VAL:HG23	1.86	0.56
12:AW:79:ARG:HB3	12:AW:266:TRP:CZ3	2.41	0.56
11:BG:78:VAL:O	11:BG:79:THR:HG23	2.06	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
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
14:BC:146:TYR:HA	14:BC:233:GLY:HA3	1.88	0.55
12:BA:535:GLY:O	12:BA:536:GLU:C	2.45	0.55
7:BB:41:LYS:O	7:BB:42:LEU:HB3	2.05	0.55
12:BA:763:THR:O	12:BA:764:ARG:HB3	2.06	0.55
14:BC:213:ILE:HB	14:BC:214:ASP:C	2.27	0.55
2:BS:2:DA:C2'	2:BS:3:DT:C5'	2.85	0.55
6:AO:3:ILE:HG22	6:AO:52:HIS:CG	2.41	0.55
12:AW:70:GLY:O	12:AW:71:HIS:HB2	2.05	0.55
7:BB:39:ARG:HG3	7:BB:40:ASN:N	2.22	0.55
11:AV:18:ILE:HG22	11:AV:29:ILE:HG23	1.88	0.55
11:BG:79:THR:HB	11:BG:80:GLU:CB	2.36	0.55
4:AJ:36:LEU:O	4:AJ:37:SER:HB2	2.06	0.55
14:AY:213:ILE:HB	14:AY:214:ASP:C	2.27	0.55
12:BA:146:CYS:HB2	12:BA:151:GLU:HA	1.87	0.55
12:BA:99:ARG:O	12:BA:100:ARG:HB3	2.05	0.55
9:BE:145:ARG:NH2	10:BF:86:ILE:HD11	2.21	0.55
7:BB:596:ASP:HA	7:BB:599:LYS:HG2	1.88	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
11:BG:34:ASN:O	11:BG:35:ASP:HB2	2.07	0.55
12:BA:416:VAL:HG21	12:BA:477:LYS:HB2	1.89	0.55
4:BQ:36:LEU:HD13	4:BQ:41:ILE:HD11	1.89	0.55
11:AV:78:VAL:O	11:AV:79:THR:HG23	2.06	0.55
14:BC:149:ILE:HD13	14:BC:230:LYS:HB2	1.87	0.55
14:AY:146:TYR:HA	14:AY:233:GLY:HA3	1.88	0.55
11:AV:34:ASN:O	11:AV:35:ASP:HB2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:AR:323:SER:HA	7:AR:326:ILE:HD11	1.87	0.55
12:AW:423:PRO:HB2	12:AW:425:LEU:CD1	2.37	0.55
11:BG:18:ILE:HG22	11:BG:29:ILE:HG23	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
12:BA:353:ILE:HD11	12:BA:407:VAL:HG23	1.89	0.55
4:AJ:36:LEU:HD13	4:AJ:41:ILE:HD11	1.89	0.55
7:BB:734:GLY:HA3	7:BB:735:TYR:CD2	2.42	0.55
14:AY:176:ASP:N	14:AY:177:LYS:HB2	2.21	0.55
7:BB:1014:ILE:O	7:BB:1015:LEU:HB3	2.05	0.55
15:AZ:43:PRO:HB2	15:AZ:79:ARG:HG2	1.89	0.55
13:BP:5:ARG:HA	13:BP:6:CYS:SG	2.47	0.55
7:AR:916:HIS:CD2	12:AW:500:GLN:HB2	2.42	0.55
10:BF:78:ILE:H	10:BF:78:ILE:HD13	1.72	0.55
12:AW:106:ILE:CG2	12:AW:143:ALA:HB3	2.37	0.55
15:BH:42:LEU:HB3	15:BH:43:PRO:HD2	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
12:AW:353:ILE:HD11	12:AW:407:VAL:HG23	1.88	0.55
12:AW:47:PRO:HB2	12:AW:59:PRO:CG	2.36	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
7:BB:732:PHE:CD1	7:BB:733:THR:HB	2.43	0.54
14:AY:176:ASP:HB2	14:AY:177:LYS:HD2	1.90	0.54
10:AU:78:ILE:H	10:AU:78:ILE:HD13	1.72	0.54
7:BB:196:THR:O	7:BB:197:ALA:CB	2.54	0.54
7:AR:196:THR:HG21	7:AR:302:PRO:HB2	1.88	0.54
11:BG:101:LEU:O	11:BG:105:ILE:HG12	2.07	0.54
14:AY:140:VAL:O	14:AY:144:LEU:HG	2.08	0.54
7:AR:39:ARG:HG3	7:AR:40:ASN:N	2.22	0.54
8:BD:180:ALA:HA	8:BD:188:PHE:HB2	1.89	0.54
4:BQ:36:LEU:O	4:BQ:37:SER:HB2	2.06	0.54
9:BE:164:MET:HB3	9:BE:170:GLY:HA2	1.89	0.54
10:AU:76:CYS:HB2	10:AU:104:ILE:HG23	1.90	0.54
8:AS:250:ILE:O	8:AS:253:ILE:HG22	2.08	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
12:BA:441:LEU:HD22	7:BB:1004:ILE:HD13	1.89	0.54
11:AV:88:ASN:HB2	12:AW:538:ALA:HB1	1.88	0.54
9:BE:102:GLY:O	10:BF:36:ARG:HD3	2.06	0.54
7:BB:935:TYR:CD2	7:BB:956:LEU:HD22	2.43	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
12:BA:574:LEU:HD23	12:BA:575:CYS:N	2.23	0.54
14:BC:176:ASP:HB2	14:BC:177:LYS:HD2	1.90	0.54
12:BA:238:LYS:HE2	12:BA:275:THR:HB	1.90	0.54
11:BG:16:ASN:O	11:BG:17:SER:CB	2.56	0.54
7:AR:406:TRP:CA	7:AR:407:VAL:CB	2.85	0.54
7:AR:380:ARG:CB	7:AR:381:LYS:HA	2.36	0.54
10:BF:76:CYS:HB2	10:BF:104:ILE:HG23	1.90	0.54
14:BC:294:ILE:HD13	14:BC:314:LEU:HD23	1.90	0.54
8:AS:180:ALA:HA	8:AS:188:PHE:HB2	1.89	0.54
12:AW:823:LEU:CD1	14:AY:75:ALA:HB1	2.37	0.54
2:AD:14:DA:H5'	12:AW:818:TYR:OH	2.08	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
12:AW:842:TYR:CZ	14:AY:339:ASN:O	2.61	0.54
5:AM:79:MET:SD	8:AS:21:PRO:HD2	2.48	0.54
14:AY:294:ILE:HD13	14:AY:314:LEU:HD23	1.90	0.54
8:BD:250:ILE:O	8:BD:253:ILE:HG22	2.08	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:283:GLY:CA	12:AW:284:LEU:HB2	2.38	0.54
9:AT:56:GLU:HG2	14:AY:391:ARG:CG	2.38	0.54
12:BA:692:LEU:HD12	12:BA:692:LEU:N	2.23	0.54
11:AV:16:ASN:O	11:AV:17:SER:CB	2.56	0.54
7:AR:833:GLN:N	7:AR:834:ALA:CB	2.69	0.54
15:AZ:42:LEU:HB3	15:AZ:43:PRO:HD2	1.88	0.54
14:AY:120:PRO:HG2	14:AY:255:GLY:HA2	1.89	0.54
7:AR:953:ILE:HD13	7:AR:953:ILE:N	2.23	0.54
12:AW:535:GLY:O	12:AW:536:GLU:C	2.45	0.54
12:AW:547:THR:HG23	12:AW:550:GLN:HB2	1.90	0.54
11:AV:72:CYS:SG	11:AV:114:LYS:HD2	2.48	0.53
11:BG:72:CYS:SG	11:BG:114:LYS:HD2	2.49	0.53
9:AT:164:MET:HB3	9:AT:170:GLY:HA2	1.89	0.53
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
7:BB:953:ILE:HD13	7:BB:953:ILE:N	2.24	0.53
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:BC:120:PRO:HG2	14:BC:255:GLY:HA2	1.90	0.53
3:AI:91:SER:O	3:AI:92:LEU:HB2	2.09	0.53
7:AR:352:LEU:HD12	7:AR:406:TRP:NE1	2.22	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
12:AW:238:LYS:HE2	12:AW:275:THR:HB	1.90	0.53
7:AR:1064:CYS:HB3	7:AR:1067:CYS:HB2	1.91	0.53
7:AR:732:PHE:CD1	7:AR:733:THR:HB	2.43	0.53
12:AW:146:CYS:SG	12:AW:154:PHE:CZ	3.01	0.53
14:BC:322:ARG:O	14:BC:323:THR:HB	2.08	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:416:VAL:HG21	12:AW:477:LYS:HB2	1.89	0.53
2:AD:15:DT:H1'	2:AD:16:DA:P	2.48	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
12:AW:574:LEU:HD23	12:AW:575:CYS:N	2.23	0.53
7:AR:852:LEU:HB3	7:AR:868:ARG:HG2	1.89	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
7:AR:108:ASN:O	7:AR:109:ASN:HB2	2.09	0.53
12:BA:851:GLY:O	12:BA:852:ASP:HB2	2.09	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:HB2	2.39	0.53
14:AY:214:ASP:HB2	14:AY:215:SER:HA	1.89	0.53
14:BC:214:ASP:HB2	14:BC:215:SER:HA	1.89	0.53
12:BA:451:PRO:N	12:BA:452:PRO:HD2	2.23	0.53
5:BL:83:TYR:CZ	5:BL:87:ILE:HD11	2.43	0.53
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
13:AX:5:ARG:HA	13:AX:6:CYS:SG	2.48	0.53
7:AR:190:ALA:HB2	7:AR:325:VAL:HG22	1.91	0.53
12:BA:868:VAL:HG12	14:BC:35:LEU:CD1	2.38	0.53
7:BB:406:TRP:CA	7:BB:407:VAL:CB	2.85	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
12:AW:105:LYS:CE	12:AW:195:LEU:HD21	2.39	0.53
15:BH:43:PRO:HB2	15:BH:79:ARG:HG2	1.90	0.53
9:BE:114:THR:HG21	9:BE:134:LYS:HD3	1.91	0.53
1:BR:13:DT:H1'	1:BR:14:DC:P	2.49	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:BE:126:ILE:HD11	9:BE:128:PHE:CD1	2.44	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
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
14:BC:154:SER:HB3	14:BC:170:ASP:HB2	1.91	0.53
7:AR:874:ILE:HG23	7:AR:875:PRO:HD2	1.90	0.53
7:AR:133:ILE:HD13	7:AR:136:TYR:CE2	2.44	0.53
7:AR:1064:CYS:HA	7:AR:1091:LEU:CD2	2.39	0.52
7:AR:734:GLY:N	7:AR:735:TYR:HB2	2.24	0.52
12:BA:97:THR:HA	12:BA:103:ARG:CZ	2.39	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
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
12:BA:549:LYS:HD2	12:BA:593:LEU:HD22	1.91	0.52
7:AR:52:ILE:CB	7:AR:53:PRO:CD	2.86	0.52
12:BA:284:LEU:HD22	12:BA:285:PRO:CD	2.39	0.52
12:BA:101:CYS:SG	12:BA:152:LYS:HG3	2.49	0.52
12:AW:160:LYS:HB3	12:AW:161:PRO:CD	2.40	0.52
12:AW:147:PRO:O	12:AW:148:HIS:HB2	2.10	0.52
7:BB:918:LEU:H	7:BB:919:PRO:HD2	1.74	0.52
7:BB:108:ASN:O	7:BB:109:ASN:HB2	2.09	0.52
14:BC:70:ILE:HA	14:BC:73:VAL:HG22	1.91	0.52
7:BB:1064:CYS:HA	7:BB:1091:LEU:CD2	2.39	0.52
4:AJ:44:LEU:HD21	15:AZ:59:PRO:CB	2.39	0.52
15:AZ:45:ILE:HG13	15:AZ:79:ARG:CB	2.40	0.52
12:AW:237:HIS:O	12:AW:240:VAL:HB	2.10	0.52
7:BB:545:GLU:HG3	7:BB:546:ARG:N	2.24	0.52
7:BB:665:GLN:HG2	7:BB:667:PRO:HD2	1.91	0.52
14:BC:104:LEU:N	14:BC:105:PRO:CD	2.73	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
14:AY:322:ARG:O	14:AY:323:THR:CB	2.57	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
8:AS:78:TRP:HB3	8:AS:79:PRO:HD2	1.91	0.52
15:BH:59:PRO:CB	4:BQ:44:LEU:HD21	2.39	0.52
12:AW:40:ILE:HG22	12:AW:41:GLU:N	2.24	0.52
15:BH:45:ILE:HG13	15:BH:79:ARG:CB	2.39	0.52
14:BC:165:ILE:HD13	14:BC:223:ARG:HB2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:AO:64:ARG:HB2	6:AO:65:PRO:CD	2.39	0.52
12:AW:97:THR:HA	12:AW:103:ARG:CZ	2.39	0.52
7:AR:372:LEU:HD23	7:AR:387:LEU:HD13	1.92	0.52
14:AY:124:ILE:HB	14:AY:251:ILE:HB	1.92	0.52
7:AR:1064:CYS:SG	7:AR:1067:CYS:HB2	2.49	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
9:AT:136:ILE:HG12	9:AT:171:LYS:HB2	1.92	0.52
9:AT:126:ILE:HD11	9:AT:128:PHE:CD1	2.45	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: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:BA:532:ILE:HD13	12:BA:554:ALA:HB1	1.90	0.52
7:AR:72:ARG:HB3	7:AR:82:GLU:HA	1.92	0.52
7:BB:1053:LEU:HD23	7:BB:1053:LEU:C	2.30	0.52
12:AW:851:GLY:O	12:AW:852:ASP:HB2	2.08	0.52
7:AR:52:ILE:CG2	7:AR:53:PRO:HD3	2.39	0.52
12:BA:282:PRO:O	12:BA:284:LEU:HG	2.10	0.52
12:AW:283:GLY:CA	12:AW:284:LEU:CB	2.86	0.52
12:BA:548:GLY:HA2	12:BA:551:VAL:HG12	1.92	0.52
11:AV:36:PHE:CD1	11:AV:96:ILE:HD13	2.45	0.52
8:BD:93:TYR:CE1	8:BD:146:ARG:HG2	2.45	0.52
6:AO:5:ILE:HD11	8:AS:61:ARG:CZ	2.40	0.52
7:BB:406:TRP:CB	7:BB:407:VAL:HB	2.40	0.52
12:BA:146:CYS:SG	12:BA:154:PHE:CE2	3.03	0.52
12:BA:687:ILE:HG13	12:BA:688:PRO:HD2	1.91	0.52
12:AW:763:THR:O	12:AW:764:ARG:CB	2.58	0.52
12:BA:691:THR:HG22	12:BA:692:LEU:N	2.25	0.52
7:AR:170:LEU:HD23	7:AR:171:ALA:N	2.25	0.52
12:BA:606:GLN:O	12:BA:608:PRO:HD3	2.10	0.52
11:BG:57:ALA:HA	11:BG:115:ILE:HD13	1.90	0.52
14:AY:154:SER:HB3	14:AY:170:ASP:HB2	1.91	0.52
12:AW:549:LYS:HD2	12:AW:593:LEU:HD22	1.92	0.52
12:BA:36:ASP:N	12:BA:37:GLY:CA	2.71	0.51
12:AW:282:PRO:O	12:AW:284:LEU:HG	2.09	0.51
10:BF:62:ILE:O	10:BF:63:ILE:HB	2.11	0.51
12:BA:40:ILE:HG22	12:BA:41:GLU:N	2.24	0.51
14:BC:322:ARG:O	14:BC:323:THR:CB	2.58	0.51
12:BA:868:VAL:HG12	14:BC:35:LEU:HD12	1.91	0.51
3:AI:75:PRO:HB3	14:AY:394:LEU:HD11	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:AS:93:TYR:CE1	8:AS:146:ARG:HG2	2.45	0.51
7:BB:736:ASN:HB3	7:BB:742:ILE:HG13	1.92	0.51
12:BA:848:VAL:O	12:BA:849:ALA:CB	2.58	0.51
12:AW:548:GLY:HA2	12:AW:551:VAL:HG12	1.92	0.51
12:BA:868:VAL:CG1	14:BC:35:LEU:HD12	2.41	0.51
6:AO:43:TYR:OH	7:AR:907:VAL:HG11	2.09	0.51
7:BB:974:TYR:CE2	7:BB:981:LYS:HB3	2.46	0.51
12:BA:830:LEU:HD11	14:BC:319:VAL:HG21	1.92	0.51
14:AY:104:LEU:N	14:AY:105:PRO:CD	2.73	0.51
7:AR:736:ASN:HB3	7:AR:742:ILE:HG13	1.92	0.51
7:BB:72:ARG:HB3	7:BB:82:GLU:HA	1.91	0.51
7:AR:406:TRP:CB	7:AR:407:VAL:HB	2.40	0.51
11:BG:79:THR:O	11:BG:84:SER:HB2	2.11	0.51
9:BE:136:ILE:HG12	9:BE:171:LYS:HB2	1.92	0.51
12:BA:524:ILE:CG2	12:BA:634:VAL:HG13	2.41	0.51
9:BE:88:GLU:HG2	9:BE:89:VAL:N	2.26	0.51
7:AR:665:GLN:HG2	7:AR:667:PRO:HD2	1.91	0.51
7:BB:636:LEU:HD21	7:BB:643:LEU:HD12	1.92	0.51
7:BB:628:TYR:CE2	7:BB:640:HIS:CE1	2.98	0.51
7:AR:52:ILE:HG22	7:AR:53:PRO:N	2.26	0.51
11:BG:64:LEU:N	11:BG:64:LEU:HD22	2.25	0.51
12:BA:665:ILE:O	12:BA:668:ALA:HB3	2.11	0.51
7:AR:545:GLU:HG3	7:AR:546:ARG:N	2.24	0.51
7:BB:235:ILE:HD12	7:BB:235:ILE:N	2.26	0.51
7:AR:66:ILE:HG13	7:AR:101:LEU:HD23	1.92	0.51
14:AY:348:GLU:CG	14:AY:349:VAL:N	2.74	0.51
10:BF:6:ILE:HD12	10:BF:6:ILE:N	2.25	0.51
12:BA:763:THR:O	12:BA:764:ARG:CB	2.58	0.51
9:AT:91:GLN:HA	9:AT:138:LYS:HE2	1.93	0.51
7:AR:918:LEU:H	7:AR:919:PRO:HD2	1.74	0.51
7:BB:52:ILE:HG22	7:BB:53:PRO:N	2.26	0.51
7:BB:734:GLY:N	7:BB:735:TYR:HB2	2.24	0.51
12:BA:103:ARG:HG3	12:BA:187:VAL:HG13	1.93	0.51
7:BB:1080:TYR:HB3	7:BB:1091:LEU:HD12	1.92	0.51
11:AV:16:ASN:O	11:AV:17:SER:HB3	2.10	0.51
7:AR:628:TYR:CE2	7:AR:640:HIS:CE1	2.98	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
