Full wwPDB X-ray Structure Validation Report ⓘ

Jan 10, 2017 – 01:30 PM EST

PDB ID	:	5TW1
Title	:	Crystal structure of a Mycobacterium smegmatis transcription initiation complex with RbpA
Authors	:	Hubin, E.A.; Darst, S.A.; Campbell, E.A.
Deposited on	:	2016-11-10
Resolution	:	2.76 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 ⓘ symbol.

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

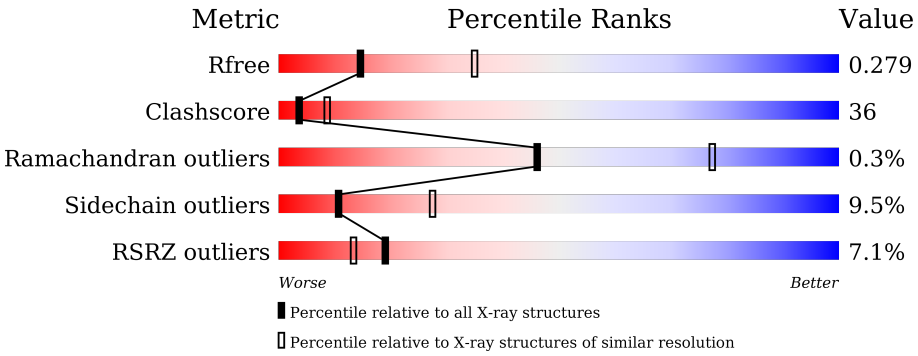
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028442

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.76 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	3340 (2.80-2.72)
Clashscore	102246	3829 (2.80-2.72)
Ramachandran outliers	100387	3767 (2.80-2.72)
Sidechain outliers	100360	3770 (2.80-2.72)
RSRZ outliers	91569	3352 (2.80-2.72)

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	J	114	9% 34% 33% 5% 27%
2	A	350	% 23% 36% • 38%
2	B	350	10% 26% 36% 5% 33%
2	T	350	13% 9% 5% • 85%
3	C	1169	8% 44% 45% 6% 6%
4	D	1317	3% 50% 40% • 5%

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Mol	Chain	Length	Quality of chain
5	E	107	4% 34% 28% 8% 29%
6	F	466	% 38% 23% 35%
7	O	31	35% 65%
8	P	26	62% 38%
9	G	17	100%

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
10	SO4	C	1203	-	-	X	-
10	SO4	D	2005	-	-	X	-
10	SO4	F	505	-	-	-	X
12	ZN	D	2001	-	-	-	X

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 26644 atoms, of which 36 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called RNA polymerase-binding protein RbpA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	J	83	Total	C	N	O	S	0	0	0
			667	419	118	128	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	218	Total	C	N	O	S	0	0	0
			1617	1020	276	318	3			
2	B	233	Total	C	N	O	S	0	0	0
			1667	1054	289	322	2			
2	T	53	Total	C	N	O	S	0	0	0
			374	236	65	72	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	1099	Total	C	N	O	S	0	0	0
			8250	5164	1448	1603	35			

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	1248	Total	C	N	O	S	0	0	0
			9588	6016	1727	1805	40			

- Molecule 5 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	76	Total	C	N	O	0	0	0
			592	378	100	114			

- Molecule 6 is a protein called RNA polymerase sigma factor SigA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	302	Total	C	N	O	S	0	0	0
			2396	1502	433	454	7			

- Molecule 7 is a DNA chain called DNA (31-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	O	31	Total	C	N	O	P	0	0	0
			634	305	114	185	30			

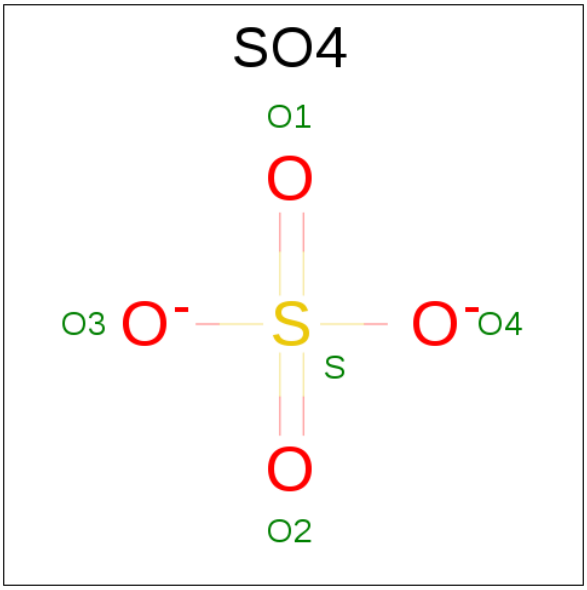
- Molecule 8 is a DNA chain called DNA (26-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	P	26	Total	C	N	O	P	0	0	0
			526	254	94	153	25			

- Molecule 9 is a protein called Unknown peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	G	17	Total	C	N	O	0	0	0
			85	51	17	17			

- Molecule 10 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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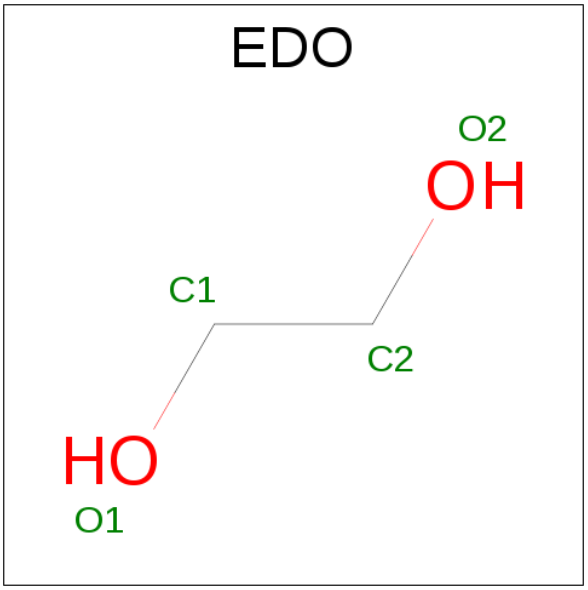
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	C	1	Total O S 5 4 1	0	0
10	C	1	Total O S 5 4 1	0	0
10	D	1	Total O S 5 4 1	0	0
10	D	1	Total O S 5 4 1	0	0
10	D	1	Total O S 5 4 1	0	0
10	D	1	Total O S 5 4 1	0	0
10	F	1	Total O S 5 4 1	0	0
10	F	1	Total O S 5 4 1	0	0
10	F	1	Total O S 5 4 1	0	0
10	F	1	Total O S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

- Molecule 11 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	C	1	Total C H O 10 2 6 2	0	0
11	C	1	Total C H O 10 2 6 2	0	0
11	D	1	Total C H O 10 2 6 2	0	0
11	D	1	Total C H O 10 2 6 2	0	0
11	D	1	Total C H O 10 2 6 2	0	0
11	F	1	Total C H O 10 2 6 2	0	0

- Molecule 12 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	D	2	Total Zn 2 2	0	0

- Molecule 13 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	D	1	Total Mg 1 1	0	0

- Molecule 14 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	J	2	Total O 2 2	0	0
14	A	2	Total O 2 2	0	0
14	B	2	Total O 2 2	0	0
14	C	30	Total O 30 30	0	0
14	D	57	Total O 57 57	0	0
14	E	3	Total O 3 3	0	0
14	F	16	Total O 16 16	0	0

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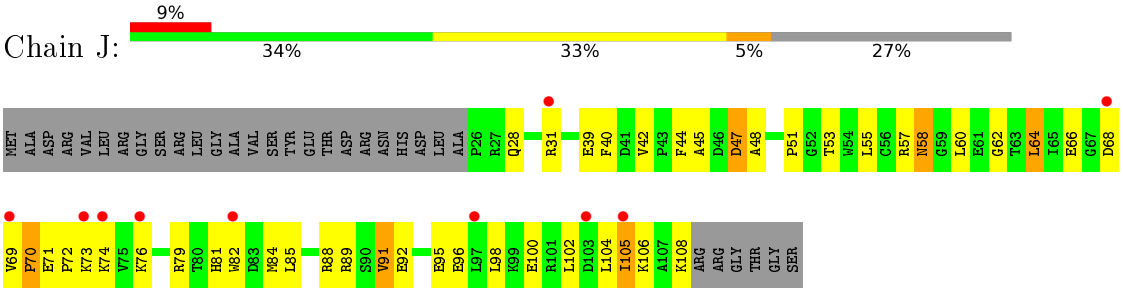
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	O	10	Total O 10 10	0	0
14	P	3	Total O 3 3	0	0

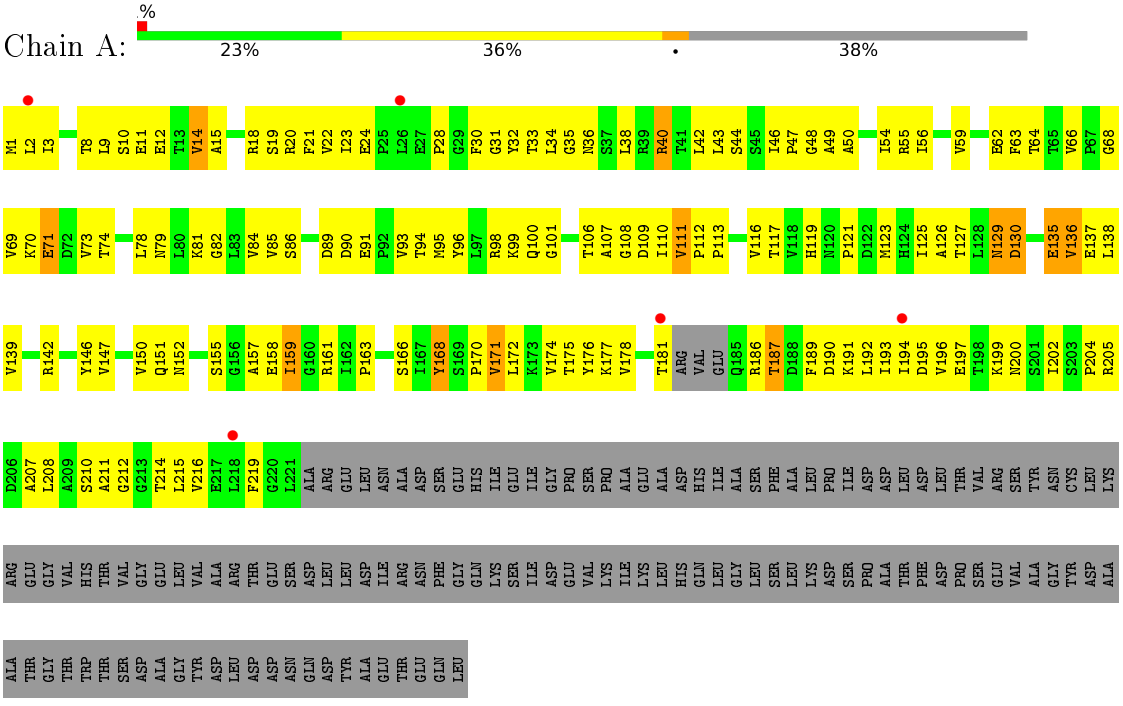
3 Residue-property plots

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.

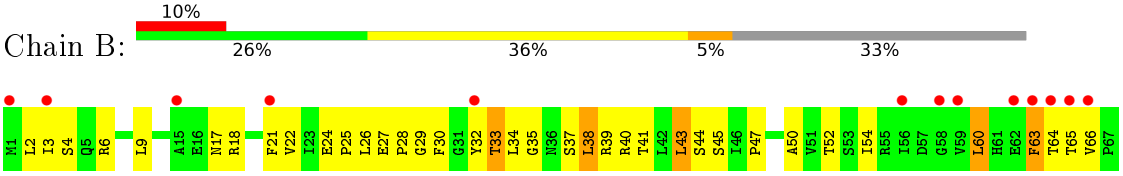
- Molecule 1: RNA polymerase-binding protein RbpA

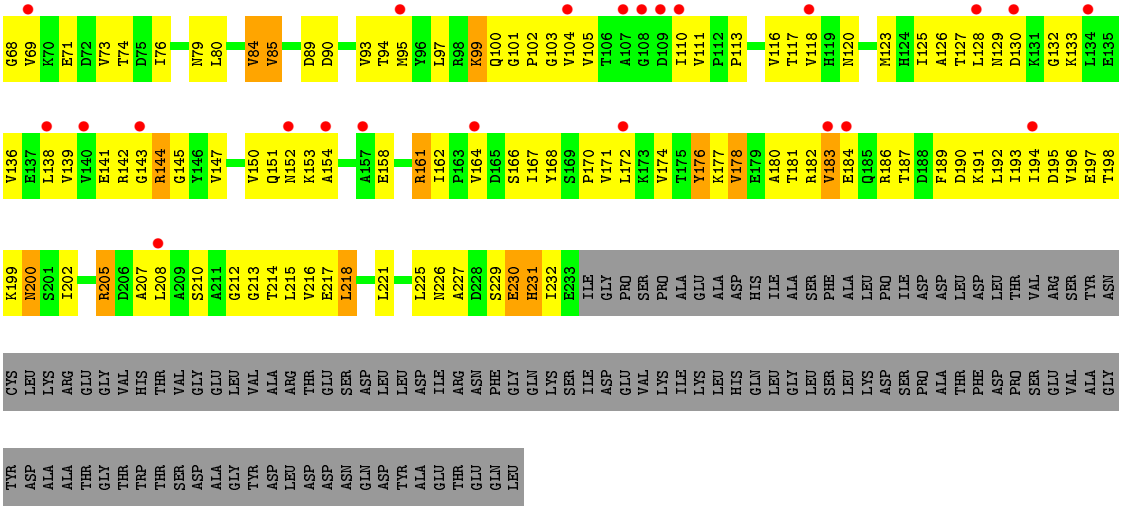


- Molecule 2: DNA-directed RNA polymerase subunit alpha



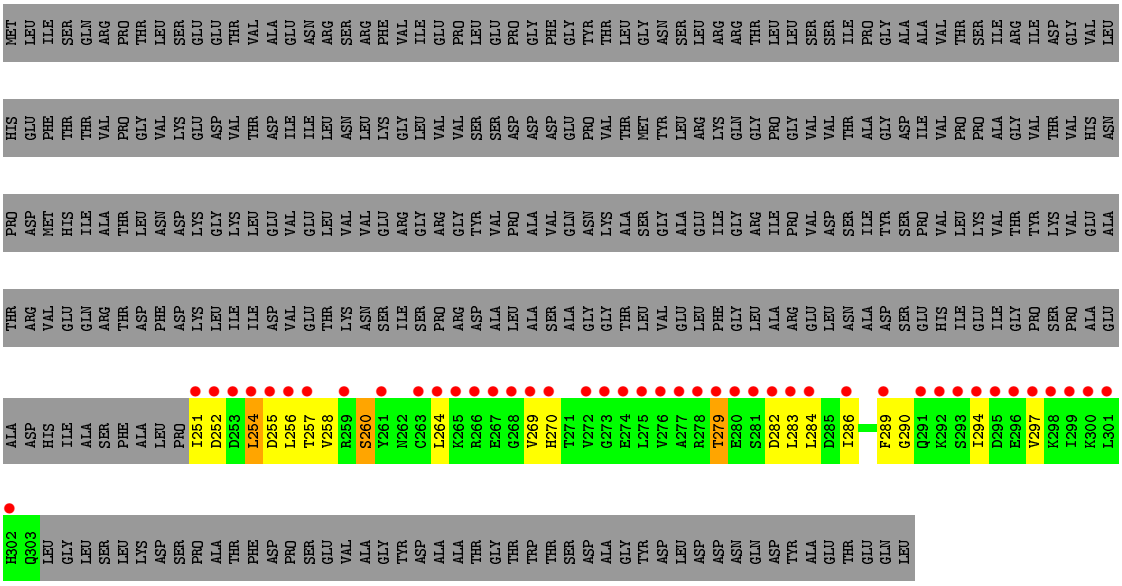
- Molecule 2: DNA-directed RNA polymerase subunit alpha