7:BB:372:LEU:HD23	7:BB:387:LEU:HD13	1.92	0.51
10:AU:65:ARG:O	10:AU:69:ARG:HG3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:AR:235:ILE:HD12	7:AR:235:ILE:N	2.26	0.51
7:AR:974:TYR:CE2	7:AR:981:LYS:HB3	2.46	0.51
11:AV:79:THR:O	11:AV:84:SER:HB2	2.11	0.51
12:BA:147:PRO:O	12:BA:148:HIS:HB2	2.10	0.51
12:AW:687:ILE:HG13	12:AW:688:PRO:HD2	1.91	0.51
11:BG:16:ASN:O	11:BG:17:SER:HB3	2.10	0.51
12:AW:691:THR:HG22	12:AW:692:LEU:N	2.25	0.51
7:AR:242:VAL:CG1	7:AR:252:GLN:HG3	2.41	0.51
8:BD:78:TRP:HB3	8:BD:79:PRO:HD2	1.91	0.51
12:AW:606:GLN:O	12:AW:608:PRO:HD3	2.11	0.51
12:BA:363:GLN:O	12:BA:366:ILE:HG22	2.11	0.51
10:AU:6:ILE:N	10:AU:6:ILE:HD12	2.25	0.51
7:AR:284:LYS:O	7:AR:285:ARG:C	2.49	0.51
7:BB:242:VAL:CG1	7:BB:252:GLN:HG3	2.41	0.51
14:AY:165:ILE:HD13	14:AY:223:ARG:HB2	1.91	0.51
12:AW:21:LYS:O	12:AW:24:VAL:HG13	2.11	0.51
4:AJ:77:LYS:O	4:AJ:81:ARG:HG2	2.11	0.51
14:AY:244:LYS:HB3	14:AY:249:TYR:CD1	2.46	0.51
4:BQ:77:LYS:O	4:BQ:81:ARG:HG2	2.11	0.51
12:AW:363:GLN:O	12:AW:366:ILE:HG22	2.11	0.51
12:AW:185:GLU:HA	12:AW:205:GLU:CG	2.41	0.51
12:BA:185:GLU:HA	12:BA:205:GLU:CG	2.41	0.51
9:AT:88:GLU:HG2	9:AT:89:VAL:N	2.26	0.51
8:AS:219:ILE:HD12	8:AS:219:ILE:N	2.26	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
12:AW:703:THR:HG22	12:AW:707:LEU:CD1	2.41	0.51
11:AV:88:ASN:HB2	12:AW:538:ALA:CB	2.40	0.51
12:AW:765:THR:HG22	12:AW:766:LEU:HD22	1.92	0.51
7:AR:364:PHE:CE1	7:AR:388:VAL:HG13	2.46	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
7:BB:734:GLY:HA3	7:BB:735:TYR:HB2	1.90	0.51
12:BA:502:TYR:CD1	12:BA:632:PHE:HB3	2.46	0.51
12:AW:378:VAL:HG22	12:AW:386:ILE:HB	1.92	0.51
6:AO:53:ILE:HD11	7:AR:701:PRO:HG2	1.92	0.51
4:BQ:54:LEU:HA	4:BQ:59:ILE:HG22	1.93	0.50
11:AV:64:LEU:N	11:AV:64:LEU:HD22	2.26	0.50
10:BF:78:ILE:HG12	10:BF:79:THR:N	2.26	0.50
10:BF:65:ARG:O	10:BF:69:ARG:HG3	2.10	0.50
9:BE:91:GLN:HA	9:BE:138:LYS:HE2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:AW:17:ASP:HA	12:AW:20:ARG:HG2	1.93	0.50
8:AS:153:HIS:O	8:AS:154:ALA:HB3	2.11	0.50
7:BB:284:LYS:O	7:BB:285:ARG:C	2.49	0.50
12:BA:106:ILE:HG12	12:BA:154:PHE:CZ	2.47	0.50
12:AW:104:VAL:HA	12:AW:191:ASP:OD2	2.12	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: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
8:AS:41:ILE:HB	8:AS:63:ALA:HA	1.93	0.50
7:AR:636:LEU:HD21	7:AR:643:LEU:HD12	1.93	0.50
12:AW:84:VAL:HG11	12:AW:274:ALA:HB1	1.93	0.50
7:BB:66:ILE:HG13	7:BB:101:LEU:HD23	1.93	0.50
7:AR:1053:LEU:HD23	7:AR:1053:LEU:C	2.31	0.50
12:BA:104:VAL:HA	12:BA:191:ASP:OD2	2.12	0.50
12:AW:70:GLY:O	12:AW:71:HIS:CB	2.59	0.50
7:AR:631:LEU:CD2	12:AW:768:HIS:CD2	2.95	0.50
14:BC:216:ILE:O	14:BC:217:ALA:HB2	2.12	0.50
12:BA:17:ASP:HA	12:BA:20:ARG:HG2	1.93	0.50
14:BC:124:ILE:HB	14:BC:251:ILE:HB	1.92	0.50
12:BA:378:VAL:HG22	12:BA:386:ILE:HB	1.92	0.50
12:BA:703:THR:HG22	12:BA:707:LEU:CD1	2.41	0.50
12:AW:848:VAL:O	12:AW:849:ALA:CB	2.58	0.50
11:BG:99:PHE:CD2	11:BG:99:PHE:O	2.65	0.50
11:AV:94:THR:HG22	11:AV:96:ILE:HD11	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
6:BN:35:LEU:HD13	6:BN:46:ARG:HG3	1.94	0.50
12:BA:765:THR:HG22	12:BA:766:LEU:HD22	1.93	0.50
8:BD:219:ILE:N	8:BD:219:ILE:HD12	2.26	0.50
12:AW:600:LYS:HG2	12:AW:600:LYS:O	2.11	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
15:BH:23:LEU:HD21	15:BH:64:ARG:HD2	1.93	0.50
12:BA:21:LYS:O	12:BA:24:VAL:HG13	2.11	0.50
14:AY:216:ILE:O	14:AY:217:ALA:HB2	2.12	0.50
12:BA:84:VAL:HG11	12:BA:274:ALA:HB1	1.93	0.50
11:BG:106:ILE:O	11:BG:107:SER:HB2	2.11	0.50
8:BD:41:ILE:HB	8:BD:63:ALA:HA	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:AR:774:ASP:O	7:AR:775:LYS:HB3	2.11	0.50
7:BB:406:TRP:CG	7:BB:407:VAL:HB	2.47	0.50
7:AR:406:TRP:HA	7:AR:407:VAL:HG23	1.94	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
15:BH:45:ILE:HG13	15:BH:79:ARG:HB3	1.94	0.50
7:AR:592:VAL:HG23	7:AR:615:LYS:HD3	1.93	0.50
7:BB:900:MET:SD	7:BB:912:ILE:HD11	2.52	0.50
10:AU:60:SER:HA	10:AU:69:ARG:NE	2.27	0.50
7:BB:364:PHE:CE1	7:BB:388:VAL:HG13	2.46	0.50
2:AD:13:DG:OP1	14:AY:352:LYS:HE3	2.12	0.50
7:BB:54:THR:OG1	7:BB:55:GLU:N	2.45	0.50
11:BG:65:SER:CB	11:BG:66:TYR:CA	2.87	0.50
7:BB:348:LEU:O	7:BB:352:LEU:HD23	2.12	0.50
2:BS:14:DA:C5	2:BS:15:DT:C7	2.94	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
8:BD:153:HIS:O	8:BD:154:ALA:HB3	2.11	0.50
12:BA:402:ALA:HB1	12:BA:403:PRO:HD2	1.93	0.50
2:AD:16:DA:OP2	12:AW:814:SER:HB3	2.12	0.50
7:AR:406:TRP:CG	7:AR:407:VAL:HB	2.47	0.50
14:BC:81:PRO:CB	14:BC:306:LEU:HG	2.42	0.50
12:BA:70:GLY:O	12:BA:71:HIS:CB	2.59	0.50
9:BE:125:GLY:C	9:BE:126:ILE:HG23	2.32	0.50
5:AM:23:THR:HG23	8:AS:27:ALA:HA	1.94	0.50
14:BC:244:LYS:HB3	14:BC:249:TYR:CD1	2.46	0.50
7:BB:854:LEU:C	7:BB:854:LEU:HD23	2.33	0.50
7:AR:448:LEU:HD22	12:AW:796:PHE:CZ	2.46	0.50
7:BB:226:PHE:CZ	7:BB:230:MET:HG3	2.47	0.50
12:BA:33:TYR:H	12:BA:34:ASP:CB	2.25	0.49
12:AW:106:ILE:HG12	12:AW:154:PHE:CZ	2.47	0.49
14:BC:80:GLU:N	14:BC:81:PRO:HD3	2.27	0.49
15:AZ:45:ILE:HG13	15:AZ:79:ARG:HB3	1.93	0.49
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:BA:830:LEU:HD13	14:BC:315:LEU:HD21	1.94	0.49
10:BF:60:SER:HA	10:BF:69:ARG:NE	2.27	0.49
15:AZ:38:ARG:HB3	15:AZ:39:PRO:HD2	1.93	0.49
7:BB:774:ASP:O	7:BB:775:LYS:HB3	2.12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:BG:94:THR:HG22	11:BG:96:ILE:HD11	1.93	0.49
14:BC:301:LEU:HD13	14:BC:308:VAL:CG1	2.41	0.49
7:BB:730:ILE:HG23	7:BB:986:ILE:HD12	1.94	0.49
12:AW:747:LEU:HD22	12:AW:786:PHE:CE2	2.48	0.49
9:AT:166:GLN:HB3	9:AT:167:PRO:HD2	1.94	0.49
14:AY:80:GLU:N	14:AY:81:PRO:HD3	2.26	0.49
12:AW:75:ILE:HD12	12:AW:243:VAL:HG22	1.94	0.49
11:AV:99:PHE:O	11:AV:99:PHE:CD2	2.65	0.49
7:AR:900:MET:SD	7:AR:912:ILE:HD11	2.52	0.49
13:BP:7:GLY:HA3	13:BP:34:ILE:HD11	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
3:AI:88:ILE:HD12	3:AI:88:ILE:N	2.27	0.49
12:BA:105:LYS:HE2	12:BA:136:VAL:HG12	1.94	0.49
7:BB:592:VAL:HG23	7:BB:615:LYS:HD3	1.94	0.49
10:BF:60:SER:HA	10:BF:69:ARG:CZ	2.42	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
12:AW:868:VAL:HG13	14:AY:32:LEU:HD23	1.94	0.49
9:BE:15:PRO:HD3	9:BE:65:ALA:HB2	1.94	0.49
14:AY:102:LEU:HB2	14:AY:106:ARG:HB2	1.94	0.49
15:BH:38:ARG:HB3	15:BH:39:PRO:HD2	1.94	0.49
9:AT:15:PRO:HD3	9:AT:65:ALA:HB2	1.94	0.49
7:AR:138:LEU:HG	7:AR:148:PRO:HB3	1.94	0.49
12:BA:600:LYS:HG2	12:BA:600:LYS:O	2.11	0.49
7:AR:733:THR:HG23	7:AR:735:TYR:HD2	1.76	0.49
9:AT:125:GLY:C	9:AT:126:ILE:HG23	2.32	0.49
11:BG:93:ILE:HG22	11:BG:94:THR:N	2.27	0.49
7:BB:201:VAL:HG23	7:BB:218:PRO:HG2	1.94	0.49
15:AZ:23:LEU:HD21	15:AZ:64:ARG:HD2	1.93	0.49
7:BB:566:ILE:HD13	7:BB:568:GLU:CD	2.33	0.49
13:AX:7:GLY:HA3	13:AX:34:ILE:HD11	1.95	0.49
7:AR:743:MET:HE1	7:AR:891:ILE:HD11	1.93	0.49
7:BB:658:ILE:HG12	7:BB:672:GLN:HG2	1.94	0.49
14:AY:349:VAL:HB	14:AY:353:HIS:CE1	2.47	0.49
12:BA:703:THR:HG22	12:BA:707:LEU:HD12	1.95	0.49
11:BG:96:ILE:CD1	11:BG:99:PHE:HB2	2.42	0.49
12:AW:118:TYR:O	12:AW:121:ILE:HG22	2.13	0.49
7:BB:138:LEU:HG	7:BB:148:PRO:HB3	1.94	0.49
12:BA:440:GLY:HA3	12:BA:444:ARG:NH2	2.27	0.49
7:BB:647:SER:N	7:BB:648:PRO:CD	2.75	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:BA:77:LEU:CD2	12:BA:77:LEU:N	2.76	0.49
7:BB:228:ILE:HG23	7:BB:271:ALA:HB1	1.94	0.49
14:AY:348:GLU:O	14:AY:349:VAL:HB	2.12	0.49
12:BA:131:ARG:NH1	4:BQ:36:LEU:HD21	2.26	0.49
10:AU:88:ILE:CG2	10:AU:88:ILE:O	2.60	0.49
12:AW:105:LYS:HE2	12:AW:136:VAL:HG12	1.93	0.49
14:AY:176:ASP:CA	14:AY:177:LYS:HB2	2.42	0.49
12:AW:103:ARG:HG3	12:AW:187:VAL:HG13	1.93	0.49
14:BC:349:VAL:HB	14:BC:353:HIS:CE1	2.47	0.49
7:AR:201:VAL:HG23	7:AR:218:PRO:HG2	1.94	0.49
12:BA:118:TYR:O	12:BA:121:ILE:HG22	2.13	0.49
7:AR:226:PHE:CZ	7:AR:230:MET:HG3	2.48	0.49
14:AY:209:SER:O	14:AY:210:PHE:CB	2.61	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
7:BB:380:ARG:CB	7:BB:381:LYS:HA	2.36	0.49
14:AY:366:PHE:O	14:AY:367:LYS:HB2	2.12	0.49
14:AY:210:PHE:CE1	14:AY:214:ASP:O	2.66	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
14:AY:85:MET:SD	14:AY:304:GLN:HG3	2.53	0.49
5:AM:82:HIS:CE1	5:AM:86:GLU:OE2	2.66	0.49
7:BB:904:VAL:HG23	7:BB:972:VAL:HG13	1.95	0.49
7:AR:647:SER:N	7:AR:648:PRO:CD	2.76	0.49
1:BR:1:DT:H2"	1:BR:2:DC:C6	2.48	0.49
12:BA:91:TYR:CE1	12:BA:95:LYS:HD2	2.47	0.49
1:AC:1:DT:H2"	1:AC:2:DC:C6	2.48	0.49
12:BA:393:ASP:O	12:BA:394:ARG:HB3	2.13	0.49
4:AJ:37:SER:OG	4:AJ:39:GLN:HG2	2.13	0.49
12:AW:703:THR:HG22	12:AW:707:LEU:HD12	1.95	0.49
10:BF:88:ILE:O	10:BF:88:ILE:CG2	2.60	0.49
12:BA:418:LEU:HD21	7:BB:1047:LEU:HD21	1.95	0.49
7:BB:874:ILE:CG2	7:BB:875:PRO:HD2	2.43	0.49
12:BA:842:TYR:CZ	14:BC:339:ASN:O	2.66	0.49
7:AR:968:ASP:O	7:AR:969:ALA:HB3	2.13	0.49
7:AR:854:LEU:HD23	7:AR:854:LEU:C	2.33	0.49
7:AR:53:PRO:CB	7:AR:54:THR:HB	2.39	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
11:BG:79:THR:CB	11:BG:80:GLU:HB2	2.38	0.48
9:BE:166:GLN:HB3	9:BE:167:PRO:HD2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:AU:100:ILE:O	10:AU:104:ILE:HG13	2.13	0.48
12:AW:102:GLY:O	12:AW:103:ARG:C	2.52	0.48
11:BG:77:ILE:CD1	11:BG:106:ILE:HG21	2.42	0.48
7:BB:748:VAL:HG13	7:BB:875:PRO:HG2	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
11:BG:39:SER:HB3	11:BG:93:ILE:HB	1.94	0.48
11:AV:93:ILE:HG22	11:AV:94:THR:N	2.27	0.48
7:AR:666:SER:N	7:AR:667:PRO:HD2	2.28	0.48
7:AR:242:VAL:HG13	7:AR:252:GLN:HG3	1.95	0.48
7:BB:209:LYS:O	7:BB:210:ASP:CB	2.60	0.48
7:AR:730:ILE:HG23	7:AR:986:ILE:HD12	1.95	0.48
7:AR:566:ILE:HD13	7:AR:568:GLU:CD	2.34	0.48
12:AW:393:ASP:O	12:AW:394:ARG:HB3	2.13	0.48
11:AV:43:ILE:HG22	11:AV:44:ASP:N	2.28	0.48
9:AT:30:LEU:HD22	9:AT:72:PHE:CE2	2.47	0.48
12:AW:557:PRO:HG2	12:AW:619:TYR:CZ	2.48	0.48
7:AR:54:THR:OG1	7:AR:55:GLU:N	2.45	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
14:BC:348:GLU:O	14:BC:349:VAL:HB	2.13	0.48
12:BA:743:MET:SD	7:BB:922:MET:HG2	2.53	0.48
9:AT:56:GLU:CG	14:AY:391:ARG:HG2	2.42	0.48
7:BB:666:SER:N	7:BB:667:PRO:HD2	2.27	0.48
8:AS:96:ILE:HG12	8:AS:145:LEU:HD11	1.95	0.48
12:BA:747:LEU:HD22	12:BA:786:PHE:CE2	2.48	0.48
5:BL:82:HIS:CE1	5:BL:86:GLU:OE2	2.66	0.48
11:BG:43:ILE:HG22	11:BG:44:ASP:N	2.28	0.48
14:BC:366:PHE:O	14:BC:367:LYS:HB2	2.12	0.48
12:AW:505:GLY:CA	12:AW:639:VAL:CG2	2.91	0.48
14:BC:101:THR:C	14:BC:102:LEU:HD22	2.33	0.48
7:AR:52:ILE:HG22	7:AR:53:PRO:CD	2.43	0.48
14:AY:151:ASN:O	14:AY:173:MET:HG2	2.13	0.48
7:AR:323:SER:HA	7:AR:326:ILE:CG1	2.44	0.48
7:AR:136:TYR:HB2	7:AR:141:LEU:CD1	2.43	0.48
8:BD:96:ILE:HG12	8:BD:145:LEU:HD11	1.95	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
9:BE:30:LEU:HD22	9:BE:72:PHE:CE2	2.47	0.48
3:BK:88:ILE:N	3:BK:88:ILE:HD12	2.28	0.48
12:AW:203:ARG:HB2	12:AW:206:TRP:CD2	2.48	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
12:AW:33:TYR:H	12:AW:34:ASP:CB	2.25	0.48
14:AY:146:TYR:HB2	14:AY:234:ILE:O	2.13	0.48
14:BC:85:MET:SD	14:BC:304:GLN:HG3	2.54	0.48
11:AV:96:ILE:CD1	11:AV:99:PHE:HB2	2.42	0.48
14:AY:101:THR:C	14:AY:102:LEU:HD22	2.33	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
15:BH:63:ILE:HD13	15:BH:81:VAL:CG2	2.42	0.48
7:BB:35:ASN:O	7:BB:38:VAL:HG12	2.14	0.48
12:AW:58:CYS:HB3	12:AW:62:GLY:H	1.79	0.48
13:AX:44:ILE:N	13:AX:44:ILE:HD12	2.28	0.48
12:AW:40:ILE:HD13	12:AW:47:PRO:CG	2.43	0.48
7:AR:1096:VAL:HG12	7:AR:1097:SER:N	2.28	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
10:BF:62:ILE:CD1	10:BF:100:ILE:HG12	2.44	0.48
14:BC:348:GLU:HG3	14:BC:349:VAL:N	2.28	0.48
9:AT:134:LYS:HE3	9:AT:171:LYS:HB3	1.95	0.48
7:BB:584:ILE:HB	7:BB:591:LEU:HD12	1.96	0.48
11:BG:96:ILE:HD12	11:BG:99:PHE:HB2	1.94	0.48
12:AW:868:VAL:HG12	14:AY:35:LEU:HD12	1.95	0.48
7:AR:904:VAL:HG23	7:AR:972:VAL:HG13	1.94	0.48
12:BA:557:PRO:HG2	12:BA:619:TYR:CZ	2.49	0.48
12:BA:505:GLY:CA	12:BA:639:VAL:CG2	2.91	0.48
7:AR:68:ILE:N	7:AR:68:ILE:HD12	2.29	0.48
3:AI:79:ARG:HD2	14:AY:389:THR:CG2	2.44	0.48
12:BA:203:ARG:HB2	12:BA:206:TRP:CD2	2.48	0.48
9:AT:8:ARG:HG2	9:AT:71:GLU:HG2	1.94	0.48
7:BB:1112:ILE:O	7:BB:1114:PRO:HD3	2.14	0.48
14:BC:209:SER:O	14:BC:210:PHE:CB	2.61	0.48
12:AW:191:ASP:O	12:AW:195:LEU:HG	2.14	0.48
14:AY:185:LYS:HA	14:AY:188:ILE:HD12	1.95	0.48
9:BE:134:LYS:HE3	9:BE:171:LYS:HB3	1.96	0.48
9:BE:126:ILE:HG13	9:BE:127:ILE:N	2.26	0.48
7:BB:242:VAL:HG13	7:BB:252:GLN:HG3	1.95	0.48
1:AC:11:DT:H2"	1:AC:12:DA:C5'	2.44	0.48
15:AZ:63:ILE:HD13	15:AZ:81:VAL:CG2	2.43	0.48
7:BB:1096:VAL:HG12	7:BB:1097:SER:N	2.28	0.48
9:AT:75:ILE:HG21	10:AU:21:LEU:HD11	1.93	0.48
2:AD:14:DA:C5	2:AD:15:DT:H73	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:BC:151:ASN:O	14:BC:173:MET:HG2	2.13	0.48
12:AW:33:TYR:CA	12:AW:34:ASP:HB2	2.44	0.48
14:AY:81:PRO:CB	14:AY:306:LEU:HG	2.42	0.48
7:BB:781:PRO:HA	7:BB:786:TYR:CZ	2.49	0.48
14:AY:237:ILE:HG12	14:AY:238:LYS:N	2.29	0.48
14:AY:188:ILE:HG12	14:AY:230:LYS:NZ	2.29	0.48
12:AW:764:ARG:HD2	12:AW:769:PHE:O	2.14	0.48
7:BB:605:ILE:HG22	7:BB:609:ASP:HB2	1.96	0.48
5:BL:11:ASN:HB3	5:BL:59:THR:HG23	1.96	0.48
4:BQ:37:SER:OG	4:BQ:39:GLN:HG2	2.13	0.48
12:AW:865:THR:HG22	14:AY:28:ILE:HD11	1.96	0.48
11:AV:102:LEU:HA	11:AV:105:ILE:HG12	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
12:AW:77:LEU:CD2	12:AW:77:LEU:N	2.76	0.48
7:BB:422:TRP:CZ3	7:BB:426:LEU:HD11	2.49	0.48
7:AR:191:LYS:HE2	7:AR:193:ILE:HD11	1.96	0.48
12:BA:541:ALA:HB3	12:BA:542:PRO:HD2	1.96	0.48
12:AW:281:ILE:HG13	12:AW:284:LEU:HD12	1.95	0.48
10:AU:62:ILE:CD1	10:AU:100:ILE:HG12	2.44	0.48
12:BA:47:PRO:O	12:BA:59:PRO:HD2	2.14	0.48
14:AY:277:ILE:O	14:AY:278:ARG:CB	2.62	0.48
14:BC:277:ILE:O	14:BC:278:ARG:CB	2.62	0.48
8:AS:161:LEU:HD12	8:AS:163:ILE:HD13	1.95	0.48
7:BB:53:PRO:CB	7:BB:54:THR:HB	2.39	0.47
10:BF:100:ILE:O	10:BF:104:ILE:HG13	2.14	0.47
7:AR:781:PRO:HA	7:AR:786:TYR:CZ	2.49	0.47
14:BC:85:MET:HE3	14:BC:104:LEU:HD12	1.96	0.47
12:AW:185:GLU:HA	12:AW:205:GLU:HG2	1.95	0.47
14:BC:102:LEU:HB2	14:BC:106:ARG:HB2	1.94	0.47
12:BA:130:ARG:O	12:BA:134:GLU:HG2	2.14	0.47
12:AW:667:ARG:O	12:AW:670:VAL:HG22	2.14	0.47
7:AR:605:ILE:HG22	7:AR:609:ASP:HB2	1.96	0.47
7:AR:422:TRP:CZ3	7:AR:426:LEU:HD11	2.49	0.47
7:BB:403:THR:HG23	7:BB:405:ASN:N	2.29	0.47
8:AS:237:LYS:HA	8:AS:237:LYS:HE2	1.96	0.47
7:BB:52:ILE:HG22	7:BB:53:PRO:CD	2.43	0.47
11:AV:63:ARG:C	11:AV:64:LEU:HD22	2.35	0.47
12:BA:33:TYR:HB3	12:BA:34:ASP:CB	2.44	0.47
7:BB:1064:CYS:HB3	7:BB:1067:CYS:HB2	1.95	0.47
12:AW:32:VAL:O	12:AW:44:VAL:HG21	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:AY:143:LYS:O	14:AY:234:ILE:HB	2.14	0.47
9:BE:126:ILE:HG12	9:BE:128:PHE:CE2	2.49	0.47
7:BB:918:LEU:HD13	7:BB:927:ILE:HD11	1.96	0.47
12:BA:185:GLU:HA	12:BA:205:GLU:HG2	1.95	0.47
14:AY:157:SER:HB3	14:AY:166:ILE:HB	1.96	0.47
12:BA:78:VAL:HG21	12:BA:249:LEU:HB3	1.96	0.47
7:BB:68:ILE:N	7:BB:68:ILE:HD12	2.29	0.47
13:BP:44:ILE:HD12	13:BP:44:ILE:N	2.29	0.47
8:BD:237:LYS:HA	8:BD:237:LYS:HE2	1.96	0.47
12:BA:40:ILE:HD13	12:BA:47:PRO:CG	2.43	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
14:BC:237:ILE:HG12	14:BC:238:LYS:N	2.29	0.47
7:BB:323:SER:HA	7:BB:326:ILE:CG1	2.44	0.47
12:BA:764:ARG:HD2	12:BA:769:PHE:O	2.14	0.47
12:AW:70:GLY:HA2	12:AW:216:PRO:CB	2.45	0.47
14:BC:188:ILE:HG12	14:BC:230:LYS:NZ	2.29	0.47
7:BB:233:LEU:HD11	7:BB:311:ARG:C	2.34	0.47
12:AW:78:VAL:HG21	12:AW:249:LEU:HB3	1.96	0.47
14:AY:245:LYS:HE2	14:AY:250:ILE:HD11	1.97	0.47
9:AT:42:LEU:N	9:AT:42:LEU:HD12	2.30	0.47
5:AM:3:ILE:N	5:AM:3:ILE:HD12	2.29	0.47
7:BB:220:VAL:O	7:BB:221:PRO:C	2.53	0.47
7:AR:356:LEU:HA	7:AR:407:VAL:CG1	2.44	0.47
12:BA:191:ASP:O	12:BA:195:LEU:HG	2.14	0.47
12:BA:33:TYR:N	12:BA:34:ASP:CB	2.78	0.47
12:BA:102:GLY:O	12:BA:103:ARG:C	2.52	0.47
12:BA:32:VAL:O	12:BA:44:VAL:HG21	2.14	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
7:AR:233:LEU:HD11	7:AR:311:ARG:C	2.35	0.47
12:AW:65:LEU:HD23	12:AW:65:LEU:C	2.34	0.47
2:AD:14:DA:H1'	2:AD:15:DT:H5'	1.96	0.47
14:AY:331:ARG:O	14:AY:336:GLY:HA3	2.14	0.47
7:BB:53:PRO:CB	7:BB:54:THR:CA	2.89	0.47
11:BG:72:CYS:HB3	11:BG:114:LYS:HD2	1.96	0.47
12:AW:281:ILE:CD1	12:AW:284:LEU:HD12	2.44	0.47
12:AW:107:SER:HB3	12:AW:140:ALA:HA	1.96	0.47
2:AD:5:DG:C2	2:AD:6:DA:C2	3.03	0.47
12:BA:33:TYR:CA	12:BA:34:ASP:HB2	2.44	0.47
7:AR:1104:ILE:HG23	7:AR:1114:PRO:HG2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:AU:95:TYR:CE1	10:AU:97:SER:HB2	2.50	0.47
12:BA:65:LEU:HD23	12:BA:65:LEU:C	2.34	0.47
7:AR:220:VAL:O	7:AR:221:PRO:C	2.53	0.47
4:AJ:39:GLN:OE1	4:AJ:78:ARG:CZ	2.63	0.47
14:AY:209:SER:O	14:AY:210:PHE:HB2	2.14	0.47
14:AY:130:TYR:CD2	14:AY:136:LYS:HB3	2.50	0.47
9:AT:113:ILE:CG2	9:AT:136:ILE:HD12	2.45	0.47
7:BB:136:TYR:HB2	7:BB:141:LEU:CD1	2.44	0.47
7:AR:457:CYS:HB3	7:AR:460:GLU:HB2	1.96	0.47
7:AR:287:ASN:O	7:AR:291:LYS:N	2.48	0.47
14:BC:331:ARG:O	14:BC:336:GLY:HA3	2.14	0.47
12:BA:667:ARG:O	12:BA:670:VAL:HG22	2.14	0.47
12:AW:646:MET:HE2	12:AW:725:ALA:HB2	1.97	0.47
11:BG:63:ARG:C	11:BG:64:LEU:HD22	2.34	0.47
14:BC:209:SER:O	14:BC:210:PHE:HB2	2.14	0.47
7:AR:734:GLY:HA3	7:AR:735:TYR:HB2	1.91	0.47
12:AW:33:TYR:HB3	12:AW:34:ASP:CB	2.44	0.47
12:AW:47:PRO:O	12:AW:59:PRO:HD2	2.14	0.47
12:AW:33:TYR:N	12:AW:34:ASP:CB	2.78	0.47
12:AW:146:CYS:HB3	12:AW:149:CYS:HB2	1.81	0.47
14:BC:81:PRO:HB3	14:BC:306:LEU:HG	1.97	0.47
11:BG:102:LEU:HA	11:BG:105:ILE:HG12	1.95	0.47
12:BA:70:GLY:HA2	12:BA:216:PRO:CB	2.44	0.47
9:BE:113:ILE:CG2	9:BE:136:ILE:HD12	2.45	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
13:AX:24:VAL:O	13:AX:24:VAL:HG13	2.15	0.47
6:BN:19:GLN:HB3	6:BN:20:PRO:HD3	1.97	0.47
12:BA:302:LEU:HD23	12:BA:308:ARG:HG3	1.95	0.47
15:AZ:18:PRO:HB3	15:AZ:67:ARG:HB3	1.97	0.47
9:BE:42:LEU:HD12	9:BE:42:LEU:N	2.30	0.47
1:BR:11:DT:H2"	1:BR:12:DA:C5'	2.44	0.47
8:BD:150:GLY:HA2	8:BD:156:PHE:HB2	1.96	0.47
7:AR:403:THR:HG23	7:AR:405:ASN:N	2.29	0.47
12:BA:671:GLU:O	12:BA:674:ASN:OD1	2.33	0.47
11:AV:61:LYS:O	11:AV:62:ASN:HB2	2.15	0.47
4:BQ:39:GLN:OE1	4:BQ:78:ARG:CZ	2.63	0.47
7:BB:356:LEU:HA	7:BB:407:VAL:CG1	2.43	0.47
7:AR:406:TRP:HB3	7:AR:407:VAL:C	2.35	0.47
12:AW:145:VAL:HG13	12:AW:146:CYS:N	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BS:14:DA:C5	2:BS:15:DT:H73	2.49	0.47
12:AW:27:ILE:CG2	12:AW:74:HIS:CE1	2.98	0.47
14:BC:245:LYS:HE2	14:BC:250:ILE:HD11	1.96	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
5:AM:11:ASN:HB3	5:AM:59:THR:HG23	1.96	0.47
2:AD:14:DA:N7	2:AD:15:DT:H73	2.29	0.47
7:BB:406:TRP:HB3	7:BB:407:VAL:C	2.35	0.47
12:BA:277:PHE:CZ	7:BB:1111:ILE:HD13	2.50	0.47
7:AR:953:ILE:HG12	7:AR:954:GLU:H	1.80	0.47
9:AT:126:ILE:HG13	9:AT:127:ILE:N	2.26	0.47
14:AY:85:MET:HE3	14:AY:104:LEU:HD12	1.95	0.47
12:AW:492:GLY:HA3	12:AW:862:HIS:HA	1.97	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
8:AS:133:LEU:HD21	8:AS:139:ILE:HG12	1.96	0.47
5:BL:3:ILE:HD12	5:BL:3:ILE:N	2.30	0.47
12:BA:864:LYS:CD	12:BA:867:ASP:HA	2.45	0.47
7:AR:584:ILE:HB	7:AR:591:LEU:HD12	1.95	0.47
14:AY:122:MET:HE1	14:AY:124:ILE:HD11	1.97	0.47
7:AR:855:ILE:O	13:AX:34:ILE:HG22	2.14	0.47
12:BA:475:GLU:OE1	7:BB:1046:MET:HB2	2.15	0.47
12:AW:302:LEU:HD23	12:AW:308:ARG:HG3	1.95	0.47
7:BB:421:ASN:OD1	7:BB:421:ASN:C	2.54	0.47
7:AR:208:LEU:HD11	7:AR:214:HIS:CD2	2.50	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
7:AR:421:ASN:C	7:AR:421:ASN:OD1	2.54	0.47
2:AD:14:DA:OP1	14:AY:348:GLU:OE2	2.34	0.46
12:AW:541:ALA:HB3	12:AW:542:PRO:HD2	1.96	0.46
12:BA:125:TRP:CZ2	4:BQ:48:THR:HG21	2.50	0.46
14:AY:184:VAL:HG12	14:AY:188:ILE:HD11	1.98	0.46
14:BC:184:VAL:HG12	14:BC:188:ILE:HD11	1.97	0.46
7:AR:1096:VAL:CG1	7:AR:1097:SER:N	2.78	0.46
1:BR:11:DT:H2"	1:BR:12:DA:O5'	2.15	0.46
14:BC:394:LEU:N	14:BC:394:LEU:HD22	2.31	0.46
12:AW:818:TYR:CE1	12:AW:822:ARG:HG3	2.50	0.46
12:AW:36:ASP:N	12:AW:37:GLY:CA	2.72	0.46
11:BG:78:VAL:HG12	11:BG:79:THR:OG1	2.15	0.46
4:AJ:39:GLN:HG2	4:AJ:40:ASP:H	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:AW:127:SER:O	12:AW:131:ARG:HG3	2.15	0.46
11:BG:101:LEU:HD13	11:BG:102:LEU:H	1.80	0.46
7:BB:1104:ILE:HG23	7:BB:1114:PRO:HG2	1.96	0.46
7:BB:1096:VAL:CG1	7:BB:1097:SER:N	2.78	0.46
7:BB:961:LEU:HG	7:BB:967:PRO:HD3	1.97	0.46
7:AR:905:LYS:HG3	7:AR:965:TYR:CE2	2.50	0.46
4:AJ:45:MET:HB2	12:AW:122:LYS:HE2	1.98	0.46
12:BA:38:THR:N	12:BA:39:PRO:HD2	2.30	0.46
7:AR:8:LEU:N	7:AR:8:LEU:HD22	2.31	0.46
12:BA:9:ILE:HA	7:BB:1115:ARG:O	2.14	0.46
7:BB:88:ALA:HA	7:BB:93:LEU:HB2	1.97	0.46
14:BC:41:VAL:O	14:BC:42:LEU:C	2.53	0.46
7:AR:379:GLY:O	7:AR:380:ARG:HB2	2.16	0.46
12:BA:105:LYS:HZ2	12:BA:140:ALA:CB	2.27	0.46
9:BE:134:LYS:CE	9:BE:171:LYS:HB3	2.44	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
7:BB:208:LEU:HD11	7:BB:214:HIS:CD2	2.50	0.46
12:AW:775:SER:HB2	12:AW:776:PRO:HD2	1.97	0.46
7:AR:844:HIS:CD2	7:AR:1026:GLU:HG2	2.50	0.46
7:BB:457:CYS:HB3	7:BB:460:GLU:HB2	1.96	0.46
7:BB:287:ASN:O	7:BB:291:LYS:N	2.48	0.46
12:AW:864:LYS:CD	12:AW:867:ASP:HA	2.45	0.46
15:BH:83:SER:HB3	4:BQ:44:LEU:HD11	1.97	0.46
10:BF:76:CYS:HB2	10:BF:104:ILE:CG2	2.45	0.46
12:AW:691:THR:HG22	12:AW:692:LEU:H	1.80	0.46
7:AR:483:ILE:HG13	7:AR:555:GLU:HB2	1.97	0.46
7:BB:17:ILE:O	7:BB:20:TYR:HB3	2.15	0.46
12:BA:94:LEU:HD21	12:BA:180:ILE:HG23	1.98	0.46
1:BR:7:DA:C2	2:BS:9:DA:C2	3.03	0.46
12:BA:827:LEU:O	14:BC:71:GLY:HA3	2.14	0.46
13:BP:24:VAL:O	13:BP:24:VAL:HG13	2.15	0.46
4:BQ:39:GLN:HG2	4:BQ:40:ASP:H	1.81	0.46
12:BA:145:VAL:HG13	12:BA:146:CYS:N	2.29	0.46
11:AV:101:LEU:HD13	11:AV:102:LEU:H	1.80	0.46
12:AW:687:ILE:CG1	12:AW:688:PRO:HD2	2.46	0.46
7:BB:953:ILE:HG12	7:BB:954:GLU:H	1.80	0.46
8:AS:145:LEU:N	8:AS:145:LEU:HD12	2.31	0.46
7:BB:8:LEU:N	7:BB:8:LEU:HD22	2.30	0.46
8:AS:150:GLY:HA2	8:AS:156:PHE:HB2	1.97	0.46
6:AO:19:GLN:HB3	6:AO:20:PRO:HD3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:BB:844:HIS:CD2	7:BB:1026:GLU:HG2	2.51	0.46
2:BS:5:DG:C2	2:BS:6:DA:C2	3.03	0.46
7:BB:256:PHE:N	7:BB:257:PRO:CD	2.78	0.46
14:AY:394:LEU:N	14:AY:394:LEU:HD22	2.31	0.46
12:AW:671:GLU:O	12:AW:674:ASN:OD1	2.33	0.46
8:BD:133:LEU:HD21	8:BD:139:ILE:HG12	1.97	0.46
7:AR:922:MET:SD	12:AW:739:ASN:HB2	2.55	0.46
7:BB:483:ILE:HG13	7:BB:555:GLU:HB2	1.97	0.46
7:BB:191:LYS:HE2	7:BB:193:ILE:HD11	1.96	0.46
7:AR:1044:THR:O	7:AR:1044:THR:HG23	2.16	0.46
14:AY:41:VAL:O	14:AY:41:VAL:HG22	2.15	0.46
12:BA:372:TRP:CB	12:BA:373:PRO:CD	2.94	0.46
9:AT:166:GLN:HB2	9:AT:169:LEU:HD12	1.97	0.46
12:AW:105:LYS:CE	12:AW:136:VAL:HG12	2.45	0.46
10:AU:76:CYS:HB2	10:AU:104:ILE:CG2	2.45	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
8:BD:98:ILE:HB	8:BD:141:LEU:HG	1.97	0.46
7:AR:17:ILE:O	7:AR:20:TYR:HB3	2.16	0.46
7:BB:1044:THR:O	7:BB:1044:THR:HG23	2.16	0.46
14:AY:214:ASP:N	14:AY:215:SER:HA	2.31	0.46
7:BB:379:GLY:O	7:BB:380:ARG:HB2	2.16	0.46
4:AJ:44:LEU:O	4:AJ:48:THR:HG23	2.16	0.46
14:AY:192:LYS:CA	14:AY:193:LEU:HB2	2.46	0.46
12:BA:747:LEU:HB2	12:BA:782:ILE:HB	1.97	0.46
7:AR:233:LEU:HD11	7:AR:311:ARG:O	2.16	0.46
7:BB:680:LEU:HD22	7:BB:696:HIS:CB	2.46	0.46
15:BH:28:ALA:HB1	15:BH:62:ILE:HD11	1.98	0.46