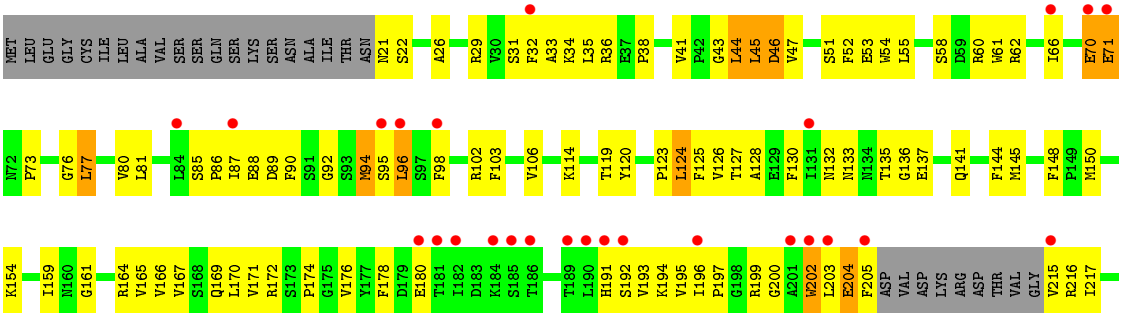
• Molecule 2: DNA-directed RNA polymerase subunit alpha

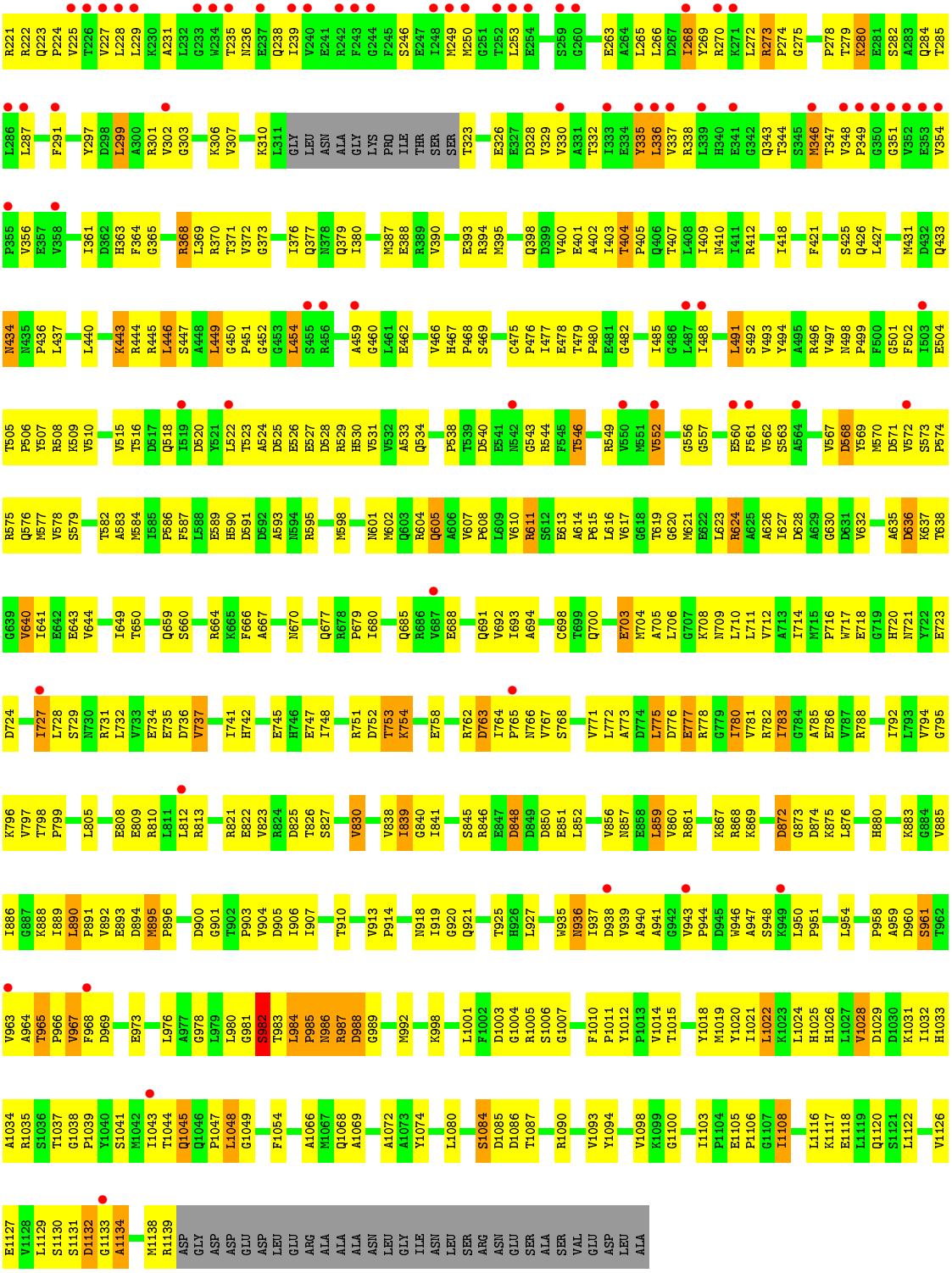
Chain T:



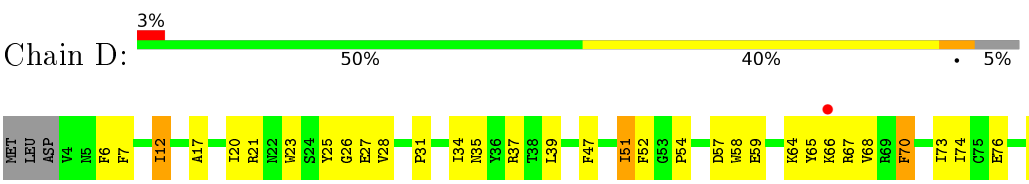
• Molecule 3: DNA-directed RNA polymerase subunit beta

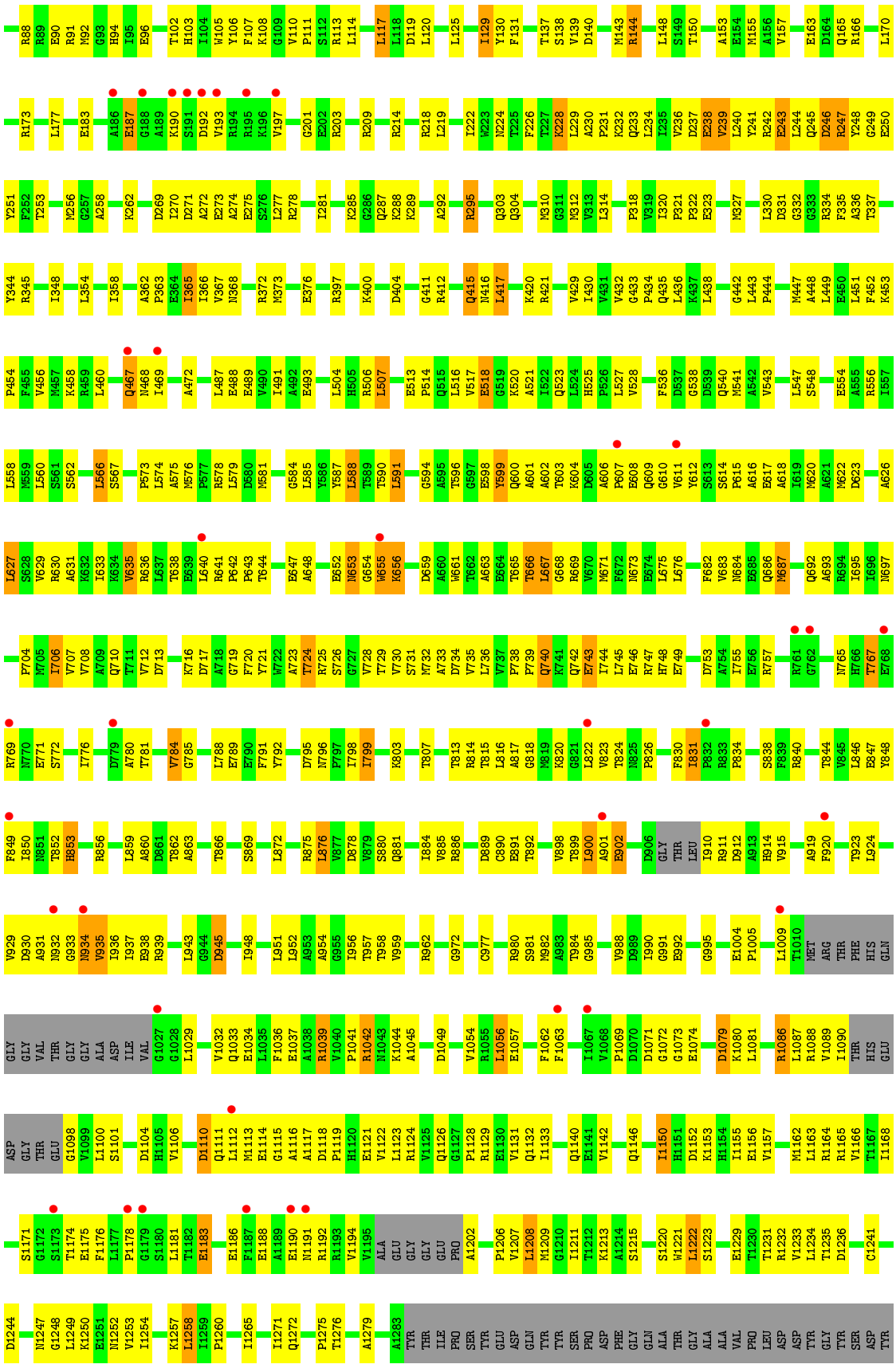
Chain C:



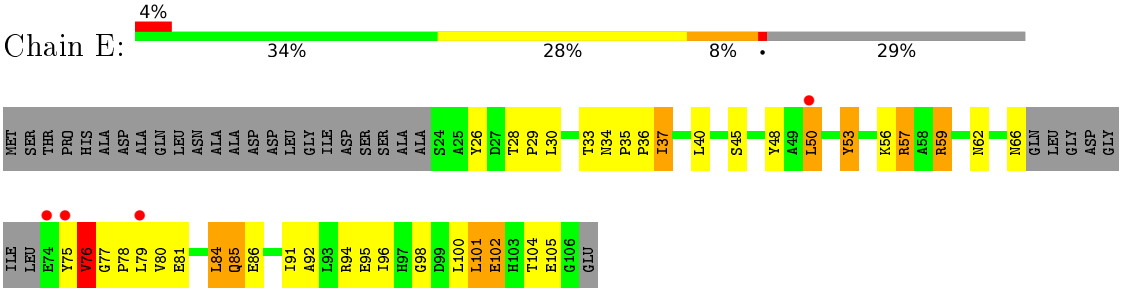


• Molecule 4: DNA-directed RNA polymerase subunit beta'

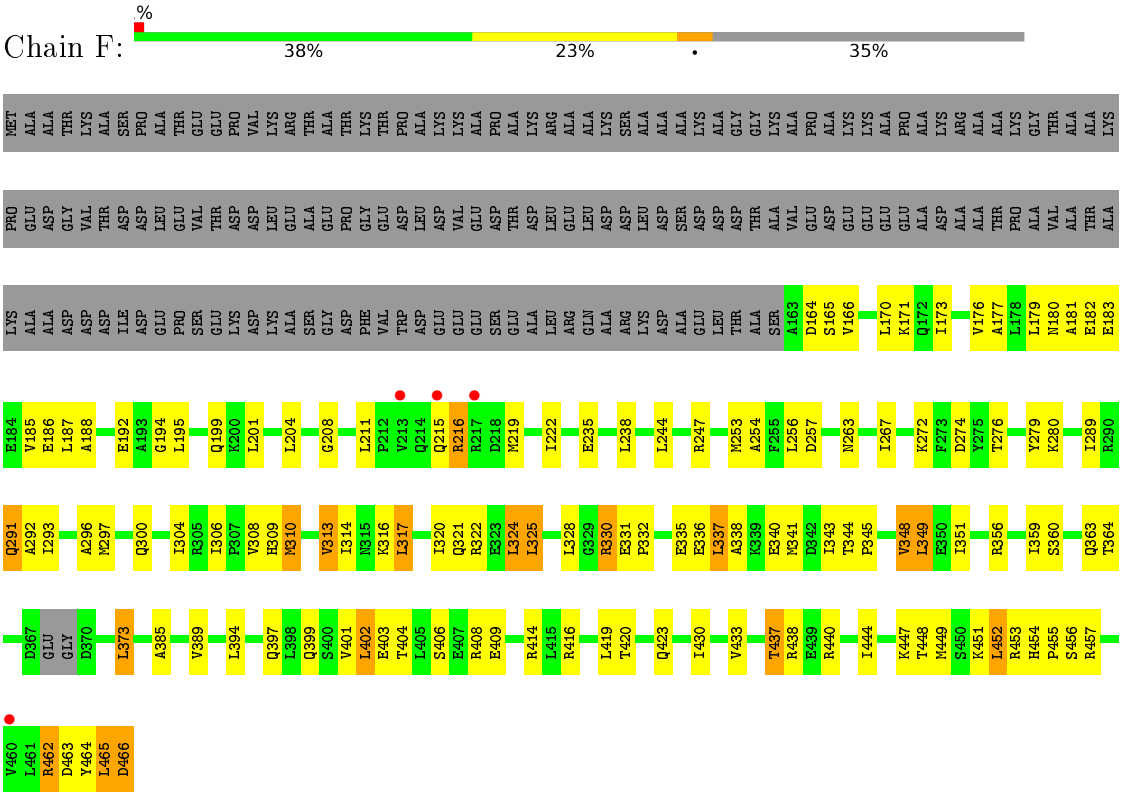




• Molecule 5: DNA-directed RNA polymerase subunit omega



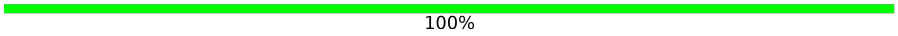
• Molecule 6: RNA polymerase sigma factor SigA



• Molecule 7: DNA (31-MER)

• Molecule 8: DNA (26-MER)

• Molecule 9: Unknown peptide

Chain G: 

There are no outlier residues recorded for this chain.

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	133.01Å 161.63Å 139.21Å 90.00° 107.72° 90.00°	Depositor
Resolution (Å)	54.91 – 2.76 54.91 – 2.75	Depositor EDS
% Data completeness (in resolution range)	99.5 (54.91-2.76) 99.4 (54.91-2.75)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.16 (at 2.77Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.239 , 0.280 0.236 , 0.279	Depositor DCC
R_{free} test set	1974 reflections (1.38%)	DCC
Wilson B-factor (Å^2)	78.4	Xtriage
Anisotropy	0.150	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 53.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	0.003 for l,-k,h	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	26644	wwPDB-VP
Average B, all atoms (Å^2)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.46% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	J	0.27	0/681	0.47	0/923
2	A	0.27	0/1641	0.50	0/2236
2	B	0.26	0/1693	0.49	0/2316
2	T	0.24	0/376	0.39	0/511
3	C	0.28	0/8394	0.50	1/11410 (0.0%)
4	D	0.30	0/9742	0.49	0/13189
5	E	0.28	0/604	0.49	0/822
6	F	0.26	0/2426	0.45	1/3273 (0.0%)
7	O	0.68	0/710	0.96	0/1095
8	P	0.69	0/589	0.96	0/906
All	All	0.31	0/26856	0.53	2/36681 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	J	0	1
3	C	0	5
All	All	0	6

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	890	LEU	CA-CB-CG	5.46	127.85	115.30
6	F	330	ARG	C-N-CA	-5.05	109.07	121.70

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	1131	SER	Peptide
3	C	368	ARG	Peptide
3	C	433	GLN	Peptide
3	C	982	SER	Peptide
3	C	985	PRO	Peptide
1	J	70	PRO	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	J	667	0	649	51	0
2	A	1617	0	1636	179	0
2	B	1667	0	1636	193	0
2	T	374	0	344	29	0
3	C	8250	0	7989	692	0
4	D	9588	0	9552	631	0
5	E	592	0	583	53	0
6	F	2396	0	2422	142	0
7	O	634	0	350	33	0
8	P	526	0	296	16	0
9	G	85	0	19	0	0
10	C	15	0	0	2	0
10	D	20	0	0	2	0
10	F	25	0	0	1	0
11	C	8	12	12	1	0
11	D	12	18	18	3	0
11	F	4	6	6	1	0
12	D	2	0	0	0	0
13	D	1	0	0	0	0
14	A	2	0	0	0	0
14	B	2	0	0	0	0
14	C	30	0	0	16	0
14	D	57	0	0	17	0
14	E	3	0	0	0	0
14	F	16	0	0	3	0
14	J	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	O	10	0	0	3	0
14	P	3	0	0	1	0
All	All	26608	36	25512	1851	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 36.