7:BB:653:ILE:HG23	7:BB:654:THR:N	2.31	0.46
12:AW:111:ILE:HG22	12:AW:112:GLU:N	2.30	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:BA:107:SER:HB3	12:BA:140:ALA:HA	1.97	0.46
12:BA:105:LYS:CE	12:BA:136:VAL:HG12	2.46	0.46
14:BC:104:LEU:HB3	14:BC:105:PRO:HD3	1.98	0.46
8:AS:154:ALA:HA	8:AS:157:ILE:HG13	1.98	0.46
12:BA:431:MET:HB2	12:BA:453:TYR:OH	2.16	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
10:BF:95:TYR:CE1	10:BF:97:SER:HB2	2.50	0.46
1:AC:7:DA:C2	2:AD:9:DA:C2	3.03	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:BA:775:SER:HB2	12:BA:776:PRO:HD2	1.97	0.46
14:BC:41:VAL:O	14:BC:41:VAL:HG22	2.15	0.46
11:AV:78:VAL:HG12	11:AV:79:THR:OG1	2.15	0.46
9:AT:168:TYR:CG	10:AU:83:VAL:HG11	2.50	0.46
12:BA:29:THR:OG1	12:BA:30:PRO:CD	2.63	0.46
10:BF:64:SER:HB2	10:BF:69:ARG:CZ	2.45	0.46
1:AC:11:DT:H2"	1:AC:12:DA:O5'	2.15	0.46
10:AU:13:PRO:HG2	10:AU:16:VAL:HG12	1.98	0.46
12:AW:512:LYS:HE3	12:AW:583:ASP:HB2	1.98	0.46
7:AR:88:ALA:HA	7:AR:93:LEU:HB2	1.97	0.46
11:AV:72:CYS:HB3	11:AV:114:LYS:HD2	1.98	0.45
14:AY:214:ASP:HB2	14:AY:215:SER:CA	2.46	0.45
12:AW:187:VAL:HG21	12:AW:204:PRO:HG3	1.98	0.45
6:BN:3:ILE:CG2	6:BN:52:HIS:CD2	3.00	0.45
11:AV:95:ILE:C	11:AV:96:ILE:HG13	2.37	0.45
12:AW:747:LEU:HB2	12:AW:782:ILE:HB	1.98	0.45
7:AR:73:VAL:HG11	7:AR:93:LEU:HD23	1.98	0.45
4:BQ:35:LYS:HD3	4:BQ:35:LYS:HA	1.71	0.45
12:AW:94:LEU:HD21	12:AW:180:ILE:HG23	1.98	0.45
11:BG:61:LYS:O	11:BG:62:ASN:HB2	2.15	0.45
12:AW:431:MET:HB2	12:AW:453:TYR:OH	2.16	0.45
8:AS:98:ILE:HB	8:AS:141:LEU:HG	1.97	0.45
13:BP:10:TRP:CE3	13:BP:11:LYS:HB3	2.51	0.45
12:AW:162:TYR:CD1	12:AW:162:TYR:O	2.69	0.45
9:BE:10:ILE:N	9:BE:10:ILE:HD12	2.32	0.45
12:BA:127:SER:O	12:BA:131:ARG:HG3	2.16	0.45
12:AW:372:TRP:HB3	12:AW:373:PRO:CD	2.42	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
15:BH:83:SER:CB	4:BQ:44:LEU:HD11	2.46	0.45
7:AR:256:PHE:N	7:AR:257:PRO:CD	2.79	0.45
14:AY:81:PRO:HB3	14:AY:306:LEU:HG	1.96	0.45
12:BA:691:THR:HG22	12:BA:692:LEU:H	1.80	0.45
11:BG:96:ILE:HG22	11:BG:97:SER:N	2.32	0.45
11:AV:96:ILE:HG22	11:AV:97:SER:N	2.31	0.45
6:BN:19:GLN:HB3	6:BN:20:PRO:CD	2.47	0.45
14:BC:125:TYR:CE1	14:BC:250:ILE:HD13	2.51	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:BA:864:LYS:CA	12:BA:865:THR:CB	2.93	0.45
7:AR:1015:LEU:HD12	7:AR:1016:THR:HG23	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:BC:348:GLU:HG2	2:BS:14:DA:H5"	1.98	0.45
9:BE:121:ASP:C	9:BE:125:GLY:HA2	2.37	0.45
8:BD:145:LEU:HD12	8:BD:145:LEU:N	2.31	0.45
8:AS:41:ILE:HA	8:AS:145:LEU:HG	1.98	0.45
8:BD:79:PRO:HG3	8:BD:148:GLY:HA2	1.98	0.45
12:BA:77:LEU:HD23	12:BA:77:LEU:N	2.32	0.45
13:AX:10:TRP:CE3	13:AX:11:LYS:HB3	2.51	0.45
5:AM:69:LEU:HD23	8:AS:260:LEU:HD11	1.99	0.45
14:BC:13:LEU:HD23	14:BC:13:LEU:C	2.37	0.45
7:BB:1015:LEU:HD12	7:BB:1016:THR:HG23	1.98	0.45
6:AO:3:ILE:CG2	6:AO:52:HIS:CD2	3.00	0.45
14:AY:26:GLN:O	14:AY:29:VAL:HG12	2.16	0.45
14:BC:192:LYS:CA	14:BC:193:LEU:HB2	2.46	0.45
14:BC:182:ASP:HA	14:BC:185:LYS:HB2	1.99	0.45
12:BA:238:LYS:HG2	12:BA:276:TYR:HA	1.97	0.45
11:BG:95:ILE:C	11:BG:96:ILE:HG13	2.37	0.45
14:AY:125:TYR:CE1	14:AY:250:ILE:HD13	2.51	0.45
7:BB:333:ARG:O	7:BB:334:GLU:HB3	2.17	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
7:AR:961:LEU:HG	7:AR:967:PRO:HD3	1.98	0.45
11:BG:18:ILE:CG2	11:BG:29:ILE:HG12	2.46	0.45
12:AW:105:LYS:HE3	12:AW:140:ALA:HB2	1.99	0.45
12:BA:97:THR:HG23	12:BA:103:ARG:HD3	1.98	0.45
14:BC:277:ILE:HG22	14:BC:278:ARG:N	2.32	0.45
14:BC:235:LYS:CE	14:BC:264:VAL:HG21	2.46	0.45
8:AS:153:HIS:O	8:AS:153:HIS:CG	2.70	0.45
15:AZ:65:ILE:HD12	15:AZ:65:ILE:N	2.31	0.45
4:AJ:45:MET:CB	12:AW:122:LYS:HE2	2.46	0.45
15:BH:69:SER:HB2	15:BH:75:VAL:HG23	1.97	0.45
14:BC:100:VAL:O	14:BC:100:VAL:HG12	2.16	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
12:AW:541:ALA:HB1	12:AW:542:PRO:HD3	1.99	0.45
12:BA:187:VAL:HG21	12:BA:204:PRO:HG3	1.99	0.45
12:AW:29:THR:OG1	12:AW:30:PRO:CD	2.63	0.45
14:BC:26:GLN:O	14:BC:29:VAL:HG12	2.17	0.45
12:AW:324:THR:HG22	12:AW:443:PHE:CE2	2.52	0.45
14:AY:235:LYS:CE	14:AY:264:VAL:HG21	2.47	0.45
11:BG:99:PHE:O	11:BG:103:VAL:HG12	2.17	0.45
8:BD:153:HIS:O	8:BD:153:HIS:CG	2.70	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:AV:92:TYR:CE2	11:AV:113:LEU:HD21	2.52	0.45
12:AW:419:PHE:CE2	12:AW:462:MET:CE	3.00	0.45
9:BE:146:VAL:CG1	9:BE:149:VAL:HG23	2.47	0.45
15:BH:18:PRO:HB3	15:BH:67:ARG:HB3	1.98	0.45
7:AR:539:LEU:HD11	7:AR:543:ILE:HD11	1.99	0.45
12:BA:131:ARG:NE	4:BQ:36:LEU:HD11	2.32	0.45
6:AO:2:MET:HG2	6:AO:56:ILE:HD12	1.99	0.45
14:BC:184:VAL:O	14:BC:188:ILE:HG13	2.17	0.45
6:BN:43:TYR:HA	6:BN:46:ARG:HB3	1.99	0.45
7:AR:647:SER:HB2	7:AR:648:PRO:HD3	1.99	0.45
12:BA:393:ASP:O	12:BA:394:ARG:CB	2.65	0.45
12:AW:393:ASP:O	12:AW:394:ARG:CB	2.65	0.45
7:BB:233:LEU:HD11	7:BB:311:ARG:O	2.16	0.45
9:BE:108:VAL:HG22	9:BE:162:LEU:CB	2.47	0.45
7:AR:653:ILE:HG23	7:AR:654:THR:N	2.31	0.45
8:AS:59:ALA:HB1	13:AX:47:ALA:HB2	1.97	0.45
12:AW:342:ILE:CG2	12:AW:343:ILE:N	2.80	0.45
8:AS:236:LEU:HD12	8:AS:236:LEU:N	2.31	0.45
7:AR:783:VAL:HB	7:AR:784:ARG:HA	1.99	0.45
12:BA:492:GLY:HA3	12:BA:862:HIS:HA	1.98	0.45
9:AT:49:LEU:HD12	9:AT:49:LEU:N	2.31	0.45
14:AY:13:LEU:HD23	14:AY:13:LEU:C	2.37	0.45
14:BC:214:ASP:N	14:BC:215:SER:HA	2.31	0.45
12:AW:105:LYS:HZ2	12:AW:140:ALA:CB	2.28	0.45
14:BC:173:MET:HA	14:BC:177:LYS:HD2	1.98	0.45
7:BB:1081:VAL:C	7:BB:1091:LEU:HD11	2.36	0.45
7:BB:197:ALA:HA	7:BB:198:GLY:HA2	1.72	0.45
7:BB:322:ILE:O	7:BB:326:ILE:HG12	2.17	0.45
12:AW:79:ARG:HB3	12:AW:80:PRO:HD2	1.99	0.45
7:AR:251:ILE:CG2	7:AR:326:ILE:HD12	2.46	0.45
8:BD:161:LEU:HD12	8:BD:163:ILE:HD13	1.97	0.45
1:BR:13:DT:C1'	1:BR:14:DC:P	3.05	0.45
14:BC:104:LEU:N	14:BC:105:PRO:HD2	2.32	0.45
8:AS:79:PRO:HG3	8:AS:148:GLY:HA2	1.98	0.45
7:BB:226:PHE:CE1	7:BB:230:MET:CG	3.00	0.45
14:BC:157:SER:HB3	14:BC:166:ILE:HB	1.97	0.45
12:AW:708:ARG:CD	12:AW:748:GLY:HA3	2.46	0.45
7:AR:582:LEU:HD12	7:AR:619:LEU:HD12	1.98	0.45
12:BA:52:ILE:CG2	12:BA:217:ILE:HG22	2.47	0.45
9:BE:147:ILE:HD11	9:BE:163:THR:HG21	1.99	0.45
3:BK:43:LEU:HD11	3:BK:68:GLU:OE2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:AR:516:GLU:O	7:AR:517:TYR:HB2	2.17	0.45
12:BA:162:TYR:O	12:BA:162:TYR:CD1	2.69	0.45
9:BE:166:GLN:HB2	9:BE:169:LEU:HD12	1.97	0.45
12:AW:97:THR:HG23	12:AW:103:ARG:HD3	1.99	0.45
12:AW:450:CYS:C	12:AW:452:PRO:HD2	2.37	0.45
12:AW:44:VAL:HG13	12:AW:45:MET:N	2.32	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
14:AY:184:VAL:O	14:AY:188:ILE:HG13	2.17	0.45
9:AT:172:LEU:HD23	9:AT:173:GLU:N	2.32	0.45
11:AV:95:ILE:N	11:AV:95:ILE:HD12	2.31	0.45
7:AR:68:ILE:HG13	7:AR:99:LEU:CD2	2.47	0.45
7:AR:8:LEU:HD11	7:AR:593:THR:HA	1.98	0.45
12:AW:336:GLU:HA	12:AW:434:ARG:O	2.17	0.45
7:AR:778:MET:HE2	7:AR:779:PRO:O	2.17	0.45
7:AR:1081:VAL:C	7:AR:1091:LEU:HD11	2.37	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
12:BA:450:CYS:C	12:BA:452:PRO:HD2	2.37	0.45
14:BC:25:PRO:O	14:BC:26:GLN:CB	2.65	0.45
2:BS:16:DA:C5'	2:BS:17:DG:OP1	2.65	0.45
12:AW:108:GLU:HG3	12:AW:147:PRO:HG3	1.99	0.45
7:BB:591:LEU:O	7:BB:592:VAL:HG12	2.17	0.45
9:AT:121:ASP:C	9:AT:125:GLY:HA2	2.37	0.45
5:BL:15:LEU:HB3	5:BL:55:VAL:CG2	2.47	0.45
11:AV:92:TYR:CE2	11:AV:113:LEU:CD2	3.00	0.45
12:BA:512:LYS:HE3	12:BA:583:ASP:HB2	1.99	0.45
7:BB:682:LEU:HD22	6:BN:55:ILE:HD12	1.99	0.45
12:AW:517:THR:O	12:AW:518:LYS:C	2.56	0.45
12:BA:646:MET:HE2	12:BA:725:ALA:HB2	1.98	0.45
7:AR:683:TYR:CZ	7:AR:687:TYR:HB2	2.52	0.45
7:BB:582:LEU:HD12	7:BB:619:LEU:HD12	1.98	0.45
9:BE:49:LEU:N	9:BE:49:LEU:HD12	2.31	0.45
8:BD:254:GLU:OE1	5:BL:77:ARG:HD3	2.16	0.45
11:AV:18:ILE:CG2	11:AV:29:ILE:HG12	2.47	0.44
13:AX:17:GLN:HG3	13:AX:18:LEU:N	2.32	0.44
9:BE:172:LEU:HD23	9:BE:173:GLU:N	2.32	0.44
7:BB:209:LYS:O	7:BB:210:ASP:HB2	2.18	0.44
7:BB:68:ILE:HG13	7:BB:99:LEU:CD2	2.47	0.44
6:AO:19:GLN:HB3	6:AO:20:PRO:CD	2.47	0.44
7:BB:783:VAL:HB	7:BB:784:ARG:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:BA:423:PRO:HB2	12:BA:425:LEU:CD1	2.47	0.44
12:BA:342:ILE:CG2	12:BA:343:ILE:N	2.80	0.44
7:BB:898:VAL:HG12	8:BD:30:ARG:NH2	2.32	0.44
15:AZ:69:SER:HB2	15:AZ:75:VAL:HG23	1.97	0.44
11:BG:92:TYR:CE2	11:BG:113:LEU:HD21	2.52	0.44
7:BB:273:ASP:HB2	7:BB:289:ILE:HD11	1.99	0.44
14:BC:351:VAL:HG23	14:BC:352:LYS:H	1.82	0.44
14:AY:340:SER:O	14:AY:344:ARG:HD3	2.17	0.44
14:BC:176:ASP:HB3	14:BC:177:LYS:HG3	1.99	0.44
6:BN:2:MET:HG2	6:BN:56:ILE:HD12	1.99	0.44
14:BC:192:LYS:HG2	14:BC:193:LEU:HD13	1.99	0.44
12:BA:417:VAL:HG11	12:BA:464:LEU:CD2	2.48	0.44
12:AW:417:VAL:HG11	12:AW:464:LEU:CD2	2.48	0.44
12:BA:687:ILE:CG1	12:BA:688:PRO:HD2	2.46	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
7:BB:73:VAL:HG11	7:BB:93:LEU:HD23	1.99	0.44
9:AT:108:VAL:HG22	9:AT:162:LEU:CB	2.47	0.44
12:AW:509:LEU:HA	12:AW:638:PHE:CE2	2.53	0.44
3:AI:43:LEU:HD11	3:AI:68:GLU:OE2	2.17	0.44
14:BC:65:ALA:HA	3:BK:23:TRP:CZ2	2.53	0.44
14:AY:258:LEU:HD22	14:AY:280:ILE:HD13	1.99	0.44
12:BA:419:PHE:CE2	12:BA:462:MET:CE	3.00	0.44
14:AY:41:VAL:O	14:AY:42:LEU:C	2.53	0.44
12:AW:112:GLU:O	12:AW:116:ARG:HD3	2.17	0.44
7:BB:683:TYR:CZ	7:BB:687:TYR:HB2	2.52	0.44
4:BQ:70:ASP:O	4:BQ:73:LYS:HG2	2.18	0.44
7:BB:856:THR:HG23	7:BB:857:GLU:N	2.33	0.44
12:BA:122:LYS:HG2	12:BA:122:LYS:O	2.17	0.44
14:AY:211:ALA:HB1	14:AY:213:ILE:N	2.32	0.44
2:AD:3:DT:H2"	2:AD:4:DA:N7	2.32	0.44
14:BC:311:ARG:HA	14:BC:314:LEU:HD12	1.99	0.44
12:AW:823:LEU:HD13	14:AY:75:ALA:CA	2.47	0.44
6:AO:43:TYR:HA	6:AO:46:ARG:HB3	1.99	0.44
14:AY:104:LEU:N	14:AY:105:PRO:HD2	2.32	0.44
7:AR:774:ASP:O	7:AR:775:LYS:CB	2.65	0.44
7:BB:647:SER:HB2	7:BB:648:PRO:HD3	1.98	0.44
12:AW:77:LEU:HD23	12:AW:77:LEU:N	2.32	0.44
7:AR:1115:ARG:O	12:AW:9:ILE:HA	2.17	0.44
11:BG:92:TYR:CE2	11:BG:113:LEU:CD2	3.01	0.44
7:AR:1086:GLY:O	7:AR:1087:ASP:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:BA:708:ARG:CD	12:BA:748:GLY:HA3	2.48	0.44
12:AW:228:GLY:O	12:AW:229:ILE:HG12	2.18	0.44
14:AY:113:ALA:O	14:AY:114:LYS:HB3	2.18	0.44
8:BD:236:LEU:N	8:BD:236:LEU:HD12	2.31	0.44
4:AJ:36:LEU:HD21	12:AW:131:ARG:NH1	2.33	0.44
12:AW:864:LYS:CA	12:AW:865:THR:CB	2.93	0.44
12:AW:98:CYS:O	12:AW:101:CYS:SG	2.75	0.44
2:BS:3:DT:H2"	2:BS:4:DA:N7	2.32	0.44
15:BH:45:ILE:HG22	15:BH:46:ARG:H	1.83	0.44
12:BA:42:GLY:O	12:BA:43:SER:HB3	2.17	0.44
14:AY:192:LYS:HG2	14:AY:193:LEU:HD13	1.99	0.44
7:AR:322:ILE:O	7:AR:326:ILE:HG12	2.18	0.44
12:AW:823:LEU:HD13	14:AY:75:ALA:HB1	1.98	0.44
7:BB:952:PRO:O	7:BB:953:ILE:C	2.56	0.44
11:AV:99:PHE:O	11:AV:103:VAL:HG12	2.17	0.44
8:BD:41:ILE:HA	8:BD:145:LEU:HG	1.99	0.44
7:AR:981:LYS:HE2	8:AS:205:LEU:HD13	2.00	0.44
14:BC:122:MET:HE1	14:BC:124:ILE:HD11	2.00	0.44
14:AY:351:VAL:HG23	14:AY:352:LYS:H	1.82	0.44
12:AW:122:LYS:O	12:AW:122:LYS:HG2	2.17	0.44
7:BB:8:LEU:HD11	7:BB:593:THR:HA	1.98	0.44
15:AZ:62:ILE:HG13	15:AZ:62:ILE:O	2.18	0.44
10:BF:13:PRO:HG2	10:BF:16:VAL:HG12	1.98	0.44
7:BB:1110:MET:HG2	7:BB:1110:MET:O	2.17	0.44
12:AW:818:TYR:CD1	12:AW:818:TYR:C	2.91	0.44
11:AV:46:ILE:HG12	12:AW:542:PRO:HG2	2.00	0.44
15:AZ:45:ILE:HG22	15:AZ:46:ARG:H	1.83	0.44
12:BA:443:PHE:CE2	12:BA:464:LEU:HB2	2.53	0.44
7:AR:592:VAL:CG2	7:AR:615:LYS:HD3	2.48	0.44
11:BG:95:ILE:HD12	11:BG:95:ILE:N	2.33	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
7:BB:774:ASP:O	7:BB:775:LYS:CB	2.66	0.44
7:BB:212:THR:HG21	7:BB:214:HIS:NE2	2.33	0.44
12:BA:614:TRP:O	12:BA:618:GLU:HG2	2.16	0.44
8:AS:13:ILE:HG21	8:AS:238:PRO:HB2	2.00	0.44
5:AM:15:LEU:HB3	5:AM:55:VAL:CG2	2.48	0.44
3:AI:61:VAL:O	3:AI:64:ILE:HB	2.17	0.44
12:BA:818:TYR:CE1	12:BA:822:ARG:HG3	2.51	0.44
12:BA:4:LYS:HG3	7:BB:1092:PHE:CD2	2.52	0.44
14:AY:333:GLY:O	14:AY:337:GLU:HG2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:AT:146:VAL:CG1	9:AT:149:VAL:HG23	2.47	0.44
7:BB:745:ARG:HB2	7:BB:894:LEU:HB3	2.00	0.44
14:BC:258:LEU:HD22	14:BC:280:ILE:HD13	2.00	0.44
7:BB:572:ASN:HB3	7:BB:577:ARG:HD3	2.00	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
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:651:VAL:HG12	12:BA:651:VAL:O	2.17	0.44
14:BC:235:LYS:HE2	14:BC:261:VAL:HA	2.00	0.44
7:AR:952:PRO:O	7:AR:953:ILE:C	2.56	0.44
9:AT:30:LEU:HD22	9:AT:72:PHE:CZ	2.52	0.44
7:BB:399:HIS:O	7:BB:403:THR:HG22	2.17	0.44
7:AR:399:HIS:O	7:AR:403:THR:HG22	2.17	0.44
7:BB:961:LEU:HD23	7:BB:961:LEU:O	2.17	0.44
8:BD:73:LEU:HD11	8:BD:236:LEU:CD2	2.48	0.44
12:AW:592:ILE:O	12:AW:594:LEU:HD22	2.17	0.44
14:BC:113:ALA:O	14:BC:114:LYS:HB3	2.18	0.44
14:BC:372:ASN:HA	14:BC:375:ILE:HG22	2.00	0.44
12:BA:495:ILE:O	12:BA:605:ASN:HB2	2.17	0.44
7:AR:333:ARG:O	7:AR:334:GLU:HB3	2.17	0.44
14:AY:100:VAL:HG12	14:AY:100:VAL:O	2.17	0.44
9:AT:10:ILE:N	9:AT:10:ILE:HD12	2.32	0.44
12:AW:449:VAL:O	12:AW:449:VAL:HG12	2.17	0.44
7:BB:855:ILE:HD12	7:BB:855:ILE:N	2.33	0.44
2:AD:14:DA:C5'	12:AW:818:TYR:OH	2.66	0.44
12:AW:818:TYR:CE1	12:AW:822:ARG:CG	3.00	0.44
7:AR:1064:CYS:CB	7:AR:1067:CYS:HB2	2.47	0.44
11:BG:72:CYS:CB	11:BG:114:LYS:HD2	2.48	0.44
14:AY:173:MET:HA	14:AY:177:LYS:HD2	1.99	0.44
12:AW:42:GLY:O	12:AW:43:SER:HB3	2.17	0.44
14:AY:25:PRO:O	14:AY:26:GLN:CB	2.65	0.44
7:AR:591:LEU:O	7:AR:592:VAL:HG12	2.17	0.44
14:AY:104:LEU:HB3	14:AY:105:PRO:HD3	1.99	0.44
7:AR:742:ILE:HB	7:AR:912:ILE:HB	2.00	0.44
7:AR:212:THR:HG21	7:AR:214:HIS:NE2	2.33	0.44
9:AT:146:VAL:HG11	9:AT:149:VAL:CG2	2.48	0.44
7:AR:273:ASP:HB2	7:AR:289:ILE:HD11	1.99	0.44
12:BA:318:VAL:HG11	7:BB:1051:ARG:O	2.17	0.44
7:AR:89:ARG:NH1	7:AR:156:ILE:HD11	2.33	0.44
7:AR:520:TRP:N	7:AR:520:TRP:CD1	2.85	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:BA:449:VAL:O	12:BA:449:VAL:HG12	2.17	0.44
4:AJ:57:GLY:O	4:AJ:59:ILE:HG22	2.17	0.44
12:BA:105:LYS:NZ	12:BA:140:ALA:HB3	2.31	0.44
12:AW:105:LYS:NZ	12:AW:140:ALA:HB3	2.31	0.44
10:BF:62:ILE:O	10:BF:62:ILE:HG22	2.17	0.44
12:BA:324:THR:HG22	12:BA:443:PHE:CE2	2.53	0.44
7:BB:323:SER:HA	7:BB:326:ILE:CD1	2.48	0.44
12:AW:548:GLY:O	12:AW:551:VAL:HG12	2.18	0.44
12:BA:548:GLY:O	12:BA:551:VAL:HG12	2.18	0.44
14:BC:257:ASN:O	14:BC:261:VAL:HG23	2.18	0.44
7:AR:323:SER:HA	7:AR:326:ILE:CD1	2.48	0.44
9:BE:30:LEU:HD22	9:BE:72:PHE:CZ	2.52	0.44
9:BE:108:VAL:HG22	9:BE:162:LEU:HB2	2.00	0.44
12:BA:818:TYR:CE1	12:BA:822:ARG:CG	3.01	0.44
7:BB:743:MET:HE1	7:BB:891:ILE:HD11	2.00	0.44
14:AY:369:VAL:HG23	14:AY:370:VAL:N	2.33	0.44
3:BK:59:THR:CG2	3:BK:63:SER:HB3	2.48	0.44
7:AR:583:ILE:HD13	7:AR:616:ILE:HG12	2.00	0.44
12:BA:592:ILE:O	12:BA:594:LEU:HD22	2.18	0.44
7:BB:675:MET:HE1	7:BB:888:LYS:HD3	1.98	0.44
12:BA:541:ALA:HB2	11:BG:72:CYS:HB2	2.00	0.43
12:BA:160:LYS:HD3	12:BA:165:TYR:CE2	2.53	0.43
12:AW:159:GLU:HG2	12:AW:160:LYS:O	2.18	0.43
12:AW:651:VAL:O	12:AW:651:VAL:HG12	2.17	0.43
7:AR:1111:ILE:HG22	7:AR:1111:ILE:O	2.18	0.43
12:BA:79:ARG:HB3	12:BA:80:PRO:HD2	1.99	0.43
14:AY:226:ILE:HG23	14:AY:230:LYS:NZ	2.33	0.43
12:BA:769:PHE:CE2	12:BA:778:ALA:HA	2.52	0.43
12:AW:842:TYR:CE1	14:AY:367:LYS:HB2	2.53	0.43
6:AO:5:ILE:CD1	8:AS:61:ARG:CZ	2.96	0.43
12:BA:516:LEU:N	12:BA:516:LEU:HD12	2.33	0.43
7:BB:361:PHE:O	7:BB:364:PHE:HB3	2.18	0.43
3:BK:68:GLU:HG3	3:BK:74:LEU:HD21	2.00	0.43
11:BG:8:GLU:HB2	11:BG:60:SER:HB2	2.00	0.43
12:BA:509:LEU:HA	12:BA:638:PHE:CE2	2.53	0.43
7:AR:524:ILE:HD12	7:AR:524:ILE:N	2.33	0.43
11:AV:72:CYS:CB	11:AV:114:LYS:HD2	2.49	0.43
14:AY:196:PHE:HB2	14:AY:209:SER:OG	2.18	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
12:BA:105:LYS:HE3	12:BA:140:ALA:HB2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:AU:62:ILE:O	10:AU:62:ILE:HG22	2.17	0.43
12:BA:44:VAL:HG13	12:BA:45:MET:N	2.32	0.43
14:AY:182:ASP:HA	14:AY:185:LYS:HB2	1.99	0.43
14:BC:104:LEU:HD23	14:BC:104:LEU:C	2.39	0.43
12:AW:747:LEU:HD21	12:AW:786:PHE:CD2	2.53	0.43
7:BB:903:THR:HG22	7:BB:904:VAL:N	2.32	0.43
7:AR:646:TRP:CE2	7:AR:648:PRO:HG2	2.53	0.43
12:BA:112:GLU:O	12:BA:116:ARG:HD3	2.17	0.43
4:BQ:35:LYS:O	4:BQ:35:LYS:HD2	2.18	0.43
7:AR:961:LEU:O	7:AR:961:LEU:HD23	2.18	0.43
12:BA:336:GLU:HA	12:BA:434:ARG:O	2.17	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:BB:539:LEU:HD11	7:BB:543:ILE:HD11	1.99	0.43
7:BB:778:MET:HE2	7:BB:779:PRO:O	2.19	0.43
12:BA:3:GLU:HG3	7:BB:1093:PRO:HD2	2.00	0.43
14:BC:108:ILE:HA	14:BC:111:VAL:HG12	1.99	0.43
2:AD:14:DA:C5	2:AD:15:DT:H72	2.53	0.43
12:AW:160:LYS:HD3	12:AW:165:TYR:CE2	2.53	0.43
7:AR:197:ALA:HA	7:AR:198:GLY:HA2	1.72	0.43
7:BB:592:VAL:CG2	7:BB:615:LYS:HD3	2.48	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
12:BA:517:THR:O	12:BA:518:LYS:C	2.55	0.43
10:BF:106:ILE:O	10:BF:107:ILE:C	2.56	0.43
12:BA:812:ARG:HG3	14:BC:86:THR:HG22	2.01	0.43
10:AU:106:ILE:O	10:AU:107:ILE:C	2.56	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
7:AR:833:GLN:CA	7:AR:834:ALA:CB	2.97	0.43
14:BC:211:ALA:HB1	14:BC:213:ILE:N	2.32	0.43
12:AW:823:LEU:HD13	14:AY:75:ALA:CB	2.48	0.43
9:BE:125:GLY:O	9:BE:126:ILE:HG12	2.19	0.43
9:AT:125:GLY:O	9:AT:126:ILE:HG12	2.19	0.43
14:AY:104:LEU:C	14:AY:104:LEU:HD23	2.38	0.43
7:BB:271:ALA:O	7:BB:274:PHE:HB3	2.18	0.43
7:AR:226:PHE:CE1	7:AR:230:MET:CG	3.01	0.43
11:BG:8:GLU:CB	11:BG:60:SER:HB2	2.48	0.43
11:AV:8:GLU:CB	11:AV:60:SER:HB2	2.48	0.43
9:AT:13:ILE:CD1	9:AT:22:LEU:HG	2.48	0.43
7:BB:10:ILE:HA	7:BB:13:ARG:HD3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:BC:340:SER:O	14:BC:344:ARG:HD3	2.18	0.43
14:BC:274:THR:HG22	14:BC:276:ASN:H	1.84	0.43
12:AW:738:LEU:C	12:AW:738:LEU:HD12	2.38	0.43
7:BB:768:TYR:HB3	7:BB:769:PRO:HD2	2.00	0.43
11:BG:10:ILE:CD1	11:BG:58:PHE:CD2	3.02	0.43
13:BP:33:ILE:HD12	13:BP:33:ILE:N	2.34	0.43
7:AR:1110:MET:HG2	7:AR:1110:MET:O	2.18	0.43
2:AD:14:DA:OP1	14:AY:348:GLU:CD	2.57	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:1111:ILE:O	7:BB:1111:ILE:HG22	2.18	0.43
12:AW:417:VAL:O	12:AW:432:ALA:HA	2.19	0.43
12:BA:95:LYS:HE2	12:BA:141:MET:HE2	2.00	0.43
7:AR:903:THR:HG22	7:AR:904:VAL:N	2.33	0.43
4:AJ:42:GLU:O	4:AJ:45:MET:HB3	2.19	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
3:AI:53:ILE:O	3:AI:54:ASN:C	2.57	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
3:BK:53:ILE:O	3:BK:54:ASN:C	2.56	0.43
7:BB:520:TRP:CD1	7:BB:520:TRP:N	2.85	0.43
7:AR:760:LEU:C	7:AR:760:LEU:HD23	2.39	0.43
11:AV:72:CYS:H	12:AW:541:ALA:CB	2.31	0.43
12:BA:108:GLU:HG3	12:BA:147:PRO:HG3	1.99	0.43
10:AU:62:ILE:O	10:AU:63:ILE:CB	2.67	0.43
12:BA:662:TYR:O	12:BA:665:ILE:HG12	2.19	0.43
6:AO:1:MET:O	6:AO:2:MET:HB2	2.18	0.43
2:BS:14:DA:C5	2:BS:15:DT:H72	2.53	0.43
12:AW:443:PHE:CE2	12:AW:464:LEU:HB2	2.54	0.43
12:AW:769:PHE:CE2	12:AW:778:ALA:HA	2.53	0.43
8:BD:41:ILE:HD13	8:BD:145:LEU:HG	2.00	0.43
12:AW:516:LEU:N	12:AW:516:LEU:HD12	2.33	0.43
8:BD:141:LEU:HD12	8:BD:141:LEU:C	2.39	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
12:BA:259:GLN:HA	12:BA:262:ILE:HG22	2.00	0.43
7:BB:583:ILE:HD13	7:BB:616:ILE:HG12	1.99	0.43
12:BA:738:LEU:HD12	12:BA:738:LEU:C	2.38	0.43
12:AW:259:GLN:HA	12:AW:262:ILE:HG22	2.00	0.43
14:AY:372:ASN:HA	14:AY:375:ILE:HG22	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:BB:524:ILE:HD12	7:BB:524:ILE:N	2.33	0.43
12:BA:752:VAL:O	12:BA:752:VAL:HG23	2.18	0.43
7:BB:833:GLN:N	7:BB:834:ALA:CA	2.82	0.43
11:AV:79:THR:CG2	11:AV:80:GLU:HB2	2.48	0.43
11:BG:79:THR:CG2	11:BG:80:GLU:HB2	2.48	0.43
4:AJ:78:ARG:HD3	4:AJ:79:ASP:N	2.33	0.43
12:BA:165:TYR:CE1	12:BA:174:LYS:HB2	2.54	0.43
12:AW:165:TYR:CE1	12:AW:174:LYS:HB2	2.54	0.43
14:BC:226:ILE:HG23	14:BC:230:LYS:NZ	2.33	0.43
12:BA:238:LYS:HA	12:BA:238:LYS:HD2	1.90	0.43
12:BA:27:ILE:HG22	12:BA:74:HIS:NE2	2.34	0.43
7:AR:856:THR:HG23	7:AR:857:GLU:N	2.33	0.43
7:BB:516:GLU:O	7:BB:517:TYR:HB2	2.17	0.43
14:AY:119:THR:HG22	14:AY:121:MET:HE2	2.00	0.43
14:BC:369:VAL:HG23	14:BC:370:VAL:N	2.34	0.43
7:BB:26:LEU:H	7:BB:26:LEU:HD23	1.84	0.43
4:BQ:54:LEU:HA	4:BQ:59:ILE:CG2	2.49	0.43
12:AW:30:PRO:O	12:AW:243:VAL:HG11	2.18	0.43
7:AR:271:ALA:O	7:AR:274:PHE:HB3	2.18	0.43
4:AJ:45:MET:HG3	12:AW:122:LYS:HE2	2.00	0.43
13:BP:38:ARG:HG2	13:BP:39:LYS:N	2.34	0.43
12:BA:456:ASP:OD1	12:BA:460:ASP:CG	2.48	0.43
7:AR:768:TYR:HB3	7:AR:769:PRO:HD2	1.99	0.43
8:BD:13:ILE:HG21	8:BD:238:PRO:HB2	2.00	0.43
13:AX:38:ARG:HG2	13:AX:39:LYS:N	2.34	0.43
12:BA:864:LYS:HB3	12:BA:865:THR:C	2.39	0.43
12:AW:586:VAL:HG11	12:AW:611:ILE:HD11	2.01	0.43
12:BA:417:VAL:O	12:BA:432:ALA:HA	2.19	0.43
13:AX:5:ARG:N	13:AX:6:CYS:HA	2.34	0.43
13:BP:17:GLN:HG3	13:BP:18:LEU:N	2.32	0.43
7:AR:592:VAL:HG22	7:AR:596:ASP:HB2	2.01	0.43
12:AW:27:ILE:HG22	12:AW:74:HIS:NE2	2.33	0.43
8:AS:96:ILE:HG13	8:AS:143:ALA:HB3	2.00	0.43
15:BH:65:ILE:N	15:BH:65:ILE:HD12	2.34	0.43
4:AJ:45:MET:HB2	12:AW:122:LYS:CE	2.47	0.43
8:AS:73:LEU:HD11	8:AS:236:LEU:CD2	2.48	0.43
12:BA:618:GLU:CD	12:BA:874:ARG:HD3	2.40	0.43
12:AW:495:ILE:O	12:AW:605:ASN:HB2	2.18	0.43
7:BB:89:ARG:NH1	7:BB:156:ILE:HD11	2.33	0.43
14:BC:333:GLY:O	14:BC:337:GLU:HG2	2.18	0.43
7:AR:942:ILE:O	7:AR:943:VAL:HB	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:BB:547:ARG:HA	7:BB:552:ILE:CG2	2.49	0.43
12:BA:67:ASN:C	12:BA:69:PRO:HD3	2.38	0.43
11:AV:100:GLY:O	11:AV:104:LYS:HB2	2.19	0.43
7:BB:760:LEU:HD23	7:BB:760:LEU:C	2.39	0.43
7:AR:733:THR:HG23	7:AR:735:TYR:CD2	2.53	0.43
12:AW:864:LYS:HB3	12:AW:865:THR:C	2.39	0.43
12:BA:586:VAL:HG11	12:BA:611:ILE:HD11	2.01	0.43
10:BF:62:ILE:O	10:BF:63:ILE:CB	2.67	0.43
12:BA:728:MET:HA	12:BA:731:THR:HG22	2.01	0.43
8:AS:41:ILE:HD13	8:AS:145:LEU:HG	2.00	0.43
7:AR:235:ILE:HG22	7:AR:241:ILE:HG13	2.01	0.43
7:AR:361:PHE:O	7:AR:364:PHE:HB3	2.19	0.43
12:BA:747:LEU:HD21	12:BA:786:PHE:CD2	2.54	0.43
12:BA:134:GLU:O	12:BA:138:LYS:HG2	2.19	0.43
7:AR:403:THR:HG23	7:AR:405:ASN:H	1.84	0.43
7:AR:73:VAL:HG13	7:AR:83:ILE:HD13	1.99	0.43
3:AI:50:LEU:HD12	3:AI:73:VAL:HG23	2.01	0.43
12:BA:818:TYR:CD1	12:BA:818:TYR:C	2.92	0.43
9:BE:60:VAL:HG22	9:BE:61:PHE:N	2.34	0.43
7:AR:298:LYS:HG3	7:AR:299:TYR:CD2	2.54	0.43
12:AW:728:MET:HA	12:AW:731:THR:HG22	2.01	0.43
9:BE:13:ILE:CD1	9:BE:22:LEU:HG	2.48	0.43
13:BP:20:VAL:O	13:BP:20:VAL:HG23	2.19	0.43
12:BA:228:GLY:O	12:BA:229:ILE:HG12	2.18	0.43
11:AV:64:LEU:HD21	11:AV:112:PHE:HB2	2.01	0.42
12:AW:662:TYR:O	12:AW:665:ILE:HG12	2.19	0.42
7:BB:196:THR:HG22	7:BB:302:PRO:C	2.39	0.42
14:BC:348:GLU:CG	14:BC:349:VAL:N	2.82	0.42
7:BB:646:TRP:CE2	7:BB:648:PRO:HG2	2.54	0.42
12:AW:505:GLY:HA3	12:AW:639:VAL:HG23	2.01	0.42
12:BA:358:ILE:HG23	12:BA:359:GLU:N	2.34	0.42
7:AR:572:ASN:HB3	7:AR:577:ARG:HD3	2.00	0.42
11:AV:70:ASP:OD2	11:AV:116:HIS:CD2	2.72	0.42
9:AT:123:VAL:O	9:AT:124:ARG:HB2	2.19	0.42
7:AR:1118:LEU:H	7:AR:1118:LEU:HD23	1.84	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
7:AR:217:PHE:CB	7:AR:221:PRO:O	2.67	0.42
7:BB:217:PHE:CB	7:BB:221:PRO:O	2.68	0.42
11:BG:64:LEU:HD21	11:BG:112:PHE:HB2	2.01	0.42
7:AR:226:PHE:CE1	7:AR:318:LEU:HD22	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:AZ:28:ALA:CB	15:AZ:62:ILE:HD11	2.49	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
9:BE:9:SER:HB3	10:BF:4:VAL:HA	2.01	0.42
14:AY:108:ILE:HA	14:AY:111:VAL:HG12	1.99	0.42