All (1851) 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)
2:B:184:GLU:HA	2:B:187:THR:HG22	1.28	1.15
3:C:940:ALA:HB1	3:C:941:ALA:HA	1.28	1.12
3:C:228:LEU:HD21	3:C:268:ILE:HG12	1.29	1.11
3:C:982:SER:HB3	3:C:983:THR:HG23	1.35	1.08
3:C:176:VAL:HG12	3:C:195:VAL:HG22	1.35	1.07
3:C:540:ASP:HB2	3:C:546:THR:HG23	1.32	1.07
4:D:1275:PRO:HG3	5:E:76:VAL:HG11	1.34	1.04
4:D:641:ARG:HA	4:D:656:LYS:HE3	1.40	1.04
3:C:444:ARG:HH21	3:C:491:LEU:HD23	1.20	1.03
4:D:432:VAL:HG22	4:D:434:PRO:HD3	1.40	1.02
3:C:799:PRO:HA	3:C:823:VAL:HG12	1.36	1.02
3:C:215:VAL:HG23	3:C:225:VAL:HA	1.41	0.99
3:C:635:ALA:HB2	3:C:693:ILE:HD11	1.43	0.97
3:C:602:MET:HE1	3:C:883:LYS:HB3	1.42	0.97
4:D:603:THR:HG22	4:D:604:LYS:HE2	1.47	0.96
6:F:308:VAL:HG21	7:O:23:DT:H71	1.45	0.96
2:A:1:MET:N	2:B:142:ARG:O	1.97	0.96
2:A:31:GLY:HA2	2:A:192:LEU:HD23	1.48	0.96
4:D:815:THR:HG22	4:D:820:LYS:HA	1.48	0.95
3:C:41:VAL:O	3:C:624:ARG:NH2	1.98	0.95
3:C:710:LEU:HD22	3:C:1021:ILE:HD11	1.46	0.95
3:C:478:GLU:OE2	3:C:604:ARG:NH2	1.98	0.95
4:D:1174:THR:HG23	4:D:1176:PHE:H	1.31	0.94
3:C:584:MET:O	14:C:1301:HOH:O	1.85	0.93
4:D:327:MET:HG3	4:D:337:THR:HB	1.49	0.93
4:D:573:PRO:HG2	4:D:576:MET:HE3	1.51	0.93
3:C:338:ARG:HD2	3:C:346:MET:HG3	1.48	0.93
3:C:1048:LEU:HD23	3:C:1048:LEU:H	1.34	0.92
3:C:217:ILE:HD11	3:C:272:LEU:HD11	1.52	0.92
2:A:89:ASP:CB	2:A:90:ASP:HA	1.99	0.92
3:C:783:ILE:H	3:C:783:ILE:HD12	1.33	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:191:HIS:HA	3:C:192:SER:HB3	1.49	0.91
2:B:63:PHE:CE2	4:D:603:THR:HG23	2.04	0.91
4:D:365:ILE:HD12	4:D:365:ILE:H	1.35	0.91
6:F:211:LEU:HB2	6:F:216:ARG:HD2	1.52	0.91
3:C:454:LEU:HD22	3:C:459:ALA:HB2	1.53	0.90
4:D:951:LEU:HB3	4:D:956:ILE:HD11	1.53	0.90
3:C:77:LEU:HD11	3:C:124:LEU:HD11	1.52	0.89
3:C:1132:ASP:HB3	3:C:1133:GLY:HA2	1.54	0.89
6:F:253:MET:HE3	6:F:297:MET:HA	1.54	0.89
5:E:86:GLU:OE2	5:E:94:ARG:NH1	2.06	0.89
2:B:34:LEU:HD11	2:B:192:LEU:HD22	1.54	0.89
4:D:323:GLU:OE2	14:D:2102:HOH:O	1.91	0.89
4:D:599:TYR:HB2	4:D:610:GLY:HA3	1.52	0.89
4:D:740:GLN:H	4:D:740:GLN:HE21	1.19	0.89
3:C:92:GLY:O	3:C:133:ASN:ND2	2.07	0.88
4:D:1074:GLU:O	14:D:2101:HOH:O	1.89	0.88
3:C:895:MET:SD	14:C:1326:HOH:O	2.30	0.88
3:C:508:ARG:HD3	3:C:515:VAL:HG11	1.56	0.87
3:C:938:ASP:O	3:C:944:PRO:HD3	1.74	0.87
3:C:159:ILE:HB	3:C:164:ARG:HD2	1.57	0.87
3:C:758:GLU:HG2	3:C:798:THR:HG22	1.54	0.87
3:C:935:TRP:HA	3:C:983:THR:HG23	1.54	0.87
2:A:98:ARG:HG2	2:A:135:GLU:HG2	1.56	0.87
4:D:655:TRP:CE3	4:D:655:TRP:HA	2.08	0.87
2:B:84:VAL:HB	2:B:199:LYS:HD3	1.56	0.86
6:F:324:LEU:HD23	6:F:328:LEU:HD13	1.57	0.86
3:C:584:MET:HA	3:C:619:THR:HG21	1.56	0.86
4:D:269:ASP:HB3	4:D:272:ALA:HB3	1.57	0.86
2:B:153:LYS:N	2:B:154:ALA:HA	1.88	0.86
3:C:510:VAL:N	3:C:568:ASP:O	2.09	0.86
2:A:152:ASN:HB2	2:A:157:ALA:HB3	1.58	0.85
1:J:31:ARG:NH2	1:J:39:GLU:OE1	2.09	0.85
4:D:442:GLY:HA3	4:D:523:GLN:HB2	1.57	0.85
4:D:668:GLY:HA2	4:D:671:MET:HE2	1.59	0.85
2:B:95:MET:HG2	2:B:113:PRO:HD2	1.59	0.85
6:F:280:LYS:HG2	7:O:30:DC:OP2	1.75	0.85
2:B:6:ARG:O	2:B:25:PRO:HD2	1.77	0.85
4:D:1088:ARG:HG2	4:D:1089:VAL:H	1.42	0.85
2:B:152:ASN:C	2:B:154:ALA:HA	1.97	0.85
3:C:718:GLU:H	4:D:724:THR:HG21	1.42	0.85
4:D:1071:ASP:HB2	4:D:1073:GLY:N	1.93	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:612:TYR:HB2	4:D:635:VAL:HG12	1.57	0.84
2:B:32:TYR:HB3	3:C:1005:ARG:HG3	1.58	0.84
8:P:16:DT:OP2	14:P:101:HOH:O	1.95	0.84
2:A:48:GLY:HA2	2:A:49:ALA:HB3	1.58	0.84
3:C:150:MET:HA	3:C:150:MET:HE2	1.60	0.84
4:D:930:ASP:O	4:D:933:GLY:HA3	1.77	0.84
3:C:574:PRO:O	3:C:575:ARG:HG2	1.78	0.84
4:D:1174:THR:HG21	4:D:1176:PHE:HB2	1.60	0.83
3:C:170:LEU:HA	3:C:369:LEU:H	1.44	0.83
3:C:379:GLN:HG2	3:C:421:PHE:HB2	1.61	0.83
2:B:21:PHE:HB2	2:B:194:ILE:HG22	1.61	0.83
4:D:901:ALA:H	4:D:912:ASP:HB2	1.44	0.83
2:B:151:GLN:HG2	2:B:154:ALA:HB1	1.61	0.82
2:T:289:PHE:HE2	2:T:294:ILE:HG13	1.44	0.82
2:B:100:GLN:HA	2:B:133:LYS:HA	1.61	0.82
2:A:157:ALA:HB1	2:A:161:ARG:HD2	1.60	0.82
3:C:649:ILE:HD11	3:C:679:PRO:HB3	1.61	0.82
6:F:253:MET:CE	6:F:300:GLN:HB2	2.09	0.82
2:A:56:ILE:HB	2:A:59:VAL:HG22	1.62	0.81
4:D:1248:GLY:O	4:D:1252:ASN:ND2	2.12	0.81
4:D:1174:THR:HG23	4:D:1176:PHE:N	1.96	0.81
4:D:642:PRO:HD3	4:D:656:LYS:HG2	1.62	0.81
3:C:940:ALA:HB1	3:C:941:ALA:CA	2.10	0.81
3:C:88:GLU:HG2	3:C:92:GLY:HA2	1.62	0.81
4:D:929:VAL:HG12	4:D:935:VAL:HG22	1.61	0.80
2:B:64:THR:O	2:B:65:THR:OG1	1.97	0.80
3:C:410:ASN:OD1	14:C:1302:HOH:O	1.98	0.80
4:D:1275:PRO:HB3	5:E:79:LEU:HD11	1.63	0.80
5:E:84:LEU:H	5:E:84:LEU:HD12	1.45	0.80
5:E:85:GLN:H	5:E:85:GLN:HE21	1.30	0.80
1:J:102:LEU:O	1:J:105:ILE:HG22	1.81	0.80
4:D:573:PRO:HG2	4:D:576:MET:CE	2.12	0.80
3:C:891:PRO:HB2	3:C:893:GLU:HG2	1.64	0.80
2:B:18:ARG:HG3	2:B:197:GLU:HG3	1.64	0.79
4:D:1171:SER:CA	4:D:1174:THR:HG22	2.11	0.79
3:C:540:ASP:CB	3:C:546:THR:HG23	2.12	0.79
4:D:643:PRO:O	4:D:647:GLU:HB3	1.82	0.79
7:O:12:DG:N7	14:O:102:HOH:O	2.15	0.79
4:D:26:GLY:HA3	4:D:51:ILE:HG22	1.64	0.79
5:E:30:LEU:O	5:E:33:THR:HG22	1.83	0.79
4:D:818:GLY:O	4:D:838:SER:HB3	1.83	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:152:ASN:CB	2:A:157:ALA:HB3	2.13	0.78
6:F:454:HIS:ND1	6:F:455:PRO:HD2	1.98	0.78
3:C:981:GLY:O	3:C:982:SER:OG	2.01	0.78
4:D:587:TYR:O	4:D:590:THR:HG22	1.84	0.78
4:D:599:TYR:CE1	4:D:601:ALA:HB2	2.19	0.78
4:D:735:VAL:HG12	4:D:840:ARG:HD2	1.64	0.78
6:F:308:VAL:HG22	14:F:601:HOH:O	1.82	0.78
3:C:51:SER:OG	3:C:373:GLY:N	2.14	0.78
4:D:859:LEU:O	4:D:862:THR:HG22	1.83	0.78
3:C:148:PHE:HE1	3:C:380:ILE:HD11	1.48	0.77
4:D:641:ARG:CA	4:D:656:LYS:HE3	2.13	0.77
5:E:45:SER:OG	5:E:105:GLU:OE2	2.01	0.77
2:T:279:THR:HG23	2:T:282:ASP:HB2	1.67	0.77
2:A:181:THR:N	2:A:189:PHE:O	2.18	0.77
3:C:763:ASP:HB3	3:C:821:ARG:HH22	1.50	0.77
4:D:1168:ILE:HD13	4:D:1176:PHE:HB3	1.64	0.77
4:D:642:PRO:HG3	4:D:661:TRP:CE2	2.19	0.77
7:O:11:DA:H2"	7:O:12:DG:H5"	1.65	0.77
3:C:412:ARG:HD2	6:F:322:ARG:HE	1.50	0.77
4:D:772:SER:O	4:D:776:ILE:HG13	1.85	0.77
4:D:937:ILE:HD12	4:D:951:LEU:HG	1.66	0.77
3:C:132:ASN:HB3	3:C:135:THR:HG22	1.65	0.76
3:C:494:TYR:HB3	3:C:506:PRO:HG3	1.67	0.76
3:C:637:LYS:HD2	3:C:659:GLN:HE22	1.50	0.76
3:C:1127:GLU:OE1	14:C:1304:HOH:O	2.02	0.76
3:C:231:ALA:HB1	3:C:265:LEU:CD1	2.14	0.76
4:D:417:LEU:HG	4:D:1254:ILE:HG23	1.66	0.76
2:A:40:ARG:HD3	2:B:33:THR:HG22	1.67	0.76
2:A:48:GLY:CA	2:A:49:ALA:HB3	2.16	0.76
3:C:1003:ASP:OD1	3:C:1006:SER:N	2.17	0.76
3:C:509:LYS:O	3:C:516:THR:HG22	1.85	0.76
2:B:170:PRO:HB2	2:B:202:ILE:HD11	1.67	0.76
2:B:184:GLU:CA	2:B:187:THR:HG22	2.13	0.76
2:A:86:SER:OG	2:A:119:HIS:NE2	2.15	0.76
3:C:368:ARG:NH1	14:C:1309:HOH:O	2.19	0.76
4:D:47:PHE:O	4:D:88:ARG:NH2	2.18	0.76
4:D:277:LEU:HD11	4:D:295:ARG:HG2	1.65	0.76
6:F:404:THR:O	6:F:457:ARG:NH2	2.19	0.76
4:D:901:ALA:HB2	4:D:911:ARG:HA	1.68	0.76
3:C:984:LEU:HB2	3:C:985:PRO:HA	1.66	0.75
3:C:935:TRP:HA	3:C:983:THR:CG2	2.15	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:28:PRO:HA	2:A:190:ASP:OD2	1.86	0.75
3:C:348:VAL:HB	3:C:351:GLY:HA3	1.69	0.75
3:C:711:LEU:HD23	3:C:904:VAL:HA	1.68	0.75
3:C:205:PHE:CE1	3:C:215:VAL:HG13	2.21	0.75
4:D:721:TYR:O	4:D:725:ARG:HG2	1.85	0.75
6:F:201:LEU:HD11	6:F:219:MET:HB3	1.68	0.75
2:B:22:VAL:HG12	2:B:193:ILE:HD12	1.69	0.75
3:C:940:ALA:CB	3:C:941:ALA:HA	2.12	0.75
4:D:951:LEU:HB3	4:D:956:ILE:CD1	2.15	0.75
4:D:655:TRP:HE3	4:D:655:TRP:HA	1.50	0.75
4:D:822:LEU:HD23	4:D:834:PRO:HA	1.67	0.75
2:B:32:TYR:HE1	2:B:178:VAL:HG21	1.51	0.75
3:C:720:HIS:CE1	3:C:888:LYS:HD3	2.22	0.75
2:A:66:VAL:O	2:A:69:VAL:HG22	1.86	0.74
4:D:237:ASP:HB3	4:D:240:LEU:HB3	1.69	0.74
1:J:68:ASP:HA	1:J:69:VAL:HB	1.68	0.74
3:C:1138:MET:O	3:C:1139:ARG:HG3	1.86	0.74
4:D:1009:LEU:HD12	4:D:1146:GLN:HG3	1.68	0.74
4:D:644:THR:HA	4:D:647:GLU:OE1	1.88	0.74
2:T:264:LEU:HB3	2:T:269:VAL:CG2	2.18	0.74
3:C:215:VAL:HG12	3:C:217:ILE:CG2	2.17	0.74
4:D:487:LEU:HG	4:D:491:ILE:HD12	1.70	0.74
3:C:249:MET:O	3:C:253:LEU:HD23	1.87	0.74
7:O:19:DA:H2"	7:O:20:DT:O5'	1.87	0.74
4:D:111:PRO:O	4:D:113:ARG:NH1	2.20	0.74
6:F:253:MET:CE	6:F:297:MET:HA	2.18	0.74
3:C:773:ALA:O	3:C:782:ARG:NH2	2.21	0.74
7:O:14:DG:H2"	7:O:15:DT:OP2	1.86	0.74
3:C:1108:ILE:H	3:C:1108:ILE:HD12	1.52	0.73
3:C:982:SER:HB3	3:C:983:THR:CG2	2.16	0.73
4:D:1069:PRO:HG2	4:D:1073:GLY:H	1.53	0.73
4:D:647:GLU:HB2	4:D:655:TRP:CZ3	2.23	0.73
2:A:14:VAL:HG13	2:A:18:ARG:HG3	1.68	0.73
3:C:426:GLN:HE21	3:C:451:PRO:HD3	1.53	0.73
3:C:578:VAL:HG13	3:C:582:THR:HB	1.69	0.73
3:C:636:ASP:N	3:C:636:ASP:OD1	2.19	0.73
3:C:845:SER:N	3:C:850:ASP:OD2	2.19	0.73
2:A:14:VAL:HG12	2:A:19:SER:HA	1.69	0.73
4:D:26:GLY:HA3	4:D:51:ILE:CG2	2.18	0.73
4:D:278:ARG:O	4:D:281:ILE:HG13	1.88	0.73
3:C:742:HIS:CD2	3:C:868:ARG:HG3	2.23	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:720:HIS:O	4:D:432:VAL:HG11	1.89	0.73
7:O:15:DT:OP1	2:T:258:VAL:HG21	1.87	0.73
3:C:1018:TYR:O	14:C:1305:HOH:O	2.04	0.73
3:C:205:PHE:HE1	3:C:215:VAL:HG13	1.54	0.73
6:F:253:MET:HE2	6:F:300:GLN:HB2	1.69	0.73
8:P:11:DA:H2"	8:P:12:DA:O5'	1.88	0.73
2:B:24:GLU:OE2	2:B:191:LYS:HD3	1.88	0.73
6:F:320:ILE:HG23	6:F:340:GLU:HG2	1.69	0.73
3:C:496:ARG:NH2	3:C:504:GLU:OE1	2.21	0.73
3:C:87:ILE:HD12	3:C:388:GLU:HG3	1.69	0.73
3:C:593:ALA:HB2	4:D:852:THR:HG22	1.71	0.73
4:D:951:LEU:C	4:D:956:ILE:HD11	2.09	0.73
4:D:962:ARG:NH1	4:D:977:CYS:SG	2.62	0.72
3:C:204:GLU:OE1	3:C:216:ARG:NH1	2.21	0.72
3:C:191:HIS:HA	3:C:192:SER:CB	2.18	0.72
3:C:361:ILE:HD12	3:C:361:ILE:H	1.54	0.72
3:C:754:LYS:HE2	3:C:754:LYS:H	1.55	0.72
4:D:138:SER:HB3	4:D:253:THR:OG1	1.89	0.72
4:D:113:ARG:HB2	4:D:312:MET:HE3	1.70	0.72
4:D:88:ARG:NH1	14:D:2102:HOH:O	2.21	0.72
3:C:936:ASN:HD22	3:C:937:ILE:H	1.37	0.72
2:B:2:LEU:CB	2:B:231:HIS:HA	2.20	0.72
3:C:239:ILE:HG21	3:C:253:LEU:HD22	1.70	0.72
4:D:12:ILE:HD11	4:D:1221:TRP:CD2	2.25	0.72
3:C:47:VAL:HG23	3:C:497:VAL:HG21	1.71	0.72
3:C:52:PHE:HZ	3:C:150:MET:HE2	1.53	0.72
3:C:728:LEU:CD2	3:C:906:ILE:HG22	2.20	0.72
4:D:444:PRO:HG3	4:D:521:ALA:O	1.89	0.72
4:D:796:ASN:HD21	4:D:798:ILE:HB	1.54	0.72
6:F:253:MET:HE3	6:F:297:MET:CA	2.19	0.72
6:F:397:GLN:O	6:F:401:VAL:HG23	1.89	0.72
8:P:11:DA:H2"	8:P:12:DA:C5'	2.20	0.71
3:C:637:LYS:HD2	3:C:659:GLN:NE2	2.03	0.71
4:D:106:TYR:HB3	4:D:312:MET:CE	2.20	0.71
4:D:590:THR:HG21	4:D:630:ARG:HH21	1.55	0.71
3:C:390:VAL:O	3:C:394:ARG:HB2	1.91	0.71
2:A:106:THR:HA	2:A:125:ILE:HD13	1.72	0.71
3:C:482:GLY:O	3:C:485:ILE:HG13	1.90	0.71
3:C:939:VAL:CG2	3:C:940:ALA:HA	2.21	0.71
3:C:982:SER:OG	14:C:1307:HOH:O	2.08	0.71
2:B:26:LEU:HD11	2:B:34:LEU:HD21	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:622:MET:O	14:D:2104:HOH:O	2.07	0.71
2:B:158:GLU:HB3	2:B:161:ARG:HB2	1.72	0.71
3:C:265:LEU:HD11	3:C:287:LEU:HD12	1.72	0.71
4:D:488:GLU:HG3	4:D:516:LEU:HD12	1.72	0.71
7:O:28:DT:H2"	7:O:29:DA:H5'	1.72	0.71
3:C:1130:SER:HB3	3:C:1132:ASP:O	1.90	0.71
3:C:246:SER:CB	3:C:337:VAL:HG11	2.21	0.71
4:D:527:LEU:HD22	4:D:575:ALA:O	1.91	0.70
4:D:155:MET:CE	4:D:219:LEU:HB3	2.21	0.70
4:D:596:THR:HG22	4:D:626:ALA:O	1.91	0.70
3:C:239:ILE:CG2	3:C:253:LEU:HD22	2.21	0.70
3:C:328:ASP:O	3:C:332:THR:HG23	1.91	0.70
3:C:531:VAL:HG13	3:C:552:VAL:CG2	2.21	0.70
3:C:650:THR:HG22	3:C:660:SER:OG	1.90	0.70
4:D:622:MET:CE	4:D:629:VAL:HG22	2.21	0.70
4:D:588:LEU:HD22	4:D:668:GLY:HA3	1.72	0.70
2:B:32:TYR:CB	3:C:1005:ARG:HG3	2.22	0.70
3:C:1045:GLN:HG3	3:C:1090:ARG:HH21	1.55	0.70
3:C:299:LEU:HB3	3:C:323:THR:HA	1.74	0.70
3:C:667:ALA:N	14:C:1303:HOH:O	2.01	0.70
3:C:613:GLU:HB3	3:C:708:LYS:HD3	1.71	0.70
2:A:38:LEU:HD13	2:A:208:LEU:HD11	1.74	0.70
3:C:728:LEU:HB2	3:C:889:ILE:HG12	1.72	0.70
3:C:250:MET:HA	3:C:253:LEU:HD21	1.74	0.70
3:C:754:LYS:H	3:C:754:LYS:CE	2.05	0.70
2:B:32:TYR:CG	3:C:1005:ARG:HG3	2.26	0.70
2:B:181:THR:O	2:B:189:PHE:N	2.23	0.70
3:C:776:ASP:HB2	3:C:777:GLU:OE1	1.92	0.70
2:B:63:PHE:HE2	4:D:603:THR:HG23	1.52	0.70
3:C:1068:GLN:NE2	4:D:1249:LEU:HD13	2.07	0.69
3:C:780:ILE:HD11	3:C:841:ILE:HD13	1.73	0.69
6:F:164:ASP:OD1	6:F:166:VAL:HG22	1.92	0.69
5:E:35:PRO:HG2	5:E:40:LEU:HD11	1.74	0.69
2:B:30:PHE:HA	2:B:33:THR:HG23	1.73	0.69
3:C:981:GLY:O	14:C:1307:HOH:O	2.09	0.69
7:O:6:DA:H2"	7:O:7:DC:H5'	1.73	0.69
2:A:11:GLU:OE1	2:A:205:ARG:NE	2.24	0.69
3:C:727:ILE:HG22	3:C:888:LYS:HB3	1.72	0.69
3:C:910:THR:HG23	4:D:730:VAL:HG23	1.75	0.69
4:D:12:ILE:HD11	4:D:1221:TRP:CE3	2.28	0.69
4:D:139:VAL:HG12	4:D:231:PRO:HD3	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:291:GLN:HG3	6:F:292:ALA:N	2.06	0.69
1:J:91:VAL:HG22	1:J:92:GLU:OE1	1.93	0.69
2:A:158:GLU:H	2:A:161:ARG:HH11	1.41	0.69
2:B:182:ARG:N	2:B:186:ARG:O	2.25	0.69
3:C:1100:GLY:HA3	4:D:458:LYS:HE3	1.75	0.69
3:C:494:TYR:HD2	3:C:572:VAL:HG21	1.57	0.69
3:C:45:LEU:HD12	3:C:628:ASP:O	1.92	0.69
4:D:344:TYR:O	4:D:348:ILE:HG22	1.92	0.69
3:C:1026:HIS:HB3	3:C:1031:LYS:HE3	1.75	0.69
4:D:1166:VAL:HA	4:D:1207:VAL:HG23	1.75	0.69
4:D:599:TYR:CB	4:D:610:GLY:HA3	2.23	0.69
4:D:795:ASP:O	14:D:2105:HOH:O	2.10	0.69
3:C:444:ARG:NH2	3:C:492:SER:O	2.26	0.69
3:C:508:ARG:HD3	3:C:515:VAL:CG1	2.23	0.69
4:D:668:GLY:HA2	4:D:671:MET:CE	2.23	0.69
5:E:26:TYR:HE1	5:E:29:PRO:HD3	1.58	0.69
4:D:1115:GLY:N	14:D:2110:HOH:O	2.22	0.68
4:D:1174:THR:HA	4:D:1175:GLU:CB	2.22	0.68
4:D:708:VAL:O	4:D:712:VAL:HG23	1.93	0.68
1:J:79:ARG:NH2	7:O:25:DC:OP1	2.27	0.68
3:C:1045:GLN:HG2	3:C:1087:THR:HG22	1.75	0.68
3:C:718:GLU:H	4:D:724:THR:CG2	2.05	0.68
2:B:74:THR:HG21	4:D:611:VAL:HG11	1.73	0.68
4:D:780:ALA:O	4:D:784:VAL:HG22	1.93	0.68
8:P:13:DC:H2"	8:P:14:DA:C8	2.29	0.68
2:A:33:THR:HG21	2:B:37:SER:HA	1.76	0.68
3:C:507:TYR:OH	3:C:527:GLU:OE2	2.11	0.68
4:D:238:GLU:HA	4:D:241:TYR:HB3	1.74	0.68
3:C:1103:ILE:HD12	4:D:548:SER:HA	1.76	0.68
7:O:24:DG:OP2	14:O:101:HOH:O	2.11	0.68
4:D:578:ARG:HB2	11:D:2008:EDO:C2	2.24	0.68
6:F:330:ARG:NH2	6:F:336:GLU:OE2	2.25	0.68
2:T:256:LEU:HD22	2:T:297:VAL:HG22	1.76	0.68
1:J:89:ARG:NH2	6:F:276:THR:HG23	2.09	0.68
3:C:426:GLN:NE2	3:C:450:GLY:HA2	2.08	0.68
3:C:444:ARG:NH2	3:C:491:LEU:HD23	2.04	0.68
4:D:603:THR:CG2	4:D:604:LYS:HE2	2.23	0.68
4:D:931:ALA:HB1	4:D:932:ASN:HD22	1.59	0.68
3:C:729:SER:OG	3:C:905:ASP:HA	1.94	0.67
4:D:73:ILE:O	4:D:82:VAL:HG12	1.94	0.67
3:C:191:HIS:HB2	3:C:336:LEU:HD21	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:219:MET:HE2	6:F:219:MET:HA	1.77	0.67
2:B:47:PRO:HA	2:B:144:ARG:HG3	1.76	0.67
3:C:467:HIS:CG	3:C:468:PRO:HD2	2.29	0.67
2:B:216:VAL:HG13	2:B:217:GLU:H	1.59	0.67
6:F:399:GLN:O	6:F:403:GLU:HG2	1.94	0.67
2:B:143:GLY:HA3	2:B:168:TYR:CD1	2.30	0.67
6:F:254:ALA:HA	10:F:502:SO4:O3	1.94	0.67
4:D:648:ALA:O	4:D:652:GLU:HB2	1.94	0.67
4:D:1168:ILE:O	4:D:1178:PRO:HA	1.95	0.67
4:D:1232:ARG:NH1	4:D:1236:ASP:OD2	2.27	0.67
6:F:308:VAL:N	14:F:601:HOH:O	2.27	0.67
3:C:872:ASP:N	3:C:872:ASP:OD1	2.17	0.67
4:D:137:THR:HG22	4:D:253:THR:O	1.93	0.67
5:E:57:ARG:NE	5:E:95:GLU:OE1	2.23	0.67
2:A:89:ASP:CB	2:A:90:ASP:CA	2.73	0.67
2:A:40:ARG:NH1	2:B:33:THR:HG22	2.10	0.67
3:C:102:ARG:NH2	3:C:127:THR:OG1	2.27	0.67
4:D:108:LYS:HG3	4:D:108:LYS:O	1.94	0.67
3:C:44:LEU:HD13	3:C:440:LEU:HD21	1.75	0.66
1:J:42:VAL:HG13	4:D:74:ILE:HD12	1.75	0.66
2:B:3:ILE:HA	2:B:232:ILE:CB	2.25	0.66
4:D:106:TYR:HB3	4:D:312:MET:HE3	1.77	0.66
4:D:627:LEU:HD13	4:D:667:LEU:HD12	1.77	0.66
2:A:94:THR:HG22	2:A:139:VAL:HG22	1.76	0.66
3:C:772:LEU:HA	3:C:775:LEU:HD22	1.78	0.66
4:D:889:ASP:OD2	4:D:891:GLU:N	2.28	0.66
2:A:177:LYS:HE2	2:A:193:ILE:CD1	2.25	0.66
3:C:44:LEU:CD1	3:C:440:LEU:HD21	2.25	0.66
3:C:454:LEU:HD22	3:C:459:ALA:CB	2.24	0.66
3:C:799:PRO:CA	3:C:823:VAL:HG12	2.21	0.66
4:D:230:ALA:N	4:D:233:GLN:OE1	2.25	0.66
4:D:527:LEU:HD21	4:D:581:MET:CE	2.25	0.66
6:F:338:ALA:HB1	6:F:343:ILE:O	1.95	0.66
3:C:176:VAL:HG12	3:C:195:VAL:CG2	2.21	0.66
3:C:148:PHE:CE1	3:C:380:ILE:HD11	2.31	0.66
3:C:613:GLU:O	3:C:705:ALA:HB1	1.96	0.66
4:D:980:ARG:HD3	4:D:985:GLY:O	1.96	0.66
2:A:42:LEU:O	2:A:171:VAL:HG11	1.96	0.66
2:A:66:VAL:HB	2:A:69:VAL:HG21	1.76	0.66
4:D:237:ASP:OD1	4:D:239:VAL:HG13	1.96	0.66
4:D:642:PRO:CD	4:D:656:LYS:HG2	2.26	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:24:GLU:CD	2:A:191:LYS:HD3	2.16	0.66
3:C:77:LEU:CD1	3:C:124:LEU:HD11	2.25	0.66
2:A:177:LYS:HE2	2:A:193:ILE:HD11	1.77	0.66
3:C:203:LEU:HD13	3:C:217:ILE:HG22	1.78	0.66
3:C:250:MET:HA	3:C:253:LEU:CD2	2.26	0.66
3:C:533:ALA:HB2	3:C:567:VAL:HG11	1.78	0.66
3:C:732:LEU:HA	3:C:737:VAL:CG1	2.26	0.66
3:C:851:GLU:O	3:C:852:LEU:HG	1.96	0.66
4:D:878:ASP:OD2	4:D:1250:LYS:NZ	2.29	0.66
4:D:881:GLN:HE22	4:D:1250:LYS:HE2	1.61	0.66
4:D:320:ILE:HG12	4:D:321:PRO:HD2	1.78	0.66
4:D:647:GLU:HG2	4:D:648:ALA:N	2.11	0.66
3:C:1086:ASP:O	3:C:1090:ARG:HG2	1.96	0.65
3:C:1045:GLN:HG3	3:C:1090:ARG:NH2	2.10	0.65
3:C:685:GLN:OE1	14:C:1308:HOH:O	2.15	0.65
4:D:665:THR:HG22	4:D:684:ASN:ND2	2.12	0.65
5:E:40:LEU:HB3	5:E:50:LEU:HD11	1.79	0.65
3:C:721:ASN:HD22	3:C:727:ILE:HD11	1.62	0.65