10:BF:72:LEU:HG	10:BF:84:ARG:NH2	2.34	0.42
11:BG:70:ASP:OD2	11:BG:116:HIS:CD2	2.72	0.42
14:BC:119:THR:HG22	14:BC:121:MET:HE2	2.01	0.42
12:AW:67:ASN:C	12:AW:69:PRO:HD3	2.38	0.42
7:AR:745:ARG:HB2	7:AR:894:LEU:HB3	2.00	0.42
8:BD:109:LEU:HD23	8:BD:109:LEU:C	2.40	0.42
7:BB:833:GLN:CA	7:BB:834:ALA:CB	2.97	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
7:AR:110:ILE:N	7:AR:110:ILE:HD13	2.34	0.42
9:BE:121:ASP:O	9:BE:125:GLY:HA2	2.20	0.42
12:BA:505:GLY:HA3	12:BA:639:VAL:HG23	2.01	0.42
7:BB:403:THR:HG23	7:BB:405:ASN:H	1.84	0.42
7:BB:898:VAL:HG12	8:BD:30:ARG:CZ	2.50	0.42
9:BE:123:VAL:O	9:BE:124:ARG:HB2	2.19	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
7:BB:298:LYS:HG3	7:BB:299:TYR:CD2	2.54	0.42
3:AI:93:ARG:O	3:AI:94:LYS:HB2	2.18	0.42
9:AT:94:ASN:HB3	9:AT:120:TYR:CD2	2.54	0.42
12:AW:752:VAL:O	12:AW:752:VAL:HG23	2.19	0.42
2:AD:16:DA:C8	2:AD:16:DA:OP1	2.72	0.42
7:AR:217:PHE:HZ	7:AR:300:PHE:CA	2.32	0.42
10:BF:75:ILE:C	10:BF:76:CYS:SG	2.98	0.42
12:BA:40:ILE:HD13	12:BA:47:PRO:HG3	2.01	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
12:BA:324:THR:HG22	12:BA:443:PHE:CD2	2.55	0.42
12:BA:79:ARG:CB	12:BA:266:TRP:CZ3	3.02	0.42
7:BB:592:VAL:HG22	7:BB:596:ASP:HB2	2.01	0.42
14:AY:235:LYS:HE2	14:AY:261:VAL:HA	2.00	0.42
8:BD:172:ILE:HD11	8:BD:188:PHE:CE1	2.54	0.42
7:BB:226:PHE:CE1	7:BB:318:LEU:HD22	2.54	0.42
12:AW:134:GLU:O	12:AW:138:LYS:HG2	2.19	0.42
7:BB:233:LEU:CD1	7:BB:315:ALA:HB2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:AR:233:LEU:CD1	7:AR:315:ALA:HB2	2.49	0.42
8:AS:141:LEU:C	8:AS:141:LEU:HD12	2.39	0.42
7:AR:547:ARG:HA	7:AR:552:ILE:CG2	2.49	0.42
10:BF:52:ALA:O	10:BF:55:VAL:HG12	2.19	0.42
9:BE:80:VAL:HG12	9:BE:81:VAL:N	2.34	0.42
12:BA:53:GLU:HA	12:BA:54:PRO:HD3	1.93	0.42
12:AW:358:ILE:HG23	12:AW:359:GLU:N	2.33	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
11:AV:64:LEU:CD2	11:AV:64:LEU:N	2.82	0.42
12:BA:106:ILE:HD11	12:BA:154:PHE:CE1	2.54	0.42
12:AW:103:ARG:HB3	12:AW:186:LYS:HB2	2.01	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
12:BA:837:THR:HG23	12:BA:847:GLN:O	2.20	0.42
11:AV:101:LEU:HD22	11:AV:101:LEU:C	2.40	0.42
11:AV:99:PHE:O	11:AV:99:PHE:CG	2.72	0.42
7:BB:742:ILE:HB	7:BB:912:ILE:HB	1.99	0.42
7:BB:63:LEU:HD22	7:BB:101:LEU:HD11	2.02	0.42
12:AW:618:GLU:CD	12:AW:874:ARG:HD3	2.40	0.42
14:AY:274:THR:HG22	14:AY:276:ASN:H	1.83	0.42
11:BG:100:GLY:O	11:BG:104:LYS:HB2	2.20	0.42
7:AR:76:SER:HA	7:AR:77:ASP:HA	1.73	0.42
7:BB:841:VAL:HG12	7:BB:842:THR:N	2.34	0.42
7:AR:259:LEU:O	7:AR:263:SER:HB3	2.20	0.42
12:BA:683:GLU:CA	12:BA:684:LEU:CB	2.97	0.42
4:AJ:54:LEU:HA	4:AJ:59:ILE:CG2	2.49	0.42
7:BB:733:THR:HG23	7:BB:735:TYR:CD2	2.54	0.42
9:BE:169:LEU:C	9:BE:175:ILE:HD11	2.40	0.42
14:BC:173:MET:HA	14:BC:177:LYS:CD	2.50	0.42
14:BC:152:VAL:HA	14:BC:173:MET:HB3	2.02	0.42
14:AY:152:VAL:HA	14:AY:173:MET:HB3	2.02	0.42
12:AW:106:ILE:HD11	12:AW:154:PHE:CE1	2.54	0.42
14:AY:306:LEU:HD13	14:AY:306:LEU:H	1.84	0.42
9:AT:126:ILE:HG22	9:AT:137:GLN:HG2	2.02	0.42
8:AS:93:TYR:HA	8:AS:145:LEU:O	2.20	0.42
7:AR:918:LEU:N	7:AR:919:PRO:HD2	2.34	0.42
10:AU:69:ARG:HG2	10:AU:69:ARG:NH1	2.34	0.42
7:AR:633:PRO:HA	7:AR:636:LEU:HD23	2.01	0.42
14:BC:122:MET:SD	14:BC:256:SER:HA	2.59	0.42
9:AT:30:LEU:HD13	9:AT:72:PHE:CZ	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:BE:30:LEU:HD13	9:BE:72:PHE:CZ	2.54	0.42
15:BH:28:ALA:CB	15:BH:62:ILE:HD11	2.49	0.42
11:AV:23:LEU:HD12	12:AW:512:LYS:HB2	2.00	0.42
10:BF:102:LYS:O	10:BF:106:ILE:HG13	2.19	0.42
3:BK:93:ARG:O	3:BK:94:LYS:HB2	2.18	0.42
7:BB:259:LEU:O	7:BB:263:SER:HB3	2.20	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
11:AV:10:ILE:CD1	11:AV:58:PHE:CD2	3.02	0.42
7:BB:872:LEU:HD23	7:BB:873:ARG:N	2.34	0.42
2:AD:3:DT:O3'	2:AD:4:DA:C8	2.73	0.42
12:AW:687:ILE:HD12	12:AW:688:PRO:HD2	2.02	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
8:BD:78:TRP:HB3	8:BD:79:PRO:CD	2.49	0.42
7:AR:633:PRO:HA	7:AR:636:LEU:CD2	2.49	0.42
7:AR:420:THR:O	7:AR:421:ASN:CG	2.58	0.42
7:BB:94:THR:O	7:BB:96:ALA:N	2.53	0.42
10:BF:7:VAL:HG12	10:BF:8:GLU:HG2	2.01	0.42
7:AR:1008:ALA:HB2	12:AW:346:THR:HG22	2.02	0.42
12:BA:323:ARG:HB2	7:BB:1029:LEU:HD11	2.02	0.42
12:AW:370:ASP:O	12:AW:371:LYS:HB3	2.20	0.42
7:AR:840:ILE:HD12	7:AR:840:ILE:N	2.35	0.42
13:AX:33:ILE:N	13:AX:33:ILE:HD12	2.34	0.42
7:AR:450:GLY:HA3	12:AW:760:GLY:HA2	2.01	0.42
7:BB:217:PHE:HZ	7:BB:300:PHE:CA	2.32	0.42
7:AR:833:GLN:N	7:AR:834:ALA:CA	2.82	0.42
7:AR:56:ILE:CG2	7:AR:59:LEU:HB2	2.49	0.42
11:BG:101:LEU:C	11:BG:101:LEU:HD22	2.40	0.42
9:AT:171:LYS:HG3	9:AT:172:LEU:N	2.35	0.42
14:AY:122:MET:SD	14:AY:256:SER:HA	2.59	0.42
11:BG:99:PHE:CG	11:BG:99:PHE:O	2.72	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
12:BA:35:GLU:O	12:BA:39:PRO:HD2	2.20	0.42
15:BH:62:ILE:HG13	15:BH:62:ILE:O	2.19	0.42
9:AT:60:VAL:HG22	9:AT:61:PHE:N	2.34	0.42
7:BB:706:VAL:HG11	7:BB:929:GLU:HG2	2.01	0.42
9:BE:132:SER:O	9:BE:133:LYS:HG2	2.20	0.42
14:BC:268:ASP:O	14:BC:272:VAL:HG23	2.20	0.42
10:AU:52:ALA:O	10:AU:55:VAL:HG12	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:BB:521:SER:HB3	7:BB:567:ASN:ND2	2.34	0.42
4:AJ:57:GLY:O	4:AJ:58:LYS:C	2.58	0.42
4:AJ:59:ILE:HG12	4:AJ:60:SER:N	2.35	0.42
12:BA:372:TRP:HB3	12:BA:373:PRO:CD	2.42	0.42
12:AW:284:LEU:HD13	12:AW:285:PRO:HD2	2.02	0.42
14:AY:211:ALA:HA	14:AY:212:ASN:CB	2.48	0.42
12:AW:105:LYS:HZ1	12:AW:137:LYS:HA	1.85	0.42
12:BA:28:ILE:HG21	12:BA:243:VAL:HG21	2.02	0.42
7:AR:196:THR:HG22	7:AR:302:PRO:C	2.39	0.42
12:AW:417:VAL:HG11	12:AW:464:LEU:HD11	2.02	0.42
9:BE:171:LYS:HG3	9:BE:172:LEU:N	2.35	0.42
7:AR:591:LEU:O	7:AR:592:VAL:CB	2.68	0.42
7:BB:918:LEU:N	7:BB:919:PRO:HD2	2.34	0.42
7:BB:633:PRO:HA	7:BB:636:LEU:CD2	2.49	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
8:BD:61:ARG:CZ	6:BN:5:ILE:HD11	2.49	0.42
7:AR:478:GLN:HG2	7:AR:479:ILE:N	2.34	0.42
12:BA:510:THR:CG2	12:BA:552:VAL:HG21	2.50	0.42
3:AI:67:GLU:O	3:AI:71:ARG:HG2	2.19	0.42
7:BB:478:GLN:HG2	7:BB:479:ILE:N	2.35	0.42
9:AT:169:LEU:C	9:AT:175:ILE:HD11	2.40	0.42
12:BA:101:CYS:SG	12:BA:152:LYS:CG	3.07	0.42
2:AD:6:DA:C2	2:AD:7:DG:C2	3.08	0.42
2:BS:3:DT:O3'	2:BS:4:DA:C8	2.73	0.42
12:AW:103:ARG:HB3	12:AW:186:LYS:CB	2.49	0.42
6:BN:3:ILE:HD13	6:BN:18:TRP:CB	2.50	0.42
14:BC:306:LEU:H	14:BC:306:LEU:HD13	1.83	0.42
13:BP:5:ARG:N	13:BP:17:GLN:HA	2.35	0.42
7:BB:213:PHE:CZ	7:BB:326:ILE:CG2	3.03	0.42
12:AW:324:THR:HG22	12:AW:443:PHE:CD2	2.54	0.42
7:AR:592:VAL:CG2	7:AR:596:ASP:CG	2.88	0.42
11:BG:42:ILE:HG12	11:BG:43:ILE:N	2.35	0.42
12:BA:431:MET:CE	12:BA:482:VAL:HA	2.50	0.42
12:AW:52:ILE:HG21	12:AW:217:ILE:HG22	2.02	0.42
12:AW:737:VAL:HG13	12:AW:738:LEU:N	2.35	0.42
14:AY:268:ASP:O	14:AY:272:VAL:HG23	2.20	0.42
7:AR:872:LEU:HD23	7:AR:873:ARG:N	2.35	0.42
12:AW:362:ARG:O	12:AW:365:VAL:HG12	2.20	0.42
7:AR:247:LEU:HD11	7:AR:503:VAL:HG12	2.02	0.42
12:AW:830:LEU:HD11	14:AY:319:VAL:HG21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:AX:20:VAL:HG23	13:AX:20:VAL:O	2.20	0.42
7:AR:300:PHE:O	7:AR:301:LEU:C	2.58	0.41
7:BB:217:PHE:O	7:BB:221:PRO:HA	2.20	0.41
12:BA:372:TRP:C	12:BA:372:TRP:CD1	2.93	0.41
11:BG:64:LEU:N	11:BG:64:LEU:CD2	2.82	0.41
12:AW:106:ILE:HG22	12:AW:143:ALA:HB3	2.02	0.41
12:AW:79:ARG:CB	12:AW:266:TRP:CZ3	3.03	0.41
7:BB:110:ILE:N	7:BB:110:ILE:HD13	2.34	0.41
10:AU:69:ARG:HG2	10:AU:69:ARG:HH11	1.85	0.41
7:AR:632:GLU:HB3	7:AR:633:PRO:HD2	2.01	0.41
7:BB:420:THR:O	7:BB:421:ASN:CG	2.59	0.41
7:BB:73:VAL:HG13	7:BB:83:ILE:HD13	2.00	0.41
12:AW:431:MET:CE	12:AW:482:VAL:HA	2.50	0.41
13:AX:10:TRP:HB2	13:AX:31:TYR:CE2	2.55	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
12:AW:749:GLN:NE2	12:AW:756:ARG:HG2	2.35	0.41
7:AR:480:ALA:HB2	7:AR:579:ARG:HD3	2.02	0.41
8:AS:66:PRO:HG2	8:AS:124:ILE:HG12	2.01	0.41
7:AR:1059:THR:HG22	7:AR:1060:THR:N	2.35	0.41
7:BB:300:PHE:O	7:BB:301:LEU:C	2.59	0.41
14:BC:211:ALA:CB	14:BC:213:ILE:N	2.84	0.41
12:BA:146:CYS:HB3	12:BA:149:CYS:HB2	1.72	0.41
12:BA:103:ARG:HB3	12:BA:186:LYS:CB	2.49	0.41
15:AZ:45:ILE:HG22	15:AZ:46:ARG:N	2.35	0.41
14:AY:149:ILE:O	14:AY:153:VAL:HG12	2.21	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
7:BB:633:PRO:HA	7:BB:636:LEU:HD23	2.01	0.41
7:BB:632:GLU:HB3	7:BB:633:PRO:HD2	2.02	0.41
7:BB:741:ILE:HG23	7:BB:911:VAL:HG13	2.02	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
14:AY:8:LYS:N	14:AY:8:LYS:HD2	2.35	0.41
8:BD:121:ILE:N	8:BD:121:ILE:HD12	2.36	0.41
7:AR:691:THR:HG23	7:AR:691:THR:O	2.20	0.41
7:BB:1118:LEU:HD23	7:BB:1118:LEU:H	1.85	0.41
12:AW:113:LYS:O	12:AW:117:ILE:HG13	2.21	0.41
12:AW:684:LEU:HD12	12:AW:685:GLU:N	2.35	0.41
10:AU:91:SER:HB2	10:AU:92:ASN:CA	2.41	0.41
7:BB:1064:CYS:CB	7:BB:1067:CYS:HB2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:BA:32:VAL:O	12:BA:44:VAL:HG11	2.20	0.41
4:AJ:48:THR:HG22	15:AZ:80:TYR:OH	2.20	0.41
13:BP:5:ARG:N	13:BP:6:CYS:HA	2.34	0.41
12:BA:687:ILE:HD12	12:BA:688:PRO:HD2	2.02	0.41
12:AW:421:ARG:HB2	12:AW:462:MET:HE3	2.02	0.41
11:BG:10:ILE:C	11:BG:11:LEU:HD12	2.41	0.41
12:AW:510:THR:CG2	12:AW:552:VAL:HG21	2.50	0.41
12:AW:155:LYS:O	12:AW:156:ILE:C	2.59	0.41
12:AW:192:VAL:CG2	12:AW:199:PRO:HB3	2.50	0.41
14:AY:262:LEU:HD11	14:AY:283:VAL:HG11	2.02	0.41
7:BB:877:ILE:H	7:BB:877:ILE:HD12	1.85	0.41
4:AJ:35:LYS:O	4:AJ:35:LYS:HD3	2.21	0.41
12:BA:285:PRO:HA	12:BA:286:PRO:HD3	1.92	0.41
14:AY:173:MET:HA	14:AY:177:LYS:CD	2.50	0.41
10:AU:75:ILE:C	10:AU:76:CYS:SG	2.98	0.41
12:AW:184:LEU:O	12:AW:187:VAL:CG2	2.68	0.41
6:AO:3:ILE:HG22	6:AO:52:HIS:CD2	2.55	0.41
13:AX:5:ARG:N	13:AX:17:GLN:HA	2.35	0.41
12:AW:417:VAL:CG1	12:AW:418:LEU:N	2.84	0.41
10:AU:89:MET:HB3	10:AU:89:MET:HE2	1.87	0.41
14:BC:234:ILE:O	14:BC:235:LYS:HB2	2.21	0.41
14:AY:234:ILE:O	14:AY:235:LYS:HB2	2.20	0.41
7:AR:213:PHE:CZ	7:AR:326:ILE:CG2	3.04	0.41
12:AW:95:LYS:HE2	12:AW:141:MET:HE2	2.00	0.41
12:AW:249:LEU:HD21	12:AW:265:LEU:HB2	2.02	0.41
8:BD:115:LYS:O	8:BD:116:SER:HB2	2.20	0.41
7:AR:706:VAL:HG11	7:AR:929:GLU:HG2	2.02	0.41
4:BQ:42:GLU:O	4:BQ:45:MET:HB3	2.20	0.41
8:AS:115:LYS:O	8:AS:116:SER:HB2	2.20	0.41
3:BK:67:GLU:O	3:BK:71:ARG:HG2	2.20	0.41
14:BC:8:LYS:N	14:BC:8:LYS:HD2	2.35	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
12:AW:33:TYR:CA	12:AW:34:ASP:CB	2.99	0.41
2:BS:16:DA:C8	2:BS:16:DA:OP1	2.73	0.41
12:AW:837:THR:HG23	12:AW:847:GLN:O	2.19	0.41
10:AU:87:LEU:CD2	10:AU:87:LEU:O	2.69	0.41
7:BB:591:LEU:O	7:BB:592:VAL:CB	2.67	0.41
14:AY:365:GLU:O	14:AY:366:PHE:HB2	2.20	0.41
11:BG:96:ILE:HD12	11:BG:99:PHE:CB	2.51	0.41
14:BC:244:LYS:HB3	14:BC:249:TYR:HD1	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:AV:42:ILE:HG12	11:AV:43:ILE:N	2.35	0.41
15:BH:63:ILE:HG22	15:BH:65:ILE:CD1	2.50	0.41
15:AZ:63:ILE:HG22	15:AZ:65:ILE:CD1	2.50	0.41
4:BQ:34:PRO:O	4:BQ:35:LYS:CB	2.67	0.41
12:AW:162:TYR:CG	12:AW:162:TYR:O	2.73	0.41
8:AS:38:VAL:HG12	8:AS:39:MET:N	2.36	0.41
8:BD:189:GLU:HG2	8:BD:198:LYS:HE3	2.02	0.41
8:AS:109:LEU:C	8:AS:109:LEU:HD23	2.40	0.41
8:AS:121:ILE:HD12	8:AS:121:ILE:N	2.36	0.41
10:AU:88:ILE:C	10:AU:90:ASP:N	2.74	0.41
9:BE:167:PRO:O	9:BE:168:TYR:HB2	2.21	0.41
10:BF:76:CYS:N	10:BF:77:PRO:HD3	2.36	0.41
12:BA:184:LEU:O	12:BA:187:VAL:CG2	2.68	0.41
15:BH:45:ILE:HG13	15:BH:79:ARG:HB2	2.02	0.41
6:AO:3:ILE:HD13	6:AO:18:TRP:CB	2.50	0.41
2:BS:15:DT:C1'	2:BS:16:DA:P	3.08	0.41
15:AZ:45:ILE:HG12	15:AZ:79:ARG:CD	2.50	0.41
7:BB:56:ILE:CG2	7:BB:59:LEU:HB2	2.49	0.41
10:BF:41:LEU:HA	10:BF:44:VAL:HG12	2.03	0.41