4:D:1174:THR:CG2	4:D:1176:PHE:HB2	2.26	0.65
4:D:193:VAL:O	4:D:197:VAL:HG23	1.96	0.65
4:D:59:GLU:OE2	4:D:66:LYS:NZ	2.29	0.65
4:D:826:PRO:HD3	4:D:853:HIS:ND1	2.12	0.65
4:D:1100:LEU:HD23	4:D:1101:SER:N	2.11	0.65
4:D:599:TYR:CZ	4:D:601:ALA:HB2	2.31	0.65
2:B:105:VAL:HB	2:B:125:ILE:HG23	1.79	0.65
3:C:685:GLN:HB3	14:C:1308:HOH:O	1.96	0.65
3:C:712:VAL:HB	3:C:906:ILE:HD11	1.78	0.65
2:A:33:THR:CG2	2:B:37:SER:HA	2.27	0.65
2:B:79:ASN:OD1	4:D:636:ARG:NH2	2.26	0.65
3:C:236:ASN:OD1	3:C:253:LEU:HD13	1.96	0.65
3:C:796:LYS:HB3	3:C:826:THR:O	1.96	0.65
4:D:218:ARG:O	4:D:222:ILE:HG13	1.95	0.65
5:E:29:PRO:HG2	5:E:34:ASN:HB2	1.78	0.65
3:C:575:ARG:HE	3:C:967:VAL:HG22	1.61	0.65
3:C:710:LEU:HD13	3:C:1021:ILE:HG12	1.78	0.65
4:D:438:LEU:HA	4:D:525:HIS:CD2	2.31	0.65
3:C:1028:VAL:O	3:C:1032:ILE:HG22	1.97	0.65
2:B:32:TYR:CE1	2:B:178:VAL:HG21	2.31	0.65
3:C:531:VAL:HG13	3:C:552:VAL:HG23	1.79	0.65
3:C:771:VAL:HG23	3:C:772:LEU:CD1	2.27	0.65
6:F:253:MET:HE1	6:F:300:GLN:HB2	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:157:ALA:CB	2:A:161:ARG:HD2	2.27	0.64
3:C:1098:VAL:HG11	4:D:469:ILE:HD12	1.78	0.64
6:F:181:ALA:O	6:F:185:VAL:HG23	1.97	0.64
1:J:64:LEU:HD22	1:J:66:GLU:H	1.61	0.64
3:C:338:ARG:HD3	3:C:343:GLN:NE2	2.11	0.64
4:D:642:PRO:HG3	4:D:661:TRP:CD2	2.31	0.64
4:D:6:PHE:CD1	4:D:1257:LYS:HE3	2.33	0.64
4:D:706:ILE:HD12	5:E:36:PRO:HB3	1.78	0.64
4:D:177:LEU:HD23	4:D:177:LEU:O	1.98	0.64
4:D:726:SER:OG	4:D:728:VAL:HG23	1.96	0.64
2:A:14:VAL:CG1	2:A:18:ARG:HG3	2.28	0.64
3:C:846:ARG:N	3:C:857:ASN:O	2.28	0.64
4:D:527:LEU:HD21	4:D:581:MET:HE1	1.78	0.64
3:C:135:THR:HG23	3:C:137:GLU:H	1.63	0.64
6:F:462:ARG:NH1	6:F:465:LEU:HD12	2.13	0.64
4:D:661:TRP:HZ3	4:D:663:ALA:HB2	1.63	0.64
4:D:400:LYS:HE3	4:D:404:ASP:HB3	1.80	0.64
4:D:846:LEU:O	4:D:850:ILE:HG12	1.98	0.64
6:F:289:ILE:O	6:F:293:ILE:HG13	1.98	0.64
4:D:924:LEU:HD21	4:D:943:LEU:HD11	1.79	0.64
2:B:144:ARG:HB2	2:B:144:ARG:NH1	2.13	0.64
4:D:1119:PRO:HA	4:D:1122:VAL:CG1	2.27	0.63
4:D:190:LYS:HE3	4:D:193:VAL:HG23	1.80	0.63
4:D:144:ARG:NH2	4:D:229:LEU:O	2.32	0.63
4:D:638:THR:HA	4:D:659:ASP:O	1.98	0.63
4:D:1168:ILE:HD13	4:D:1176:PHE:CB	2.28	0.63
4:D:139:VAL:CG1	4:D:231:PRO:HD3	2.28	0.63
2:A:177:LYS:HG2	2:A:193:ILE:HD11	1.81	0.63
3:C:235:THR:N	3:C:238:GLN:OE1	2.31	0.63
6:F:451:LYS:O	6:F:454:HIS:HB3	1.99	0.63
2:A:48:GLY:HA2	2:A:49:ALA:CB	2.28	0.63
3:C:876:LEU:HD11	3:C:886:ILE:CD1	2.29	0.63
3:C:937:ILE:CB	3:C:939:VAL:HG12	2.27	0.63
4:D:31:PRO:HB2	4:D:345:ARG:HG2	1.80	0.63
4:D:755:ILE:HD12	4:D:776:ILE:HD11	1.79	0.63
2:A:36:ASN:HB2	2:A:176:TYR:OH	1.99	0.63
2:B:95:MET:HG2	2:B:113:PRO:CD	2.28	0.63
2:B:43:LEU:HD12	2:B:171:VAL:HG23	1.81	0.63
3:C:250:MET:O	3:C:253:LEU:HG	1.99	0.63
4:D:21:ARG:NE	4:D:96:GLU:OE2	2.27	0.63
3:C:176:VAL:HG22	3:C:307:VAL:HG12	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:1275:PRO:HG3	5:E:76:VAL:CG1	2.20	0.63
3:C:1072:ALA:HB1	4:D:554:GLU:OE2	1.99	0.63
6:F:204:LEU:O	6:F:208:GLY:N	2.32	0.63
3:C:792:ILE:HD12	3:C:792:ILE:H	1.64	0.63
3:C:727:ILE:HG13	3:C:907:ILE:HB	1.80	0.62
3:C:1048:LEU:HD23	3:C:1048:LEU:N	2.12	0.62
4:D:1188:GLU:O	4:D:1192:ARG:HG3	1.99	0.62
4:D:956:ILE:HD12	4:D:956:ILE:O	1.99	0.62
6:F:444:ILE:O	6:F:448:THR:HG23	1.99	0.62
2:B:30:PHE:HA	2:B:33:THR:CG2	2.29	0.62
2:B:85:VAL:HG23	2:B:117:THR:O	1.98	0.62
4:D:102:THR:HG23	4:D:258:ALA:HB2	1.81	0.62
4:D:238:GLU:OE2	4:D:242:ARG:NH2	2.31	0.62
4:D:275:GLU:HA	4:D:278:ARG:HB2	1.81	0.62
2:B:198:THR:HG21	2:B:202:ILE:HD12	1.81	0.62
2:B:50:ALA:HB3	2:B:168:TYR:HD2	1.63	0.62
3:C:302:VAL:HG11	3:C:368:ARG:HD3	1.81	0.62
4:D:1114:GLU:HG3	14:D:2110:HOH:O	2.00	0.62
4:D:578:ARG:HB2	11:D:2008:EDO:H21	1.81	0.62
3:C:876:LEU:HD13	3:C:886:ILE:HG13	1.81	0.62
4:D:614:SER:HB2	4:D:615:PRO:HD2	1.80	0.62
7:O:19:DA:H4'	7:O:20:DT:OP1	1.98	0.62
3:C:299:LEU:HD12	3:C:299:LEU:O	2.00	0.62
4:D:1171:SER:HA	4:D:1174:THR:HG22	1.79	0.62
1:J:45:ALA:HB2	4:D:73:ILE:HD12	1.80	0.62
8:P:11:DA:H4'	8:P:12:DA:OP1	1.99	0.62
3:C:766:ASN:O	3:C:767:VAL:HG13	2.00	0.62
3:C:876:LEU:CD1	3:C:886:ILE:HG13	2.29	0.62
4:D:1249:LEU:HD12	4:D:1250:LYS:N	2.15	0.62
4:D:363:PRO:HB2	4:D:365:ILE:CD1	2.30	0.62
4:D:602:ALA:HB3	4:D:607:PRO:O	2.00	0.62
3:C:765:PRO:HD2	3:C:825:ASP:HB2	1.81	0.61
4:D:190:LYS:NZ	4:D:192:ASP:HB3	2.15	0.61
4:D:622:MET:HE1	4:D:629:VAL:HG22	1.82	0.61
1:J:47:ASP:N	1:J:47:ASP:OD1	2.19	0.61
2:A:158:GLU:H	2:A:161:ARG:NH1	1.97	0.61
2:B:120:ASN:ND2	2:B:123:MET:SD	2.72	0.61
3:C:215:VAL:HG12	3:C:217:ILE:HG23	1.82	0.61
2:T:279:THR:HG23	2:T:282:ASP:CB	2.29	0.61
3:C:714:ILE:HG22	3:C:714:ILE:O	2.00	0.61
6:F:180:ASN:OD1	6:F:183:GLU:HG3	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:74:LYS:O	1:J:74:LYS:HG3	2.01	0.61
3:C:348:VAL:HB	3:C:351:GLY:CA	2.30	0.61
3:C:876:LEU:HD11	3:C:886:ILE:HD11	1.82	0.61
3:C:477:ILE:CD1	4:D:852:THR:HG21	2.30	0.61
4:D:647:GLU:HB2	4:D:655:TRP:CH2	2.36	0.61
4:D:676:LEU:HD12	4:D:676:LEU:N	2.16	0.61
1:J:44:PHE:HE2	4:D:76:GLU:HA	1.66	0.61
4:D:785:GLY:O	4:D:789:GLU:HG3	1.99	0.61
1:J:98:LEU:O	1:J:102:LEU:HD13	1.99	0.61
3:C:231:ALA:HB1	3:C:265:LEU:HD13	1.80	0.61
2:A:138:LEU:N	2:A:138:LEU:HD12	2.15	0.61
2:B:74:THR:CG2	4:D:611:VAL:HG11	2.30	0.61
3:C:32:PHE:O	3:C:34:LYS:HD2	2.01	0.61
4:D:957:THR:O	4:D:958:THR:HG23	2.01	0.61
2:A:3:ILE:O	2:A:3:ILE:HG13	1.99	0.61
3:C:302:VAL:O	3:C:306:LYS:HG2	2.01	0.61
4:D:88:ARG:HD2	14:D:2102:HOH:O	2.00	0.61
5:E:80:VAL:HG12	5:E:81:GLU:N	2.15	0.61
5:E:80:VAL:HG12	5:E:81:GLU:H	1.65	0.61
6:F:324:LEU:HD22	6:F:332:PRO:HB3	1.82	0.61
3:C:132:ASN:CB	3:C:135:THR:HG22	2.29	0.61
3:C:732:LEU:HD22	3:C:737:VAL:HG11	1.83	0.61
3:C:795:GLY:HA2	3:C:827:SER:OG	2.01	0.61
2:A:40:ARG:NH2	3:C:894:ASP:OD2	2.34	0.61
4:D:1089:VAL:HG13	4:D:1098:GLY:C	2.21	0.61
4:D:137:THR:HG22	4:D:253:THR:C	2.21	0.61
2:A:99:LYS:HE3	2:A:109:ASP:CG	2.22	0.61
2:A:113:PRO:HD2	2:A:116:VAL:HG21	1.83	0.61
1:J:95:GLU:OE1	1:J:95:GLU:HA	2.01	0.61
2:A:210:SER:HB3	2:B:229:SER:HB2	1.83	0.60
3:C:421:PHE:O	3:C:425:SER:HB3	2.01	0.60
4:D:275:GLU:O	4:D:278:ARG:N	2.34	0.60
2:B:39:ARG:NH2	4:D:623:ASP:OD2	2.34	0.60
6:F:176:VAL:HG12	6:F:177:ALA:N	2.16	0.60
6:F:219:MET:HA	6:F:219:MET:CE	2.31	0.60
6:F:293:ILE:O	6:F:297:MET:HG3	2.01	0.60
8:P:17:DT:O5'	2:T:290:GLY:HA3	2.00	0.60
2:A:24:GLU:OE1	2:A:191:LYS:HD3	2.01	0.60
2:B:213:GLY:HA2	2:B:216:VAL:HG12	1.83	0.60
2:B:76:ILE:HA	2:B:79:ASN:HB2	1.83	0.60
3:C:216:ARG:HG2	3:C:221:ARG:HA	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:745:GLU:OE2	3:C:861:ARG:HD2	2.02	0.60
4:D:594:GLY:HA2	4:D:598:GLU:OE1	2.01	0.60
4:D:612:TYR:HB2	4:D:635:VAL:CG1	2.31	0.60
4:D:622:MET:HE3	4:D:667:LEU:HD13	1.84	0.60
6:F:272:LYS:HE3	7:O:25:DC:OP1	2.01	0.60
3:C:363:HIS:NE2	3:C:528:ASP:OD2	2.34	0.60
3:C:38:PRO:HB3	3:C:508:ARG:HH21	1.66	0.60
3:C:584:MET:HA	3:C:619:THR:CG2	2.28	0.60
1:J:96:GLU:O	1:J:100:GLU:HG3	2.02	0.60
2:B:21:PHE:HB2	2:B:194:ILE:CG2	2.30	0.60
3:C:480:PRO:O	3:C:485:ILE:HG12	2.02	0.60
2:B:200:ASN:ND2	2:B:200:ASN:H	2.00	0.60
4:D:1079:ASP:N	4:D:1079:ASP:OD1	2.34	0.60
4:D:920:PHE:CE2	4:D:948:ILE:HG13	2.35	0.60
3:C:712:VAL:HA	3:C:906:ILE:HG13	1.84	0.60
3:C:1034:ALA:HB2	4:D:447:MET:HG3	1.84	0.60
3:C:394:ARG:HG3	3:C:398:GLN:HG3	1.84	0.59
3:C:983:THR:OG1	14:C:1306:HOH:O	2.08	0.59
3:C:998:LYS:NZ	4:D:734:ASP:OD2	2.30	0.59
3:C:982:SER:CB	3:C:983:THR:HG23	2.23	0.59
4:D:1171:SER:CB	4:D:1174:THR:HG22	2.31	0.59
4:D:846:LEU:HD12	4:D:846:LEU:H	1.66	0.59
6:F:462:ARG:HH12	6:F:465:LEU:HD12	1.66	0.59
1:J:82:TRP:CE2	6:F:199:GLN:HG2	2.37	0.59
2:B:101:GLY:N	2:B:132:GLY:O	2.35	0.59
3:C:710:LEU:CD2	3:C:1021:ILE:HD11	2.28	0.59
4:D:435:GLN:OE1	4:D:435:GLN:N	2.30	0.59
2:B:85:VAL:HG23	2:B:117:THR:C	2.23	0.59
2:B:52:THR:OG1	2:B:141:GLU:HG2	2.02	0.59
2:B:183:VAL:O	2:B:183:VAL:HG12	2.03	0.59
2:B:212:GLY:O	2:B:216:VAL:HG12	2.02	0.59
2:B:22:VAL:CG1	2:B:193:ILE:HD12	2.32	0.59
3:C:338:ARG:HB3	3:C:343:GLN:HE21	1.68	0.59
3:C:556:GLY:N	3:C:557:GLY:HA2	2.17	0.59
3:C:973:GLU:CA	4:D:732:MET:HE1	2.31	0.59
4:D:1062:PHE:CD2	4:D:1080:LYS:HD2	2.38	0.59
4:D:453:LYS:HB3	4:D:454:PRO:HD3	1.85	0.59
4:D:622:MET:CE	4:D:667:LEU:HD13	2.32	0.59
6:F:321:GLN:O	6:F:325:LEU:HB2	2.02	0.59
2:A:14:VAL:HG13	2:A:15:ALA:H	1.66	0.59
3:C:751:ARG:HG2	3:C:856:VAL:HG22	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:6:PHE:HD1	4:D:1257:LYS:HE3	1.67	0.59
5:E:85:GLN:H	5:E:85:GLN:NE2	1.97	0.59
2:A:106:THR:CA	2:A:125:ILE:HD13	2.32	0.59