9:AT:150:ALA:O	9:AT:151:SER:C	2.59	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
9:AT:80:VAL:HG12	9:AT:81:VAL:N	2.34	0.41
6:AO:40:VAL:O	6:AO:41:LYS:HB2	2.21	0.41
7:BB:691:THR:HG23	7:BB:691:THR:O	2.20	0.41
12:BA:684:LEU:HD12	12:BA:685:GLU:N	2.36	0.41
14:AY:277:ILE:HD13	14:AY:293:ILE:HD13	2.02	0.41
7:BB:592:VAL:CG2	7:BB:596:ASP:CG	2.89	0.41
12:BA:692:LEU:CD1	12:BA:692:LEU:N	2.83	0.41
6:AO:5:ILE:HD11	8:AS:61:ARG:CB	2.51	0.41
7:BB:201:VAL:HG23	7:BB:202:PRO:HD2	2.03	0.41
7:AR:743:MET:HE1	7:AR:891:ILE:CD1	2.50	0.41
12:AW:35:GLU:O	12:AW:39:PRO:HD2	2.20	0.41
10:BF:68:VAL:O	10:BF:71:VAL:HG12	2.21	0.41
8:AS:15:LEU:HD11	8:AS:242:LEU:HD13	2.03	0.41
7:BB:462:PRO:CG	7:BB:470:VAL:HG13	2.51	0.41
10:AU:7:VAL:HG12	10:AU:8:GLU:HG2	2.02	0.41
5:BL:18:GLU:HA	5:BL:52:LYS:HG2	2.03	0.41
9:AT:132:SER:O	9:AT:133:LYS:HG2	2.20	0.41
7:AR:877:ILE:H	7:AR:877:ILE:HD12	1.85	0.41
7:BB:840:ILE:HD12	7:BB:840:ILE:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:AY:211:ALA:CB	14:AY:213:ILE:N	2.83	0.41
9:AT:167:PRO:O	9:AT:168:TYR:HB2	2.21	0.41
12:BA:33:TYR:O	12:BA:41:GLU:CB	2.68	0.41
12:BA:33:TYR:CA	12:BA:34:ASP:CB	2.99	0.41
12:BA:263:GLU:O	12:BA:266:TRP:HB3	2.21	0.41
14:AY:226:ILE:HG23	14:AY:230:LYS:HE3	2.03	0.41
9:BE:126:ILE:CD1	9:BE:135:VAL:HG13	2.51	0.41
9:AT:126:ILE:CD1	9:AT:135:VAL:HG13	2.51	0.41
7:BB:938:LEU:HD23	6:BN:43:TYR:HB3	2.02	0.41
12:AW:115:SER:HA	12:AW:118:TYR:HD2	1.86	0.41
9:BE:30:LEU:CD2	9:BE:72:PHE:CE2	3.04	0.41
12:AW:77:LEU:HB2	12:AW:210:THR:O	2.21	0.41
7:AR:1117:ILE:HD11	12:AW:10:LYS:HE3	2.02	0.41
12:AW:519:GLU:O	12:AW:523:GLN:HB2	2.20	0.41
12:AW:333:SER:OG	12:AW:625:LYS:HE3	2.21	0.41
12:BA:192:VAL:CG2	12:BA:199:PRO:HB3	2.50	0.41
7:AR:283:GLN:HG3	7:AR:283:GLN:O	2.21	0.41
2:AD:15:DT:C1'	2:AD:16:DA:P	3.07	0.41
4:BQ:57:GLY:O	4:BQ:58:LYS:C	2.58	0.41
11:BG:64:LEU:HD23	11:BG:114:LYS:HE3	2.03	0.41
12:BA:107:SER:HB2	12:BA:108:GLU:HB2	2.03	0.41
12:AW:105:LYS:HZ3	12:AW:195:LEU:HD21	1.86	0.41
2:AD:4:DA:H2"	2:AD:5:DG:OP2	2.20	0.41
10:AU:104:ILE:O	10:AU:104:ILE:HG22	2.21	0.41
12:AW:33:TYR:O	12:AW:41:GLU:CB	2.68	0.41
12:AW:28:ILE:HG21	12:AW:243:VAL:HG21	2.02	0.41
12:BA:687:ILE:HG22	12:BA:695:SER:HB2	2.02	0.41
12:AW:687:ILE:HG22	12:AW:695:SER:HB2	2.02	0.41
7:BB:748:VAL:CG1	7:BB:875:PRO:HG2	2.50	0.41
7:AR:748:VAL:CG1	7:AR:875:PRO:HG2	2.50	0.41
7:BB:108:ASN:O	7:BB:110:ILE:HD13	2.21	0.41
8:AS:78:TRP:HB3	8:AS:79:PRO:CD	2.49	0.41
11:AV:96:ILE:HD12	11:AV:99:PHE:CB	2.51	0.41
8:BD:79:PRO:HG2	8:BD:149:TYR:CD2	2.56	0.41
7:AR:741:ILE:O	7:AR:891:ILE:HA	2.20	0.41
12:BA:77:LEU:HB2	12:BA:210:THR:O	2.21	0.41
9:AT:30:LEU:CD2	9:AT:72:PHE:CE2	3.04	0.41
12:BA:747:LEU:HD11	12:BA:790:LEU:HD21	2.03	0.41
14:BC:365:GLU:O	14:BC:366:PHE:HB2	2.20	0.41
15:AZ:63:ILE:N	15:AZ:63:ILE:HD12	2.36	0.41
12:BA:249:LEU:HD21	12:BA:265:LEU:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:AU:84:ARG:O	10:AU:85:SER:C	2.59	0.41
7:BB:741:ILE:O	7:BB:891:ILE:HA	2.20	0.41
14:AY:289:ALA:O	14:AY:292:ILE:HG22	2.20	0.41
12:BA:155:LYS:O	12:BA:156:ILE:C	2.59	0.41
14:AY:199:ASP:HB2	14:AY:206:LEU:HD23	2.03	0.41
14:BC:199:ASP:HB2	14:BC:206:LEU:HD23	2.03	0.41
7:AR:1020:THR:HG22	7:AR:1021:GLU:H	1.85	0.41
4:BQ:72:TYR:CE1	4:BQ:76:GLU:HG2	2.56	0.41
12:AW:812:ARG:HG3	14:AY:86:THR:HG22	2.02	0.41
14:BC:289:ALA:O	14:BC:292:ILE:HG22	2.20	0.41
13:AX:41:THR:HG22	13:AX:42:ILE:N	2.35	0.41
12:BA:870:ARG:HD2	12:BA:870:ARG:HA	1.91	0.41
14:AY:265:LYS:N	14:AY:265:LYS:HD2	2.36	0.41
3:AI:23:TRP:CZ3	3:AI:26:LYS:HE3	2.56	0.41
7:BB:359:VAL:HG13	7:BB:360:ALA:N	2.36	0.41
12:AW:827:LEU:HB3	14:AY:71:GLY:CA	2.51	0.41
12:BA:823:LEU:HD13	14:BC:75:ALA:HA	2.03	0.41
7:AR:26:LEU:H	7:AR:26:LEU:HD23	1.84	0.41
10:BF:87:LEU:O	10:BF:87:LEU:CD2	2.68	0.41
2:AD:15:DT:H1'	2:AD:16:DA:OP2	2.21	0.41
7:AR:217:PHE:O	7:AR:221:PRO:HA	2.20	0.41
10:AU:88:ILE:CG2	10:AU:92:ASN:OD1	2.69	0.41
12:BA:107:SER:OG	12:BA:140:ALA:HB2	2.20	0.41
12:AW:40:ILE:HD13	12:AW:47:PRO:HG3	2.02	0.41
12:BA:103:ARG:HB3	12:BA:186:LYS:HB2	2.01	0.41
12:AW:32:VAL:O	12:AW:44:VAL:HG11	2.20	0.41
15:BH:45:ILE:HG12	15:BH:79:ARG:CD	2.50	0.41
12:BA:417:VAL:CG1	12:BA:418:LEU:N	2.84	0.41
12:AW:687:ILE:CD1	12:AW:688:PRO:HD2	2.50	0.41
12:AW:263:GLU:O	12:AW:266:TRP:HB3	2.21	0.41
12:AW:769:PHE:CD2	12:AW:778:ALA:HA	2.56	0.41
7:BB:1061:ILE:HD11	7:BB:1101:LYS:HD2	2.02	0.41
13:BP:10:TRP:HB2	13:BP:31:TYR:CE2	2.56	0.41
12:BA:162:TYR:CG	12:BA:162:TYR:O	2.73	0.41
7:BB:273:ASP:O	7:BB:277:SER:N	2.54	0.41
3:AI:34:ARG:NE	9:AT:61:PHE:CE1	2.89	0.41
7:BB:705:LEU:O	7:BB:706:VAL:CG1	2.69	0.41
4:AJ:35:LYS:HA	4:AJ:35:LYS:HD3	1.79	0.41
8:AS:189:GLU:HG2	8:AS:198:LYS:HE3	2.03	0.41
7:AR:737:MET:SD	12:AW:447:LEU:HD13	2.61	0.41
12:BA:113:LYS:O	12:BA:117:ILE:HG13	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:BD:38:VAL:HG12	8:BD:39:MET:N	2.36	0.41
8:AS:17:PHE:O	8:AS:225:LYS:HA	2.21	0.41
7:BB:488:VAL:HG21	7:BB:573:CYS:SG	2.61	0.41
7:BB:306:THR:HG22	7:BB:306:THR:O	2.21	0.41
12:AW:879:LYS:HE3	14:AY:40:GLU:O	2.21	0.41
5:BL:5:ILE:HG13	5:BL:5:ILE:O	2.20	0.41
12:BA:98:CYS:O	12:BA:154:PHE:CE1	2.75	0.40
4:BQ:44:LEU:O	4:BQ:48:THR:HG23	2.20	0.40
12:BA:443:PHE:CZ	12:BA:464:LEU:HB2	2.56	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
7:AR:1061:ILE:HD11	7:AR:1101:LYS:HD2	2.02	0.40
8:BD:93:TYR:HA	8:BD:145:LEU:O	2.20	0.40
12:BA:516:LEU:HD23	12:BA:524:ILE:HD12	2.03	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: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
6:BN:40:VAL:O	6:BN:41:LYS:HB2	2.21	0.40
7:BB:480:ALA:HB2	7:BB:579:ARG:HD3	2.03	0.40
5:BL:32:LEU:HD13	5:BL:57:ILE:HG12	2.04	0.40
7:AR:668:ARG:HA	7:AR:668:ARG:HD3	1.94	0.40
7:BB:283:GLN:HG3	7:BB:283:GLN:O	2.21	0.40
12:BA:541:ALA:HB2	11:BG:72:CYS:N	2.36	0.40
12:BA:106:ILE:HG22	12:BA:143:ALA:HB3	2.02	0.40
12:AW:107:SER:OG	12:AW:140:ALA:HB2	2.20	0.40
12:AW:40:ILE:CG2	12:AW:41:GLU:N	2.84	0.40
14:BC:277:ILE:HD13	14:BC:293:ILE:HD13	2.03	0.40
12:BA:687:ILE:CD1	12:BA:688:PRO:HD2	2.50	0.40
7:BB:235:ILE:HG22	7:BB:241:ILE:HG13	2.01	0.40
7:BB:364:PHE:CZ	7:BB:388:VAL:HG13	2.56	0.40
12:BA:95:LYS:HD3	12:BA:141:MET:CE	2.51	0.40
7:AR:778:MET:HE3	7:AR:779:PRO:HD2	2.03	0.40
7:AR:273:ASP:O	7:AR:277:SER:N	2.54	0.40
13:BP:41:THR:HG22	13:BP:42:ILE:N	2.36	0.40
14:BC:231:ILE:O	14:BC:232:LYS:HB2	2.21	0.40
8:BD:134:GLY:N	6:BN:60:ILE:HD11	2.36	0.40
11:BG:55:VAL:HG12	11:BG:117:GLN:HA	2.03	0.40
14:BC:179:VAL:HG12	14:BC:180:THR:O	2.21	0.40
9:BE:150:ALA:O	9:BE:151:SER:C	2.58	0.40
8:BD:17:PHE:O	8:BD:225:LYS:HA	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:AY:179:VAL:HG12	14:AY:180:THR:O	2.21	0.40
7:BB:996:LEU:N	7:BB:996:LEU:HD12	2.37	0.40
11:AV:59:ILE:N	11:AV:59:ILE:HD12	2.36	0.40
10:BF:20:LEU:N	10:BF:20:LEU:HD12	2.36	0.40
2:AD:14:DA:H2"	2:AD:15:DT:O5'	2.21	0.40
14:AY:349:VAL:HB	14:AY:353:HIS:ND1	2.36	0.40
4:BQ:59:ILE:HG12	4:BQ:60:SER:N	2.36	0.40
12:BA:108:GLU:HG3	12:BA:147:PRO:HG2	2.03	0.40
14:AY:29:VAL:HG23	14:AY:52:PHE:HE1	1.86	0.40
7:AR:56:ILE:HA	7:AR:57:PRO:HD3	1.98	0.40
12:BA:83:HIS:CD2	12:BA:277:PHE:CE2	3.10	0.40
12:BA:417:VAL:HG11	12:BA:464:LEU:HD11	2.02	0.40
12:BA:769:PHE:CD2	12:BA:778:ALA:HA	2.56	0.40
7:BB:952:PRO:O	7:BB:954:GLU:N	2.54	0.40
6:AO:5:ILE:HD11	8:AS:61:ARG:HB3	2.03	0.40
7:BB:235:ILE:HG23	7:BB:240:ASP:HB3	2.04	0.40
14:AY:244:LYS:HB3	14:AY:249:TYR:HD1	1.85	0.40
12:AW:95:LYS:HD3	12:AW:141:MET:CE	2.52	0.40
5:AM:86:GLU:OE1	8:AS:3:ILE:N	2.54	0.40
12:BA:505:GLY:CA	12:BA:639:VAL:HG23	2.51	0.40
6:BN:19:GLN:N	6:BN:20:PRO:HD2	2.37	0.40
4:BQ:73:LYS:HG3	4:BQ:74:ASP:N	2.36	0.40
12:AW:815:GLN:HB3	14:AY:108:ILE:HD11	2.03	0.40
8:AS:164:VAL:HA	8:AS:227:ILE:O	2.22	0.40
11:BG:46:ILE:O	11:BG:46:ILE:HG12	2.21	0.40
8:BD:15:LEU:HD11	8:BD:242:LEU:HD13	2.03	0.40
10:AU:41:LEU:HA	10:AU:44:VAL:HG12	2.02	0.40
5:AM:1:MET:SD	8:AS:256:LEU:HB2	2.61	0.40
11:BG:59:ILE:N	11:BG:59:ILE:HD12	2.36	0.40
14:BC:265:LYS:N	14:BC:265:LYS:HD2	2.36	0.40
14:BC:42:LEU:CA	14:BC:43:VAL:HG23	2.50	0.40
12:BA:127:SER:O	12:BA:131:ARG:CD	2.69	0.40
11:AV:46:ILE:HG12	11:AV:46:ILE:O	2.21	0.40
12:BA:284:LEU:HD13	12:BA:285:PRO:HD2	2.02	0.40
12:BA:40:ILE:CG2	12:BA:41:GLU:N	2.84	0.40
2:BS:14:DA:H2"	2:BS:15:DT:O5'	2.21	0.40
5:BL:69:LEU:O	5:BL:73:ILE:HG12	2.22	0.40
12:BA:728:MET:CE	7:BB:919:PRO:HG3	2.51	0.40
7:AR:201:VAL:HG23	7:AR:202:PRO:HD2	2.04	0.40
7:AR:705:LEU:O	7:AR:706:VAL:CG1	2.69	0.40
12:BA:539:ILE:HG21	11:BG:46:ILE:HD11	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:AR:359:VAL:HG13	7:AR:360:ALA:N	2.36	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:AR:462:PRO:CG	7:AR:470:VAL:HG13	2.51	0.40
14:AY:219:LEU:HA	14:AY:222:LEU:HD23	2.03	0.40
14:BC:16:LYS:HE2	14:BC:49:ASP:HA	2.04	0.40
10:AU:20:LEU:N	10:AU:20:LEU:HD12	2.36	0.40
4:AJ:36:LEU:HD21	12:AW:131:ARG:CZ	2.51	0.40
12:BA:864:LYS:HD2	12:BA:867:ASP:CA	2.52	0.40
10:BF:88:ILE:C	10:BF:90:ASP:N	2.74	0.40
14:BC:29:VAL:HG23	14:BC:52:PHE:HE1	1.86	0.40
7:BB:808:LYS:HD2	7:BB:808:LYS:C	2.42	0.40
4:AJ:46:LYS:O	4:AJ:50:ILE:HG13	2.21	0.40
12:AW:110:GLU:OE2	12:AW:148:HIS:CE1	2.75	0.40
7:AR:108:ASN:O	7:AR:110:ILE:HD13	2.21	0.40
9:AT:126:ILE:HD12	9:AT:135:VAL:HG13	2.04	0.40
14:BC:223:ARG:HG2	14:BC:227:LEU:HD13	2.03	0.40
7:AR:72:ARG:NH1	7:AR:74:ARG:CG	2.85	0.40
11:AV:94:THR:CG2	11:AV:96:ILE:HD11	2.52	0.40
14:AY:170:ASP:O	14:AY:174:LEU:HD12	2.21	0.40
7:BB:72:ARG:NH1	7:BB:74:ARG:CG	2.85	0.40
14:AY:223:ARG:HG2	14:AY:227:LEU:HD13	2.04	0.40
7:AR:364:PHE:HB2	7:AR:393:VAL:HG22	2.04	0.40
12:AW:747:LEU:HD11	12:AW:790:LEU:HD21	2.04	0.40
7:AR:741:ILE:HG23	7:AR:911:VAL:HG13	2.03	0.40
7:AR:311:ARG:HA	7:AR:314:LYS:HE2	2.04	0.40
11:AV:61:LYS:O	11:AV:62:ASN:CB	2.70	0.40
5:BL:3:ILE:CG2	5:BL:15:LEU:HD11	2.52	0.40
7:BB:91:ARG:HB2	7:BB:93:LEU:HD13	2.04	0.40
5:AM:69:LEU:O	5:AM:73:ILE:HG12	2.22	0.40
13:BP:37:VAL:HG22	13:BP:38:ARG:N	2.37	0.40
3:AI:93:ARG:O	3:AI:94:LYS:CB	2.69	0.40
8:BD:230:LEU:HD12	8:BD:242:LEU:CD2	2.52	0.40
8:BD:205:LEU:O	8:BD:207:GLU:N	2.55	0.40
7:AR:637:THR:HB	7:AR:638:PRO:HD2	2.03	0.40
7:BB:957:GLN:HA	7:BB:960:ILE:HG12	2.04	0.40
12:BA:333:SER:OG	12:BA:625:LYS:HE3	2.20	0.40
5:AM:18:GLU:HA	5:AM:52:LYS:HG2	2.04	0.40
14:BC:262:LEU:HD11	14:BC:283:VAL:HG11	2.02	0.40
11:BG:26:LEU:C	11:BG:26:LEU:HD13	2.42	0.40
7:BB:1084:ILE:N	7:BB:1084:ILE:HD12	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%)	2	27
3	BK	82/95 (86%)	68 (83%)	9 (11%)	5 (6%)	2	27
4	AJ	47/104 (45%)	39 (83%)	4 (8%)	4 (8%)	1	17
4	BQ	48/104 (46%)	39 (81%)	4 (8%)	5 (10%)	1	12
5	AM	89/92 (97%)	82 (92%)	5 (6%)	2 (2%)	8	51
5	BL	89/92 (97%)	81 (91%)	6 (7%)	2 (2%)	8	51
6	AO	63/66 (96%)	47 (75%)	9 (14%)	7 (11%)	0	11
6	BN	63/66 (96%)	47 (75%)	9 (14%)	7 (11%)	0	11
7	AR	1097/1131 (97%)	925 (84%)	129 (12%)	43 (4%)	4	37
7	BB	1097/1131 (97%)	925 (84%)	130 (12%)	42 (4%)	4	38
8	AS	260/265 (98%)	218 (84%)	36 (14%)	6 (2%)	8	50
8	BD	260/265 (98%)	218 (84%)	36 (14%)	6 (2%)	8	50
9	AT	167/180 (93%)	150 (90%)	15 (9%)	2 (1%)	16	62
9	BE	167/180 (93%)	150 (90%)	15 (9%)	2 (1%)	16	62
10	AU	103/113 (91%)	79 (77%)	18 (18%)	6 (6%)	2	28
10	BF	103/113 (91%)	79 (77%)	18 (18%)	6 (6%)	2	28
11	AV	111/132 (84%)	80 (72%)	25 (22%)	6 (5%)	2	30
11	BG	111/132 (84%)	80 (72%)	25 (22%)	6 (5%)	2	30
12	AW	868/880 (99%)	716 (82%)	121 (14%)	31 (4%)	4	40
12	BA	868/880 (99%)	717 (83%)	121 (14%)	30 (4%)	4	41
13	AX	42/48 (88%)	29 (69%)	10 (24%)	3 (7%)	1	23
13	BP	42/48 (88%)	29 (69%)	10 (24%)	3 (7%)	1	23