7:O:6:DA:C2'	7:O:7:DC:H5'	2.32	0.59
3:C:1116:LEU:O	3:C:1120:GLN:HG3	2.03	0.59
3:C:751:ARG:NH1	4:D:332:GLY:O	2.36	0.59
3:C:1028:VAL:HG12	4:D:429:VAL:HG12	1.85	0.59
4:D:585:LEU:HD12	4:D:692:GLN:NE2	2.17	0.59
4:D:850:ILE:O	4:D:853:HIS:HB2	2.02	0.59
6:F:176:VAL:HG12	6:F:177:ALA:H	1.67	0.59
4:D:334:ARG:HD3	6:F:356:ARG:HH21	1.68	0.59
3:C:150:MET:HA	3:C:150:MET:CE	2.33	0.59
3:C:736:ASP:OD1	3:C:869:LYS:HE2	2.03	0.59
4:D:1054:VAL:HG12	4:D:1104:ASP:O	2.03	0.59
3:C:203:LEU:HD22	3:C:217:ILE:HG22	1.85	0.58
4:D:1121:GLU:OE2	4:D:1124:ARG:NH2	2.29	0.58
4:D:58:TRP:CD2	4:D:68:VAL:HG22	2.38	0.58
2:A:40:ARG:HD3	2:B:33:THR:CG2	2.33	0.58
2:B:198:THR:CG2	2:B:202:ILE:HD12	2.32	0.58
3:C:434:ASN:O	3:C:608:PRO:HD3	2.03	0.58
3:C:768:SER:O	3:C:771:VAL:HG22	2.04	0.58
4:D:745:LEU:O	4:D:749:GLU:HG2	2.02	0.58
2:A:199:LYS:O	2:A:200:ASN:HB2	2.03	0.58
2:A:89:ASP:CB	2:A:142:ARG:HD2	2.33	0.58
3:C:937:ILE:HA	3:C:938:ASP:CB	2.33	0.58
2:A:30:PHE:CE1	2:B:40:ARG:HG3	2.38	0.58
3:C:338:ARG:CD	3:C:346:MET:HG3	2.29	0.58
3:C:335:TYR:CE1	3:C:356:VAL:HG13	2.38	0.58
2:B:167:ILE:HD11	4:D:617:GLU:HG3	1.84	0.58
4:D:436:LEU:O	4:D:716:LYS:NZ	2.35	0.58
4:D:743:GLU:O	4:D:747:ARG:HG3	2.04	0.58
6:F:345:PRO:HA	6:F:348:VAL:CG1	2.33	0.58
2:B:151:GLN:CG	2:B:154:ALA:HB1	2.34	0.58
3:C:986:ASN:OD1	3:C:986:ASN:N	2.31	0.58
4:D:673:ASN:HA	4:D:676:LEU:HD13	1.84	0.58
3:C:910:THR:CG2	4:D:730:VAL:HG23	2.34	0.58
3:C:224:PRO:HB2	3:C:227:VAL:HG13	1.86	0.58
3:C:498:ASN:OD1	3:C:499:PRO:HD2	2.03	0.58
3:C:783:ILE:HG13	3:C:841:ILE:HD12	1.85	0.58
3:C:229:LEU:HD12	3:C:229:LEU:O	2.04	0.58
4:D:17:ALA:O	4:D:21:ARG:HG3	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:32:PHE:HE1	3:C:963:VAL:CG1	2.16	0.58
3:C:166:VAL:HG11	3:C:372:VAL:HG23	1.86	0.58
3:C:510:VAL:HG12	3:C:568:ASP:C	2.24	0.58
3:C:712:VAL:HG11	3:C:925:THR:HG23	1.85	0.58
3:C:412:ARG:HD2	6:F:322:ARG:NE	2.18	0.58
3:C:578:VAL:HG12	3:C:579:SER:O	2.03	0.58
3:C:590:HIS:O	3:C:919:ILE:HD11	2.04	0.58
4:D:930:ASP:HB3	4:D:954:ALA:HB1	1.85	0.58
6:F:253:MET:HE3	6:F:297:MET:N	2.19	0.58
3:C:509:LYS:HA	3:C:569:TYR:HA	1.85	0.58
4:D:1231:THR:O	4:D:1235:THR:HG23	2.03	0.58
4:D:723:ALA:O	4:D:726:SER:HB3	2.03	0.58
5:E:84:LEU:HB2	5:E:85:GLN:HE21	1.69	0.58
6:F:402:LEU:HD23	6:F:414:ARG:HE	1.68	0.58
2:A:100:GLN:OE1	2:A:101:GLY:N	2.31	0.57
2:B:34:LEU:HD12	2:B:35:GLY:N	2.19	0.57
4:D:1041:PRO:HB3	4:D:1116:ALA:HB3	1.85	0.57
4:D:269:ASP:HB3	4:D:272:ALA:CB	2.32	0.57
4:D:641:ARG:NE	4:D:655:TRP:HZ2	2.02	0.57
4:D:982:MET:HE2	4:D:1153:LYS:HE3	1.85	0.57
4:D:988:VAL:HG23	4:D:992:GLU:HG3	1.85	0.57
7:O:6:DA:H1'	7:O:7:DC:H5'	1.86	0.57
3:C:1026:HIS:HB3	3:C:1031:LYS:CE	2.32	0.57
3:C:649:ILE:HG21	3:C:693:ILE:HG21	1.86	0.57
4:D:460:LEU:HD11	4:D:472:ALA:HB1	1.86	0.57
2:T:256:LEU:CD2	2:T:297:VAL:HG22	2.34	0.57
3:C:534:GLN:NE2	4:D:846:LEU:HD11	2.19	0.57
4:D:248:TYR:HA	4:D:251:TYR:CD2	2.39	0.57
3:C:742:HIS:HD2	3:C:868:ARG:HG3	1.66	0.57
2:B:162:ILE:HG23	4:D:607:PRO:HG2	1.85	0.57
2:A:50:ALA:HB3	2:A:168:TYR:CD1	2.39	0.57
2:A:93:VAL:HG22	2:A:113:PRO:HG3	1.87	0.57
3:C:221:ARG:HG3	3:C:222:ARG:HG3	1.87	0.57
3:C:506:PRO:HB2	3:C:572:VAL:HG11	1.86	0.57
3:C:748:ILE:O	3:C:859:LEU:HD23	2.04	0.57
4:D:273:GLU:O	4:D:277:LEU:HB2	2.05	0.57
6:F:345:PRO:O	6:F:348:VAL:HG13	2.04	0.57
2:A:79:ASN:O	2:A:123:MET:HE1	2.03	0.57
2:A:9:LEU:HD13	2:A:23:ILE:CG1	2.34	0.57
3:C:203:LEU:HD22	3:C:217:ILE:CB	2.35	0.57
3:C:368:ARG:HB3	3:C:501:GLY:O	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:522:LEU:HB3	3:C:526:GLU:HG3	1.86	0.57
4:D:155:MET:HE3	4:D:219:LEU:HB3	1.85	0.57
1:J:68:ASP:HA	1:J:69:VAL:CB	2.34	0.57
2:B:97:LEU:HB3	2:B:136:VAL:CG1	2.35	0.57
3:C:540:ASP:O	3:C:543:GLY:N	2.32	0.57
3:C:710:LEU:HD13	3:C:1021:ILE:CG1	2.35	0.57
3:C:984:LEU:HD13	3:C:989:GLY:O	2.04	0.57
4:D:143:MET:CE	4:D:251:TYR:HA	2.34	0.57
2:A:112:PRO:HB2	2:A:116:VAL:HG23	1.86	0.57
2:A:85:VAL:HG22	2:A:86:SER:H	1.70	0.57
2:B:144:ARG:HH11	2:B:144:ARG:HB2	1.70	0.57
10:C:1203:SO4:O1	4:D:540:GLN:NE2	2.37	0.57
3:C:505:THR:CG2	3:C:506:PRO:HD2	2.35	0.57
3:C:38:PRO:HB3	3:C:508:ARG:NH2	2.20	0.57
3:C:575:ARG:NH2	3:C:966:PRO:HB2	2.19	0.57
4:D:368:ASN:ND2	14:D:2116:HOH:O	2.37	0.57
2:A:9:LEU:HD23	2:B:221:LEU:O	2.05	0.57
3:C:476:PRO:O	4:D:856:ARG:NH2	2.35	0.57
3:C:52:PHE:CZ	3:C:150:MET:HE2	2.37	0.57
3:C:763:ASP:CB	3:C:821:ARG:HH22	2.16	0.57
5:E:76:VAL:HG13	5:E:77:GLY:N	2.20	0.57
3:C:984:LEU:HB2	3:C:985:PRO:CA	2.33	0.57
4:D:1009:LEU:HB3	4:D:1029:LEU:HD13	1.87	0.57
4:D:641:ARG:CZ	4:D:655:TRP:HZ2	2.17	0.57
4:D:781:THR:HG22	4:D:814:ARG:HD2	1.87	0.57
4:D:885:VAL:O	4:D:990:ILE:O	2.23	0.57
8:P:3:DC:H2"	8:P:4:DA:C8	2.40	0.57
2:A:197:GLU:OE1	3:C:987:ARG:NH1	2.36	0.56
2:A:8:THR:OG1	2:A:24:GLU:O	2.13	0.56
2:B:210:SER:O	2:B:214:THR:HG23	2.05	0.56
2:B:41:THR:O	2:B:45:SER:HB3	2.05	0.56
3:C:510:VAL:HG11	3:C:567:VAL:HB	1.86	0.56
4:D:924:LEU:HD22	4:D:959:VAL:CG1	2.35	0.56
3:C:717:TRP:HH2	3:C:1005:ARG:NH2	2.03	0.56
3:C:1045:GLN:HG2	3:C:1087:THR:CG2	2.34	0.56
3:C:299:LEU:HD12	3:C:299:LEU:C	2.26	0.56
4:D:661:TRP:CZ3	4:D:663:ALA:HB2	2.38	0.56
6:F:317:LEU:HD21	6:F:337:LEU:HG	1.87	0.56
2:A:85:VAL:HG22	2:A:86:SER:N	2.19	0.56
2:A:99:LYS:HE3	2:A:109:ASP:OD1	2.05	0.56
2:B:180:ALA:HA	2:B:189:PHE:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:873:GLY:HA3	3:C:1028:VAL:HG11	1.87	0.56
3:C:45:LEU:HD21	3:C:443:LYS:HD2	1.86	0.56
3:C:966:PRO:HG2	3:C:969:ASP:O	2.05	0.56
2:B:213:GLY:HA2	2:B:216:VAL:CG1	2.36	0.56
4:D:735:VAL:HG22	4:D:798:ILE:HD11	1.87	0.56
2:B:143:GLY:HA3	2:B:168:TYR:CE1	2.41	0.56
2:B:76:ILE:HG23	2:B:125:ILE:CD1	2.35	0.56
3:C:805:LEU:HD12	3:C:809:GLU:CD	2.25	0.56
4:D:1168:ILE:CD1	4:D:1176:PHE:HB3	2.35	0.56
1:J:89:ARG:NH2	6:F:274:ASP:OD1	2.26	0.56
3:C:649:ILE:HD13	3:C:693:ILE:HG22	1.87	0.56
3:C:891:PRO:HB2	3:C:893:GLU:CG	2.34	0.56
4:D:1132:GLN:HE21	4:D:1163:LEU:HD12	1.71	0.56
3:C:1029:ASP:OD1	4:D:520:LYS:HD2	2.06	0.56
2:A:211:ALA:O	2:A:215:LEU:N	2.36	0.56
3:C:572:VAL:HG22	3:C:576:GLN:CD	2.26	0.56
3:C:721:ASN:HD22	3:C:727:ILE:CD1	2.18	0.56
3:C:973:GLU:HA	4:D:732:MET:HE1	1.86	0.56
4:D:1088:ARG:HG2	4:D:1089:VAL:N	2.18	0.56
4:D:240:LEU:HD23	4:D:244:LEU:HG	1.86	0.56
5:E:26:TYR:CE1	5:E:29:PRO:HD3	2.40	0.56
4:D:706:ILE:HD11	5:E:36:PRO:HA	1.87	0.56
2:B:105:VAL:HG23	2:B:128:LEU:CD1	2.35	0.56
3:C:171:VAL:N	3:C:368:ARG:O	2.38	0.56
4:D:203:ARG:HA	4:D:203:ARG:NE	2.20	0.56
4:D:1275:PRO:CG	5:E:76:VAL:HG11	2.23	0.56
3:C:771:VAL:HG23	3:C:772:LEU:HD12	1.86	0.56
4:D:653:ASN:HB2	4:D:654:GLY:CA	2.35	0.56
4:D:753:ASP:O	4:D:757:ARG:N	2.38	0.56
4:D:901:ALA:HB1	4:D:910:ILE:O	2.06	0.56
6:F:449:MET:O	6:F:453:ARG:HG3	2.06	0.56
6:F:465:LEU:HD23	6:F:466:ASP:N	2.21	0.56
2:T:251:ILE:O	2:T:254:LEU:HG	2.06	0.56
3:C:937:ILE:CA	3:C:938:ASP:CB	2.84	0.56
4:D:170:LEU:HD13	4:D:209:ARG:NH2	2.21	0.56
6:F:438:ARG:NH1	8:P:20:DG:N7	2.53	0.56
2:A:8:THR:O	2:A:23:ILE:HA	2.06	0.55
2:B:50:ALA:HB3	2:B:168:TYR:CD2	2.41	0.55
3:C:369:LEU:HB3	3:C:501:GLY:O	2.06	0.55
3:C:549:ARG:HB2	3:C:561:PHE:CE2	2.41	0.55
3:C:680:ILE:HD11	3:C:692:VAL:O	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:270:ILE:O	4:D:274:ALA:N	2.38	0.55
4:D:924:LEU:CD2	4:D:959:VAL:HG11	2.36	0.55
3:C:549:ARG:HA	3:C:563:SER:HA	1.88	0.55
6:F:338:ALA:HB2	6:F:348:VAL:HG11	1.87	0.55
2:A:31:GLY:HA2	2:A:192:LEU:CD2	2.29	0.55
3:C:578:VAL:HG13	3:C:582:THR:CB	2.36	0.55
4:D:1128:PRO:HG3	4:D:1206:PRO:CB	2.37	0.55
6:F:308:VAL:HG21	7:O:23:DT:C7	2.27	0.55
7:O:11:DA:C2'	7:O:12:DG:H5"	2.36	0.55
4:D:1071:ASP:HB2	4:D:1072:GLY:C	2.27	0.55
6:F:462:ARG:NH1	6:F:465:LEU:HB2	2.21	0.55
2:T:251:ILE:HG21	2:T:270:HIS:O	2.06	0.55
2:A:192:LEU:HD12	2:A:192:LEU:O	2.06	0.55
2:A:170:PRO:HB3	2:A:202:ILE:HG12	1.86	0.55
2:B:177:LYS:HG3	2:B:193:ILE:HB	1.89	0.55
3:C:1003:ASP:HB2	3:C:1010:PHE:CZ	2.42	0.55
3:C:446:LEU:HD23	3:C:446:LEU:N	2.21	0.55
3:C:839:ILE:HG22	3:C:840:GLY:N	2.21	0.55
3:C:936:ASN:HD22	3:C:937:ILE:N	2.04	0.55
4:D:183:GLU:O	4:D:187:GLU:HG2	2.07	0.55
2:B:84:VAL:HB	2:B:199:LYS:CD	2.33	0.55
3:C:338:ARG:HB3	3:C:343:GLN:NE2	2.21	0.55
4:D:962:ARG:HB3	4:D:977:CYS:HA	1.89	0.55
5:E:29:PRO:HB2	5:E:33:THR:HG23	1.87	0.55
1:J:88:ARG:HG3	1:J:89:ARG:H	1.72	0.55
2:B:97:LEU:HB3	2:B:136:VAL:HG13	1.89	0.55
3:C:132:ASN:HB3	3:C:135:THR:CG2	2.35	0.55
3:C:1126:VAL:HG12	4:D:12:ILE:HG23	1.89	0.55
4:D:631:ALA:O	4:D:666:THR:HA	2.06	0.55
4:D:844:THR:H	4:D:847:GLU:HB2	1.71	0.55
3:C:275:GLY:O	6:F:171:LYS:HD2	2.06	0.55
6:F:254:ALA:HB3	6:F:257:ASP:OD2	2.07	0.55
6:F:364:THR:HG23	6:F:364:THR:O	2.07	0.55
2:A:2:LEU:HD12	2:B:143:GLY:HA2	1.88	0.55
3:C:228:LEU:HD21	3:C:268:ILE:CG1	2.19	0.55
3:C:721:ASN:ND2	3:C:727:ILE:HD11	2.22	0.55
4:D:1056:LEU:HD21	4:D:1063:PHE:HD1	1.72	0.55
4:D:129:ILE:HD11	4:D:130:TYR:CZ	2.41	0.55
4:D:872:LEU:HG	4:D:876:LEU:HD22	1.88	0.55
4:D:937:ILE:CD1	4:D:951:LEU:HG	2.34	0.55
2:A:152:ASN:HA	2:A:155:SER:OG	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:90:ASP:O	2:A:91:GLU:HG2	2.07	0.55
3:C:1014:VAL:HG13	4:D:729:THR:HG21	1.89	0.55
3:C:348:VAL:HG13	3:C:349:PRO:HD2	1.89	0.55
3:C:523:THR:HG22	3:C:526:GLU:CD	2.27	0.55
5:E:92:ALA:O	5:E:96:ILE:HG13	2.07	0.55
2:B:66:VAL:O	2:B:69:VAL:HG22	2.06	0.55
3:C:176:VAL:HG13	3:C:307:VAL:HG11	1.87	0.55
4:D:1276:THR:HG22	5:E:102:GLU:CG	2.36	0.55
4:D:363:PRO:HG2	4:D:366:ILE:HD12	1.88	0.55
6:F:324:LEU:HD23	6:F:328:LEU:CD1	2.33	0.55
1:J:92:GLU:OE1	1:J:92:GLU:N	2.39	0.55
3:C:577:MET:HE3	4:D:849:PHE:HD1	1.71	0.54
3:C:269:TYR:CE2	3:C:278:PRO:HB3	2.41	0.54
3:C:727:ILE:CG1	3:C:907:ILE:HB	2.37	0.54
4:D:12:ILE:HG12	4:D:1221:TRP:CZ2	2.43	0.54
4:D:460:LEU:HD11	4:D:472:ALA:CB	2.37	0.54
2:B:44:SER:HA	2:B:145:GLY:HA2	1.88	0.54
3:C:346:MET:HB2	3:C:356:VAL:HG21	1.89	0.54
3:C:530:HIS:HB3	3:C:568:ASP:CG	2.27	0.54
3:C:508:ARG:HH11	3:C:570:MET:HE2	1.71	0.54
4:D:579:LEU:HG	11:D:2008:EDO:H22	1.89	0.54
4:D:581:MET:HE2	4:D:716:LYS:HA	1.90	0.54
4:D:576:MET:HE2	4:D:693:ALA:HA	1.89	0.54
3:C:1045:GLN:CG	3:C:1090:ARG:HH21	2.19	0.54
3:C:614:ALA:HB1	3:C:615:PRO:HD2	1.88	0.54
3:C:729:SER:HA	3:C:895:MET:HE1	1.89	0.54
4:D:1171:SER:C	4:D:1174:THR:HG22	2.27	0.54
2:A:210:SER:HB3	2:B:229:SER:CB	2.37	0.54
3:C:935:TRP:HB2	3:C:982:SER:CB	2.38	0.54
4:D:1037:GLU:HG2	4:D:1039:ARG:NH1	2.22	0.54
2:B:162:ILE:CG2	4:D:607:PRO:HG2	2.38	0.54
4:D:706:ILE:O	4:D:710:GLN:HG3	2.07	0.54
3:C:493:VAL:HG12	3:C:494:TYR:CD1	2.42	0.54
4:D:848:TYR:O	4:D:852:THR:HG23	2.07	0.54
2:B:24:GLU:HG3	2:B:191:LYS:HG3	1.88	0.54
3:C:1039:PRO:HB2	3:C:1048:LEU:HD21	1.89	0.54
3:C:202:TRP:C	3:C:203:LEU:HD23	2.27	0.54
3:C:885:VAL:CG1	4:D:538:GLY:HA2	2.38	0.54
4:D:932:ASN:N	4:D:933:GLY:HA2	2.22	0.54
5:E:81:GLU:OE1	5:E:81:GLU:HA	2.08	0.54
2:A:66:VAL:HB	2:A:69:VAL:CG2	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:141:GLN:OE1	3:C:404:THR:OG1	2.26	0.54
2:A:43:LEU:HD11	2:A:174:VAL:HB	1.90	0.54
4:D:1081:LEU:CB	4:D:1113:MET:HE3	2.37	0.54
4:D:706:ILE:CD1	5:E:36:PRO:HB3	2.37	0.54
6:F:385:ALA:O	6:F:389:VAL:HG23	2.08	0.54
2:A:21:PHE:HB2	2:A:194:ILE:HG12	1.89	0.54
2:A:40:ARG:HD3	2:B:33:THR:CB	2.38	0.54
3:C:380:ILE:HG12	3:C:418:ILE:HD11	1.89	0.54
3:C:921:GLN:HB2	3:C:1019:MET:HE1	1.90	0.54
4:D:106:TYR:HB3	4:D:312:MET:HE2	1.89	0.54
4:D:687:MET:HE2	4:D:695:ILE:CD1	2.38	0.54
4:D:901:ALA:N	4:D:912:ASP:HB2	2.20	0.54
4:D:468:ASN:ND2	6:F:463:ASP:OD2	2.35	0.54
2:A:111:VAL:O	2:A:111:VAL:HG22	2.08	0.53
2:A:210:SER:CB	2:B:229:SER:HB2	2.38	0.53
3:C:892:VAL:CG2	3:C:903:PRO:HG2	2.38	0.53
3:C:939:VAL:HG23	3:C:940:ALA:HA	1.88	0.53
4:D:39:LEU:HD13	4:D:335:PHE:HZ	1.72	0.53
4:D:76:GLU:H	4:D:76:GLU:CD	2.11	0.53
2:B:205:ARG:HB2	2:B:205:ARG:CZ	2.37	0.53
3:C:148:PHE:HD2	3:C:150:MET:CE	2.21	0.53
3:C:268:ILE:O	3:C:272:LEU:HD13	2.08	0.53
3:C:41:VAL:HG13	3:C:493:VAL:HG12	1.91	0.53
3:C:431:MET:O	3:C:670:ASN:ND2	2.41	0.53
3:C:876:LEU:N	3:C:876:LEU:HD12	2.24	0.53
3:C:988:ASP:N	3:C:988:ASP:OD1	2.40	0.53
4:D:915:VAL:HG23	4:D:920:PHE:CE2	2.43	0.53
6:F:215:GLN:O	6:F:219:MET:HG2	2.08	0.53
7:O:15:DT:H2"	7:O:16:DT:OP2	2.08	0.53
3:C:1117:LYS:HD2	3:C:1120:GLN:NE2	2.23	0.53
3:C:102:ARG:O	3:C:124:LEU:HD23	2.07	0.53
4:D:982:MET:CE	4:D:1153:LYS:HE3	2.38	0.53
2:A:48:GLY:CA	2:A:49:ALA:CB	2.85	0.53
3:C:338:ARG:HD3	3:C:343:GLN:HE22	1.73	0.53
3:C:712:VAL:CG1	3:C:925:THR:HG23	2.38	0.53
2:A:197:GLU:OE1	3:C:987:ARG:NH2	2.42	0.53
4:D:1229:GLU:O	4:D:1233:VAL:HG23	2.07	0.53
4:D:826:PRO:HG3	4:D:853:HIS:CE1	2.43	0.53
3:C:368:ARG:HA	3:C:369:LEU:CB	2.39	0.53
3:C:822:GLU:HG2	3:C:823:VAL:HG22	1.91	0.53
4:D:1045:ALA:O	14:D:2106:HOH:O	2.19	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:285:LYS:HA	4:D:289:LYS:HD2	1.90	0.53
2:B:103:GLY:O	2:B:128:LEU:HB2	2.08	0.53
3:C:346:MET:HE2	3:C:348:VAL:HA	1.90	0.53
4:D:1034:GLU:OE2	4:D:1042:ARG:HG2	2.09	0.53
4:D:108:LYS:NZ	14:D:2109:HOH:O	2.21	0.53
4:D:744:ILE:O	4:D:748:HIS:HD2	1.92	0.53
1:J:102:LEU:HA	1:J:105:ILE:HG22	1.90	0.53
4:D:872:LEU:HG	4:D:876:LEU:CD2	2.39	0.53
2:A:82:GLY:HA3	2:A:123:MET:CE	2.39	0.53
3:C:126:VAL:HB	3:C:145:MET:HE2	1.89	0.53
3:C:132:ASN:CG	3:C:135:THR:HG22	2.30	0.53
3:C:704:MET:CE	3:C:706:LEU:HD21	2.39	0.53
3:C:729:SER:OG	3:C:904:VAL:O	2.27	0.53
3:C:808:GLU:O	3:C:812:LEU:HD13	2.09	0.53
4:D:443:LEU:HD22	4:D:514:PRO:HB3	1.91	0.53
3:C:973:GLU:OE1	4:D:840:ARG:NH2	2.42	0.53
2:A:192:LEU:HD12	2:A:192:LEU:C	2.30	0.53
3:C:169:GLN:OE1	3:C:370:ARG:NH2	2.42	0.53
3:C:76:GLY:O	3:C:80:VAL:HG23	2.09	0.53
4:D:373:MET:SD	6:F:256:LEU:HB3	2.49	0.53
4:D:602:ALA:HB3	4:D:607:PRO:C	2.29	0.53
2:B:216:VAL:HG13	2:B:217:GLU:N	2.23	0.53
3:C:921:GLN:HB2	3:C:1019:MET:CE	2.38	0.53
1:J:40:PHE:CZ	1:J:58:ASN:HB2	2.44	0.53
2:B:97:LEU:HD21	2:B:105:VAL:HG11	1.90	0.52
3:C:280:LYS:O	3:C:284:GLN:HG2	2.10	0.52
3:C:967:VAL:HG23	3:C:968:PHE:H	1.73	0.52
4:D:1069:PRO:O	4:D:1072:GLY:HA2	2.09	0.52
2:B:60:LEU:HD22	2:B:60:LEU:N	2.24	0.52
3:C:602:MET:HE2	3:C:1024:LEU:HD21	1.90	0.52
3:C:329:VAL:O	3:C:332:THR:OG1	2.26	0.52
4:D:602:ALA:HB1	4:D:606:ALA:HB3	1.89	0.52
4:D:653:ASN:CB	4:D:654:GLY:CA	2.87	0.52
4:D:767:THR:O	4:D:771:GLU:HB2	2.09	0.52
4:D:951:LEU:CB	4:D:956:ILE:HD11	2.33	0.52
3:C:29:ARG:CD	3:C:964:ALA:HB2	2.39	0.52
3:C:62:ARG:O	3:C:66:ILE:HG13	2.09	0.52
3:C:714:ILE:O	3:C:910:THR:OG1	2.23	0.52
3:C:1084:SER:HB2	4:D:421:ARG:O	2.10	0.52
4:D:781:THR:O	4:D:784:VAL:HG23	2.09	0.52
4:D:815:THR:HG22	4:D:820:LYS:CA	2.33	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:936:ILE:CG2	4:D:951:LEU:HD23	2.38	0.52
5:E:98:GLY:O	5:E:100:LEU:HD12	2.09	0.52
6:F:335:GLU:OE1	6:F:335:GLU:N	2.41	0.52
1:J:82:TRP:CZ2	6:F:199:GLN:HG2	2.44	0.52
2:T:260:SER:O	2:T:264:LEU:HG	2.08	0.52
8:P:17:DT:P	2:T:290:GLY:HA3	2.49	0.52
2:A:33:THR:HG22	2:B:37:SER:OG	2.10	0.52
3:C:202:TRP:O	3:C:203:LEU:HD23	2.08	0.52
3:C:335:TYR:HD1	3:C:335:TYR:O	1.91	0.52
3:C:895:MET:HG3	3:C:896:PRO:HD2	1.91	0.52
3:C:90:PHE:HA	14:C:1323:HOH:O	2.09	0.52
3:C:939:VAL:HG22	3:C:940:ALA:HA	1.91	0.52
4:D:585:LEU:HD12	4:D:692:GLN:HE21	1.73	0.52
3:C:393:GLU:OE2	6:F:247:ARG:HD3	2.09	0.52
2:T:251:ILE:HD12	2:T:254:LEU:HD11	1.91	0.52
2:A:56:ILE:HB	2:A:59:VAL:CG2	2.37	0.52
3:C:494:TYR:HB3	3:C:506:PRO:CG	2.37	0.52
3:C:568:ASP:OD1	3:C:568:ASP:N	2.43	0.52
3:C:958:PRO:O	3:C:961:SER:OG	2.28	0.52
2:A:68:GLY:HA3	2:A:129:ASN:HD21	1.74	0.52
3:C:874:ASP:OD1	3:C:1028:VAL:HG22	2.10	0.52
3:C:538:PRO:HB2	3:C:546:THR:OG1	2.10	0.52
3:C:549:ARG:HD3	3:C:561:PHE:CE2	2.44	0.52
3:C:33:ALA:HB2	3:C:966:PRO:HG3	1.90	0.52
6:F:173:ILE:HG22	6:F:238:LEU:CD1	2.40	0.52
2:A:177:LYS:HG2	2:A:193:ILE:CD1	2.40	0.52
3:C:573:SER:HB2	3:C:574:PRO:HD2	1.92	0.52
3:C:44:LEU:HG	3:C:628:ASP:OD2	2.09	0.52
3:C:635:ALA:CB	3:C:693:ILE:HD11	2.30	0.52
4:D:898:VAL:HG11	4:D:919:ALA:HB2	1.91	0.52
2:A:18:ARG:HA	2:A:204:PRO:HG3	1.92	0.52
3:C:984:LEU:HD13	3:C:989:GLY:CA	2.40	0.52
6:F:394:LEU:HB2	6:F:464:TYR:CD1	2.45	0.52
1:J:89:ARG:HH22	6:F:274:ASP:CG	2.11	0.52
2:A:50:ALA:HB3	2:A:168:TYR:CE1	2.45	0.52
2:B:22:VAL:HA	2:B:192:LEU:O	2.10	0.52
3:C:299:LEU:HD23	3:C:323:THR:N	2.24	0.52
3:C:193:VAL:HG12	3:C:205:PHE:HB2	1.92	0.52
3:C:479:THR:OG1	3:C:480:PRO:HD2	2.10	0.52
4:D:248:TYR:HA	4:D:251:TYR:HD2	1.75	0.52
4:D:27:GLU:HB2	4:D:94:HIS:CE1	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:354:LEU:O	4:D:358:ILE:HG12	2.10	0.52
3:C:1133:GLY:O	3:C:1134:ALA:HB3	2.09	0.51
3:C:21:ASN:O	3:C:22:SER:OG	2.21	0.51
3:C:910:THR:O	3:C:914:PRO:HD3	2.10	0.51
4:D:432:VAL:CG2	4:D:434:PRO:HD3	2.28	0.51
4:D:607:PRO:O	4:D:609:GLN:HG2	2.10	0.51
6:F:309:HIS:O	6:F:313:VAL:HG12	2.09	0.51
3:C:641:ILE:HG21	3:C:644:VAL:HG13	1.91	0.51
4:D:1123:LEU:HA	4:D:1131:VAL:CG2	2.40	0.51
4:D:1132:GLN:CG	4:D:1163:LEU:HD12	2.40	0.51
4:D:330:LEU:H	4:D:330:LEU:HD22	1.74	0.51
4:D:653:ASN:CB	4:D:654:GLY:HA3	2.39	0.51
4:D:716:LYS:HE3	4:D:717:ASP:OD1	2.10	0.51
3:C:1132:ASP:HB3	3:C:1133:GLY:CA	2.35	0.51
3:C:624:ARG:NH1	3:C:628:ASP:OD2	2.43	0.51