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	AY	372/395 (94%)	303 (82%)	50 (13%)	19 (5%)	2	31
14	BC	372/395 (94%)	303 (82%)	50 (13%)	19 (5%)	2	31
15	AZ	74/84 (88%)	64 (86%)	6 (8%)	4 (5%)	2	30
15	BH	74/84 (88%)	64 (86%)	6 (8%)	4 (5%)	2	30
All	All	6751/7170 (94%)	5600 (83%)	876 (13%)	275 (4%)	3	36

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

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Mol	Chain	Res	Type
12	BA	229	ILE
12	BA	291	SER
12	BA	541	ALA
12	BA	684	LEU
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

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Mol	Chain	Res	Type
14	AY	127	THR
14	AY	163	MET
14	AY	193	LEU
14	AY	210	PHE
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

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Mol	Chain	Res	Type
12	AW	814	SER
12	AW	849	ALA
13	AX	9	CYS
14	AY	101	THR
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

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Mol	Chain	Res	Type
10	AU	83	VAL
12	AW	257	ALA
12	AW	308	ARG
14	AY	211	ALA
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

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Mol	Chain	Res	Type
9	AT	50	ASN
10	AU	31	SER
10	AU	93	ARG
11	AV	47	ASN
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

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Mol	Chain	Res	Type
12	AW	255	ALA
12	AW	812	ARG
14	AY	328	GLN
12	BA	39	PRO
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
4	AJ	47/96 (49%)	43 (92%)	4 (8%)	13	50
4	BQ	48/96 (50%)	44 (92%)	4 (8%)	14	51
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%)	44	77
6	BN	59/60 (98%)	57 (97%)	2 (3%)	44	77
7	AR	951/975 (98%)	915 (96%)	36 (4%)	40	74
7	BB	951/975 (98%)	915 (96%)	36 (4%)	40	74
8	AS	235/238 (99%)	234 (100%)	1 (0%)	93	96
8	BD	235/238 (99%)	234 (100%)	1 (0%)	93	96
9	AT	150/158 (95%)	143 (95%)	7 (5%)	32	69
9	BE	150/158 (95%)	143 (95%)	7 (5%)	32	69
10	AU	99/107 (92%)	92 (93%)	7 (7%)	18	58
10	BF	99/107 (92%)	92 (93%)	7 (7%)	18	58
11	AV	106/125 (85%)	102 (96%)	4 (4%)	40	74
11	BG	106/125 (85%)	102 (96%)	4 (4%)	40	74
12	AW	758/766 (99%)	717 (95%)	41 (5%)	27	66
12	BA	758/766 (99%)	717 (95%)	41 (5%)	27	66
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%)	306 (94%)	18 (6%)	26	65
14	BC	324/341 (95%)	306 (94%)	18 (6%)	26	65
15	AZ	69/75 (92%)	68 (99%)	1 (1%)	74	89
15	BH	69/75 (92%)	68 (99%)	1 (1%)	74	89
All	All	5983/6294 (95%)	5741 (96%)	242 (4%)	38	73

All (242) 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

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Mol	Chain	Res	Type
4	AJ	78	ARG
6	AO	7	CYS
6	AO	61	HIS
7	AR	54	THR
7	AR	72	ARG
7	AR	93	LEU
7	AR	110	ILE
7	AR	166	THR
7	AR	207	ARG
7	AR	217	PHE
7	AR	224	ILE
7	AR	233	LEU
7	AR	318	LEU
7	AR	330	LEU
7	AR	353	PHE
7	AR	374	LYS
7	AR	376	LYS
7	AR	406	TRP
7	AR	421	ASN
7	AR	422	TRP
7	AR	592	VAL
7	AR	651	LEU
7	AR	686	ASN
7	AR	711	LEU
7	AR	730	ILE
7	AR	733	THR
7	AR	735	TYR
7	AR	808	LYS
7	AR	899	ASP
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	1077	LYS
7	AR	1118	LEU
8	AS	209	CYS
9	AT	16	ASN
9	AT	27	LEU

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Mol	Chain	Res	Type
9	AT	61	PHE
9	AT	90	LEU
9	AT	93	ASP
9	AT	120	TYR
9	AT	126	ILE
10	AU	36	ARG
10	AU	76	CYS
10	AU	78	ILE
10	AU	86	ILE
10	AU	87	LEU
10	AU	88	ILE
10	AU	95	TYR
11	AV	7	GLN
11	AV	65	SER
11	AV	79	THR
11	AV	101	LEU
12	AW	3	GLU
12	AW	32	VAL
12	AW	52	ILE
12	AW	68	CYS
12	AW	77	LEU
12	AW	93	PHE
12	AW	99	ARG
12	AW	100	ARG
12	AW	101	CYS
12	AW	111	ILE
12	AW	116	ARG
12	AW	124	ARG
12	AW	145	VAL
12	AW	159	GLU
12	AW	162	TYR
12	AW	169	LYS
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	357	ASN
12	AW	366	ILE
12	AW	390	TYR

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Mol	Chain	Res	Type
12	AW	415	ASP
12	AW	426	HIS
12	AW	464	LEU
12	AW	478	GLU
12	AW	500	GLN
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	803	ARG
12	AW	809	THR
12	AW	865	THR
14	AY	70	ILE
14	AY	159	ASP
14	AY	176	ASP
14	AY	180	THR
14	AY	190	ARG
14	AY	196	PHE
14	AY	199	ASP
14	AY	210	PHE
14	AY	216	ILE
14	AY	219	LEU
14	AY	232	LYS
14	AY	237	ILE
14	AY	244	LYS
14	AY	247	ASP
14	AY	306	LEU
14	AY	307	ASP
14	AY	315	LEU
14	AY	319	VAL
15	AZ	14	HIS
12	BA	3	GLU
12	BA	32	VAL
12	BA	52	ILE
12	BA	68	CYS
12	BA	77	LEU
12	BA	93	PHE
12	BA	99	ARG
12	BA	100	ARG

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Mol	Chain	Res	Type
12	BA	101	CYS
12	BA	111	ILE
12	BA	116	ARG
12	BA	124	ARG
12	BA	145	VAL
12	BA	159	GLU
12	BA	162	TYR
12	BA	169	LYS
12	BA	187	VAL
12	BA	229	ILE
12	BA	232	GLU
12	BA	233	ASP
12	BA	284	LEU
12	BA	289	HIS
12	BA	342	ILE
12	BA	357	ASN
12	BA	366	ILE
12	BA	390	TYR
12	BA	415	ASP
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	803	ARG
12	BA	809	THR
12	BA	865	THR
7	BB	54	THR
7	BB	72	ARG
7	BB	93	LEU
7	BB	110	ILE
7	BB	166	THR
7	BB	207	ARG
7	BB	217	PHE
7	BB	224	ILE
7	BB	233	LEU

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Mol	Chain	Res	Type
7	BB	318	LEU
7	BB	330	LEU
7	BB	353	PHE
7	BB	374	LYS
7	BB	376	LYS
7	BB	406	TRP
7	BB	421	ASN
7	BB	422	TRP
7	BB	592	VAL
7	BB	651	LEU
7	BB	686	ASN
7	BB	711	LEU
7	BB	730	ILE
7	BB	733	THR
7	BB	735	TYR
7	BB	808	LYS
7	BB	899	ASP
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	1077	LYS
7	BB	1118	LEU
14	BC	70	ILE
14	BC	159	ASP
14	BC	176	ASP
14	BC	180	THR
14	BC	190	ARG
14	BC	196	PHE
14	BC	199	ASP
14	BC	210	PHE
14	BC	216	ILE
14	BC	219	LEU
14	BC	232	LYS
14	BC	237	ILE
14	BC	244	LYS
14	BC	247	ASP
14	BC	306	LEU

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Mol	Chain	Res	Type
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	76	CYS
10	BF	78	ILE
10	BF	86	ILE
10	BF	87	LEU
10	BF	88	ILE
10	BF	95	TYR
11	BG	7	GLN
11	BG	65	SER
11	BG	79	THR
11	BG	101	LEU
15	BH	14	HIS
6	BN	7	CYS
6	BN	61	HIS
4	BQ	33	PHE
4	BQ	35	LYS
4	BQ	46	LYS
4	BQ	78	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
5	AM	82	HIS
7	AR	1018	GLN
8	AS	26	ASN
9	AT	82	GLN
12	AW	237	HIS
12	AW	357	ASN
12	AW	485	ASN
12	AW	500	GLN
12	BA	357	ASN

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Mol	Chain	Res	Type
12	BA	485	ASN
12	BA	500	GLN
7	BB	1018	GLN
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 carbohydrates 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	AS	1001	8	0,9,12	0.00	-	0,15,24	0.00	-
17	SF4	BD	1001	8	0,9,12	0.00	-	0,15,24	0.00	-

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	AS	1001	8	-	0/0/24/48	0/0/3/5
17	SF4	BD	1001	8	-	0/0/24/48	0/0/3/5

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 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	AS	1001	SF4	2	0
17	BD	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%)	1.26	3 (23%) 1 2	263, 280, 311, 312	0
1	BR	14/14 (100%)	1.08	2 (14%) 4 4	228, 239, 287, 301	0
2	AD	15/16 (93%)	1.16	3 (20%) 1 3	264, 278, 302, 313	0
2	BS	16/16 (100%)	0.84	2 (12%) 5 6	216, 237, 276, 283	0
3	AI	84/95 (88%)	-0.01	0 100 100	139, 154, 175, 183	0
3	BK	84/95 (88%)	-0.04	0 100 100	122, 150, 173, 184	0
4	AJ	49/104 (47%)	0.81	3 (6%) 25 17	219, 247, 277, 291	0
4	BQ	50/104 (48%)	0.70	5 (10%) 9 8	216, 237, 255, 263	0
5	AM	91/92 (98%)	0.07	3 (3%) 50 39	159, 184, 196, 200	0
5	BL	91/92 (98%)	0.07	2 (2%) 65 56	139, 164, 177, 179	0
6	AO	65/66 (98%)	-0.01	0 100 100	178, 193, 215, 220	0
6	BN	65/66 (98%)	-0.03	0 100 100	137, 167, 202, 206	0
7	AR	1103/1131 (97%)	0.09	17 (1%) 76 67	132, 158, 195, 219	0
7	BB	1103/1131 (97%)	0.05	15 (1%) 78 69	117, 146, 186, 210	0
8	AS	262/265 (98%)	0.30	15 (5%) 27 20	166, 202, 222, 228	0
8	BD	262/265 (98%)	0.26	8 (3%) 52 41	138, 170, 213, 245	0
9	AT	171/180 (95%)	0.60	18 (10%) 8 7	161, 232, 291, 312	0
9	BE	171/180 (95%)	0.85	26 (15%) 3 4	160, 222, 294, 312	0
10	AU	105/113 (92%)	0.39	8 (7%) 17 12	194, 285, 328, 341	0
10	BF	105/113 (92%)	0.47	9 (8%) 13 10	182, 261, 303, 318	0
11	AV	113/132 (85%)	0.26	3 (2%) 58 48	164, 199, 234, 246	0
11	BG	113/132 (85%)	0.38	6 (5%) 30 23	140, 182, 218, 230	0
12	AW	872/880 (99%)	0.17	28 (3%) 51 40	131, 162, 230, 265	0
12	BA	872/880 (99%)	0.06	14 (1%) 74 65	116, 145, 198, 227	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	AX	44/48 (91%)	-0.00	0 100 100	164, 194, 206, 210	0
13	BP	44/48 (91%)	-0.11	0 100 100	132, 188, 206, 210	0
14	AY	376/395 (95%)	0.17	8 (2%) 67 57	148, 168, 222, 237	0
14	BC	376/395 (95%)	0.17	7 (1%) 70 61	125, 154, 209, 230	0
15	AZ	76/84 (90%)	-0.00	3 (3%) 43 34	157, 185, 200, 206	0
15	BH	76/84 (90%)	-0.17	2 (2%) 59 49	134, 156, 174, 184	0
All	All	6881/7230 (95%)	0.17	210 (3%) 52 41	116, 164, 251, 341	0

All (210) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
9	BE	132	SER	6.0
14	BC	212	ASN	5.8
12	BA	29	THR	5.6
15	AZ	8	LYS	5.3
10	AU	92	ASN	4.8
9	BE	143	ARG	4.8
12	AW	808	ASP	4.7
12	BA	103	ARG	4.6
11	BG	117	GLN	4.6
9	AT	133	LYS	4.3
9	AT	136	ILE	4.1
10	BF	92	ASN	4.1
9	BE	2	TYR	4.1
10	AU	53	GLN	4.0
9	BE	116	ASP	4.0
12	BA	80	PRO	4.0
9	BE	133	LYS	3.9
11	AV	117	GLN	3.9
2	AD	3	DT	3.9
9	BE	115	ASP	3.9
9	BE	131	LYS	3.9
9	BE	114	THR	3.8
10	BF	30	SER	3.8
1	AC	13	DT	3.7
14	BC	137	ALA	3.6
12	BA	102	GLY	3.6
10	BF	93	ARG	3.4
9	AT	81	VAL	3.3
12	AW	105	LYS	3.3

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Mol	Chain	Res	Type	RSRZ
7	AR	206	GLU	3.3
12	AW	257	ALA	3.3
7	AR	812	VAL	3.3
14	BC	192	LYS	3.3
9	BE	134	LYS	3.3
15	AZ	57	ALA	3.3
8	AS	168	PRO	3.3
9	BE	117	THR	3.3
10	BF	77	PRO	3.2
12	AW	295	LEU	3.2
9	BE	136	ILE	3.2
14	AY	243	GLN	3.2
14	BC	339	ASN	3.2
9	AT	69	GLU	3.2
7	AR	1118	LEU	3.1
9	BE	3	LYS	3.1
9	AT	162	LEU	3.1
9	BE	1	MET	3.1
12	AW	80	PRO	3.1
12	AW	28	ILE	3.0
9	AT	42	LEU	3.0
12	BA	105	LYS	3.0
8	BD	116	SER	3.0
5	AM	57	ILE	3.0
9	BE	42	LEU	3.0
5	BL	57	ILE	3.0
12	AW	56	GLN	3.0
14	AY	274	THR	3.0
12	AW	103	ARG	3.0
9	BE	17	GLU	2.9
7	AR	1080	TYR	2.9
14	BC	213	ILE	2.9
8	BD	73	LEU	2.9
11	AV	49	PHE	2.9
10	BF	53	GLN	2.9
12	BA	28	ILE	2.9
4	AJ	47	ASN	2.8
2	BS	2	DA	2.8
7	BB	1010	GLY	2.8
14	BC	252	LEU	2.8
11	BG	49	PHE	2.8
8	AS	125	SER	2.8

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Mol	Chain	Res	Type	RSRZ
9	BE	87	GLY	2.8
8	AS	17	PHE	2.8
7	AR	835	LYS	2.8
9	AT	134	LYS	2.8
14	AY	212	ASN	2.8
12	AW	531	LYS	2.8
7	AR	779	PRO	2.8
12	BA	56	GLN	2.7
8	BD	95	LYS	2.7
9	BE	107	LEU	2.7
12	AW	102	GLY	2.7
1	AC	12	DA	2.7
8	BD	176	CYS	2.6
12	BA	295	LEU	2.6
14	BC	153	VAL	2.6
7	AR	54	THR	2.6
10	BF	68	VAL	2.6
12	AW	81	VAL	2.6
12	AW	809	THR	2.6
10	BF	104	ILE	2.6
9	AT	80	VAL	2.6
1	BR	13	DT	2.6
9	BE	86	GLU	2.6
10	BF	29	SER	2.6
8	BD	67	PHE	2.6
7	BB	206	GLU	2.6
10	AU	104	ILE	2.6
8	AS	95	LYS	2.5
8	AS	124	ILE	2.5
15	BH	8	LYS	2.5
1	BR	12	DA	2.5
2	AD	17	DG	2.5
4	BQ	75	TYR	2.5
9	AT	143	ARG	2.5
5	AM	17	ILE	2.5
12	AW	26	ALA	2.5
4	BQ	81	ARG	2.5
7	BB	812	VAL	2.5
12	AW	653	LEU	2.5
8	BD	3	ILE	2.4
7	AR	200	ARG	2.4
12	AW	238	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
11	BG	71	PHE	2.4
8	AS	121	ILE	2.4
8	BD	192	ASP	2.4
5	AM	3	ILE	2.4
9	AT	132	SER	2.4
12	AW	4	LYS	2.4
8	AS	179	GLY	2.4
11	BG	116	HIS	2.4
7	BB	175	VAL	2.4
12	BA	79	ARG	2.4
9	BE	69	GLU	2.4
7	BB	178	ASP	2.4
11	AV	50	SER	2.4
12	BA	75	ILE	2.3
8	AS	123	PRO	2.3
11	BG	48	ILE	2.3
12	AW	234	ASP	2.3
9	AT	5	ILE	2.3
7	BB	811	ASP	2.3
10	AU	30	SER	2.3
7	AR	380	ARG	2.3
7	AR	504	ILE	2.3
10	AU	90	ASP	2.3
10	AU	94	THR	2.3
7	BB	787	LYS	2.3
9	BE	101	LEU	2.3
9	BE	162	LEU	2.3
10	AU	93	ARG	2.3
15	BH	60	GLY	2.3
9	BE	5	ILE	2.3
12	AW	194	ILE	2.2
4	AJ	77	LYS	2.2
10	BF	78	ILE	2.2
2	BS	17	DG	2.2
7	BB	779	PRO	2.2
4	BQ	59	ILE	2.2
9	AT	2	TYR	2.2
12	BA	857	PRO	2.2
9	BE	80	VAL	2.2
4	AJ	81	ARG	2.2
9	AT	101	LEU	2.2
8	AS	127	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
9	BE	119	LYS	2.2
10	AU	78	ILE	2.2
12	BA	119	ASN	2.2
14	AY	230	LYS	2.2
8	AS	133	LEU	2.2
7	BB	810	GLY	2.2
9	AT	39	LEU	2.2
14	AY	339	ASN	2.2
7	BB	784	ARG	2.1
11	BG	50	SER	2.1
9	AT	94	ASN	2.1
14	AY	235	LYS	2.1
14	AY	153	VAL	2.1
7	BB	813	LEU	2.1
4	BQ	76	GLU	2.1
7	AR	836	ARG	2.1
12	AW	704	LEU	2.1
4	BQ	73	LYS	2.1
8	AS	217	ILE	2.1
9	BE	168	TYR	2.1
8	AS	113	ASP	2.1
12	AW	265	LEU	2.1
15	AZ	61	ASP	2.1
12	AW	195	LEU	2.1
12	AW	181	ARG	2.1
7	AR	813	LEU	2.1
9	AT	70	VAL	2.1
9	AT	3	LYS	2.1
8	AS	188	PHE	2.1
9	AT	17	GLU	2.1
14	AY	214	ASP	2.1
8	BD	217	ILE	2.1
7	AR	175	VAL	2.1
12	AW	288	LYS	2.1
12	BA	208	ILE	2.1
1	AC	11	DT	2.1
7	BB	814	ILE	2.0
12	AW	398	ALA	2.0
9	BE	85	VAL	2.0
12	AW	145	VAL	2.0
12	BA	30	PRO	2.0
5	BL	3	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
8	AS	4	ASN	2.0
7	AR	382	LEU	2.0
7	AR	49	GLN	2.0
7	BB	283	GLN	2.0
12	AW	119	ASN	2.0
7	BB	1125	SER	2.0
7	AR	223	LYS	2.0
7	BB	380	ARG	2.0
7	AR	787	LYS	2.0
12	AW	389	ARG	2.0
8	AS	46	PHE	2.0
12	AW	688	PRO	2.0
2	AD	14	DA	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
17	SF4	AS	1001	7/8	0.97	0.24	-0.50	186,189,193,194	0
17	SF4	BD	1001	7/8	0.96	0.23	-0.80	149,150,154,157	0
16	ZN	BN	100	1/1	0.78	0.23	-0.92	153,153,153,153	0
16	ZN	AO	100	1/1	0.92	0.25	-0.92	188,188,188,188	0
16	ZN	AR	1300	1/1	0.96	0.12	-1.11	193,193,193,193	0
16	ZN	BP	101	1/1	0.86	0.09	-1.42	200,200,200,200	0
16	ZN	AX	101	1/1	0.83	0.10	-1.42	204,204,204,204	0
16	ZN	BA	902	1/1	0.94	0.17	-1.43	209,209,209,209	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
16	ZN	BB	1300	1/1	0.97	0.09	-1.45	177,177,177,177	0
16	ZN	AW	902	1/1	0.96	0.28	-1.50	245,245,245,245	0
16	ZN	BA	901	1/1	0.88	0.08	-1.56	161,161,161,161	0
16	ZN	AW	903	1/1	0.93	0.11	-1.79	134,134,134,134	0
16	ZN	AW	901	1/1	0.83	0.07	-2.02	183,183,183,183	0
16	ZN	BA	903	1/1	0.97	0.10	-2.08	118,118,118,118	0
18	MG	BA	904	1/1	0.88	0.36	-	117,117,117,117	0
18	MG	AW	904	1/1	0.92	0.29	-	132,132,132,132	0

6.5 Other polymers

There are no such residues in this entry.