3:C:852:LEU:CD2	3:C:856:VAL:HG12	2.40	0.51
4:D:1164:ARG:NH1	10:D:2005:SO4:O1	2.43	0.51
3:C:1069:ALA:HB3	4:D:506:ARG:HB3	1.93	0.51
5:E:62:ASN:O	5:E:66:ASN:ND2	2.44	0.51
2:A:147:VAL:HG12	2:A:168:TYR:HE2	1.74	0.51
2:B:102:PRO:HB3	2:B:130:ASP:HA	1.93	0.51
3:C:87:ILE:CD1	3:C:388:GLU:HG3	2.40	0.51
3:C:404:THR:HG23	3:C:407:THR:H	1.75	0.51
4:D:1009:LEU:HD23	4:D:1029:LEU:HD12	1.91	0.51
2:B:74:THR:OG1	4:D:608:GLU:OE1	2.29	0.51
3:C:764:ILE:HB	3:C:767:VAL:HG21	1.91	0.51
3:C:959:ALA:O	3:C:960:ASP:HB2	2.09	0.51
4:D:1174:THR:CA	4:D:1175:GLU:CB	2.87	0.51
1:J:64:LEU:HD22	1:J:66:GLU:HB2	1.93	0.51
2:B:79:ASN:O	2:B:123:MET:CE	2.58	0.51
3:C:1074:TYR:CE1	4:D:1258:LEU:HD21	2.46	0.51
2:A:36:ASN:CB	3:C:1007:GLY:HA3	2.41	0.51
3:C:123:PRO:HB3	3:C:144:PHE:HE1	1.75	0.51
4:D:736:LEU:N	4:D:792:TYR:OH	2.33	0.51
8:P:11:DA:H2"	8:P:12:DA:H5'	1.90	0.51
3:C:94:MET:CE	3:C:395:MET:HB3	2.40	0.51
3:C:584:MET:CA	3:C:619:THR:HG21	2.36	0.51
4:D:588:LEU:HD22	4:D:668:GLY:CA	2.38	0.51
4:D:70:PHE:O	4:D:82:VAL:HG11	2.10	0.51
4:D:932:ASN:N	4:D:933:GLY:CA	2.74	0.51
2:A:172:LEU:HD13	2:A:197:GLU:OE2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1:MET:O	2:A:1:MET:HG2	2.11	0.51
2:A:159:ILE:HD11	3:C:785:ALA:HA	1.92	0.51
3:C:171:VAL:HG12	3:C:172:ARG:N	2.26	0.50
3:C:35:LEU:HD12	3:C:35:LEU:N	2.26	0.50
3:C:578:VAL:HG13	3:C:582:THR:CG2	2.41	0.50
4:D:581:MET:HE3	4:D:716:LYS:HB2	1.93	0.50
4:D:656:LYS:HD3	4:D:656:LYS:H	1.75	0.50
6:F:164:ASP:OD1	6:F:166:VAL:N	2.42	0.50
6:F:304:ILE:HB	14:F:606:HOH:O	2.10	0.50
2:A:193:ILE:O	2:A:193:ILE:HD12	2.11	0.50
2:A:177:LYS:HE2	2:A:193:ILE:HG12	1.93	0.50
2:A:210:SER:CB	2:B:229:SER:CB	2.90	0.50
2:B:170:PRO:O	2:B:199:LYS:HB2	2.12	0.50
3:C:516:THR:HG21	3:C:518:GLN:HB2	1.92	0.50
2:B:198:THR:HG22	2:B:199:LYS:O	2.10	0.50
3:C:852:LEU:HD22	3:C:856:VAL:HG12	1.92	0.50
4:D:411:GLY:O	4:D:415:GLN:HB3	2.12	0.50
4:D:981:SER:HB3	4:D:984:THR:OG1	2.10	0.50
2:A:70:LYS:HB3	2:A:71:GLU:OE1	2.12	0.50
3:C:106:VAL:HG11	3:C:120:TYR:CE1	2.46	0.50
3:C:180:GLU:O	3:C:180:GLU:HG3	2.10	0.50
3:C:572:VAL:H	3:C:576:GLN:NE2	2.10	0.50
3:C:894:ASP:HA	3:C:1004:GLY:HA3	1.93	0.50
4:D:880:SER:O	4:D:995:GLY:HA3	2.11	0.50
2:B:171:VAL:O	2:B:171:VAL:HG23	2.12	0.50
3:C:41:VAL:HG13	3:C:493:VAL:CG1	2.41	0.50
3:C:797:VAL:CG1	3:C:823:VAL:HB	2.41	0.50
4:D:103:HIS:CE1	4:D:105:TRP:HB2	2.46	0.50
4:D:137:THR:HG23	4:D:253:THR:OG1	2.12	0.50
4:D:363:PRO:HB2	4:D:365:ILE:HD13	1.93	0.50
6:F:166:VAL:O	6:F:170:LEU:HG	2.10	0.50
2:A:113:PRO:HD2	2:A:116:VAL:CG2	2.41	0.50
3:C:508:ARG:HD2	3:C:570:MET:CE	2.41	0.50
2:B:172:LEU:O	4:D:616:ALA:HB1	2.10	0.50
4:D:54:PRO:HG3	4:D:81:GLU:O	2.12	0.50
6:F:176:VAL:CG1	6:F:177:ALA:H	2.25	0.50
6:F:462:ARG:HH11	6:F:465:LEU:HB2	1.75	0.50
3:C:762:ARG:O	3:C:762:ARG:HG3	2.10	0.50
3:C:797:VAL:HG12	3:C:823:VAL:HB	1.94	0.50
14:C:1321:HOH:O	4:D:733:ALA:HB2	2.12	0.50
2:T:289:PHE:HE2	2:T:294:ILE:CG1	2.20	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:93:VAL:HG11	2:B:116:VAL:HG11	1.92	0.50
2:B:147:VAL:HG13	2:B:166:SER:HB2	1.93	0.50
3:C:1043:ILE:HD12	3:C:1043:ILE:N	2.25	0.50
3:C:946:TRP:CZ2	3:C:978:GLY:HA3	2.46	0.50
4:D:1056:LEU:HD21	4:D:1063:PHE:CD1	2.47	0.50
4:D:1062:PHE:CE2	4:D:1080:LYS:HD2	2.47	0.50
4:D:937:ILE:HD12	4:D:951:LEU:CG	2.38	0.50
2:A:82:GLY:HA3	2:A:123:MET:HE1	1.94	0.50
3:C:199:ARG:HG2	3:C:200:GLY:N	2.27	0.50
4:D:1054:VAL:HG11	4:D:1100:LEU:HD21	1.94	0.50
4:D:155:MET:CE	4:D:219:LEU:HD22	2.42	0.50
6:F:416:ARG:HA	6:F:430:ILE:HD11	1.94	0.50
2:B:139:VAL:HG21	2:B:161:ARG:HH21	1.76	0.49
3:C:710:LEU:O	3:C:1018:TYR:HA	2.12	0.49
3:C:36:ARG:O	3:C:38:PRO:HD3	2.11	0.49
3:C:404:THR:CG2	3:C:407:THR:HG23	2.42	0.49
3:C:51:SER:OG	3:C:371:THR:HG23	2.12	0.49
3:C:754:LYS:HE2	3:C:754:LYS:N	2.24	0.49
4:D:236:VAL:HG12	4:D:236:VAL:O	2.12	0.49
4:D:704:PRO:HD2	4:D:707:VAL:HG21	1.94	0.49
4:D:890:CYS:SG	4:D:892:THR:HG22	2.52	0.49
1:J:76:LYS:HG3	1:J:76:LYS:O	2.11	0.49
2:A:130:ASP:OD1	2:A:130:ASP:N	2.44	0.49
2:B:105:VAL:HG12	2:B:125:ILE:HG21	1.93	0.49
3:C:196:ILE:O	3:C:196:ILE:HG23	2.12	0.49
3:C:268:ILE:HG23	3:C:272:LEU:HD22	1.95	0.49
3:C:467:HIS:ND1	3:C:468:PRO:HD2	2.27	0.49
3:C:475:CYS:CB	3:C:579:SER:HB3	2.42	0.49
3:C:572:VAL:O	3:C:573:SER:HB3	2.12	0.49
3:C:96:LEU:HD22	3:C:98:PHE:CE1	2.47	0.49
4:D:331:ASP:N	4:D:331:ASP:OD1	2.45	0.49
6:F:194:GLY:HA2	6:F:222:ILE:HG22	1.94	0.49
6:F:454:HIS:CD2	6:F:456:SER:HG	2.30	0.49
2:A:106:THR:C	2:A:125:ILE:HD13	2.33	0.49
2:A:24:GLU:HB3	2:A:191:LYS:HB2	1.95	0.49
3:C:370:ARG:HH22	3:C:452:GLY:HA3	1.77	0.49
4:D:285:LYS:HG3	4:D:289:LYS:HD2	1.94	0.49
4:D:432:VAL:HG22	4:D:434:PRO:CD	2.28	0.49
4:D:430:ILE:HD13	4:D:541:MET:HG3	1.93	0.49
5:E:56:LYS:HA	5:E:59:ARG:HG3	1.93	0.49
2:T:289:PHE:CE2	2:T:294:ILE:HG13	2.34	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:99:LYS:O	2:B:133:LYS:HG3	2.12	0.49
3:C:753:THR:HG21	3:C:799:PRO:HD2	1.95	0.49
3:C:965:THR:O	3:C:965:THR:OG1	2.25	0.49
4:D:362:ALA:HB3	4:D:367:VAL:HG23	1.93	0.49
3:C:1117:LYS:HE2	4:D:90:GLU:O	2.13	0.49
4:D:992:GLU:OE1	5:E:48:TYR:OH	2.31	0.49
4:D:1275:PRO:CB	5:E:79:LEU:HD11	2.38	0.49
2:A:211:ALA:O	2:A:215:LEU:HB2	2.12	0.49
2:B:183:VAL:O	2:B:184:GLU:CB	2.61	0.49
4:D:599:TYR:HA	4:D:610:GLY:HA3	1.94	0.49
4:D:936:ILE:HG23	4:D:951:LEU:HD23	1.95	0.49
2:A:108:GLY:HA2	2:A:121:PRO:HB3	1.94	0.49
2:A:32:TYR:CE1	2:A:178:VAL:HG22	2.47	0.49
2:B:26:LEU:CD1	2:B:34:LEU:HD21	2.42	0.49
3:C:523:THR:CG2	3:C:526:GLU:HG2	2.43	0.49
3:C:680:ILE:HG12	3:C:693:ILE:O	2.13	0.49
3:C:727:ILE:HG13	3:C:907:ILE:HD12	1.94	0.49
4:D:1153:LYS:O	4:D:1157:VAL:HG23	2.13	0.49
4:D:1276:THR:HG22	5:E:102:GLU:HG3	1.95	0.49
3:C:626:ALA:HB2	3:C:704:MET:HG2	1.95	0.49
4:D:1271:ILE:HG12	5:E:105:GLU:HA	1.94	0.49
4:D:603:THR:HG22	4:D:604:LYS:CE	2.30	0.49
4:D:755:ILE:HD12	4:D:776:ILE:CD1	2.43	0.49
4:D:901:ALA:HB2	4:D:911:ARG:CA	2.39	0.49
4:D:915:VAL:O	4:D:920:PHE:HD2	1.96	0.49
4:D:988:VAL:CG2	4:D:992:GLU:HG3	2.42	0.49
2:A:71:GLU:OE2	2:A:126:ALA:HA	2.11	0.49
2:A:9:LEU:HD23	2:B:221:LEU:C	2.33	0.49
2:B:85:VAL:HB	2:B:118:VAL:HA	1.94	0.49
3:C:176:VAL:O	3:C:176:VAL:HG23	2.11	0.49
4:D:1222:LEU:HD23	4:D:1244:ASP:OD2	2.12	0.49
4:D:177:LEU:HD12	4:D:201:GLY:HA3	1.95	0.49
4:D:114:LEU:HG	4:D:312:MET:HE2	1.94	0.49
2:T:283:LEU:O	2:T:286:ILE:HG22	2.13	0.49
2:A:129:ASN:H	2:A:129:ASN:HD22	1.60	0.49
3:C:26:ALA:HB1	3:C:623:LEU:HD21	1.94	0.49
4:D:618:ALA:HB1	4:D:627:LEU:CD1	2.43	0.49
5:E:95:GLU:HB3	5:E:101:LEU:CD2	2.43	0.49
6:F:253:MET:HE3	6:F:296:ALA:C	2.32	0.49
2:A:31:GLY:O	2:A:35:GLY:N	2.34	0.49
2:A:49:ALA:HB1	2:A:85:VAL:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:105:VAL:HG23	2:B:128:LEU:HD13	1.95	0.49
3:C:284:GLN:HG3	3:C:285:THR:N	2.28	0.49
3:C:326:GLU:O	3:C:330:VAL:HG23	2.13	0.49
3:C:45:LEU:HD21	3:C:443:LYS:CD	2.43	0.49
3:C:510:VAL:HG11	3:C:567:VAL:CG1	2.43	0.49
4:D:140:ASP:OD2	4:D:143:MET:HB2	2.13	0.49
4:D:243:GLU:O	4:D:247:ARG:HG3	2.13	0.49
4:D:915:VAL:HG23	4:D:920:PHE:HE2	1.78	0.49
6:F:313:VAL:CG2	6:F:351:ILE:HD13	2.43	0.49
3:C:410:ASN:ND2	3:C:412:ARG:HG3	2.28	0.48
4:D:1117:ALA:O	4:D:1119:PRO:HD3	2.13	0.48
2:B:172:LEU:HD12	4:D:620:MET:SD	2.53	0.48
6:F:317:LEU:CD2	6:F:337:LEU:HG	2.43	0.48
2:A:9:LEU:HD13	2:A:23:ILE:HG13	1.96	0.48
3:C:777:GLU:H	3:C:777:GLU:CD	2.15	0.48
3:C:781:VAL:HG21	3:C:838:VAL:HG21	1.95	0.48
4:D:105:TRP:CE2	4:D:1231:THR:HG23	2.48	0.48
4:D:1069:PRO:HG2	4:D:1073:GLY:N	2.24	0.48
4:D:1081:LEU:HB3	4:D:1113:MET:HE3	1.94	0.48
1:J:84:MET:CE	6:F:272:LYS:HB2	2.43	0.48
7:O:29:DA:N7	14:O:103:HOH:O	2.35	0.48
2:A:186:ARG:O	2:A:187:THR:HG22	2.13	0.48
3:C:505:THR:HG22	3:C:506:PRO:HD2	1.95	0.48
3:C:919:ILE:HD12	3:C:920:GLY:N	2.28	0.48
3:C:948:SER:C	3:C:950:LEU:CB	2.82	0.48
4:D:1034:GLU:OE2	4:D:1042:ARG:N	2.46	0.48
1:J:81:HIS:CG	6:F:195:LEU:HD21	2.48	0.48
7:O:15:DT:H1'	7:O:16:DT:H5"	1.95	0.48
2:A:177:LYS:HE2	2:A:193:ILE:CG1	2.44	0.48
3:C:174:PRO:HD2	3:C:302:VAL:HB	1.94	0.48
3:C:771:VAL:HG23	3:C:772:LEU:HD13	1.93	0.48
4:D:608:GLU:O	4:D:609:GLN:HB2	2.13	0.48
4:D:653:ASN:N	4:D:654:GLY:HA3	2.28	0.48
4:D:735:VAL:HG22	4:D:798:ILE:CD1	2.43	0.48
2:B:76:ILE:HG23	2:B:125:ILE:HD11	1.94	0.48
3:C:32:PHE:HE1	3:C:963:VAL:HG13	1.79	0.48
3:C:723:GLU:O	3:C:724:ASP:HB2	2.14	0.48
3:C:708:LYS:HG3	3:C:737:VAL:HG23	1.95	0.48
3:C:845:SER:O	3:C:850:ASP:HB2	2.13	0.48
4:D:1071:ASP:N	4:D:1072:GLY:HA2	2.28	0.48
4:D:363:PRO:HB2	4:D:365:ILE:HD12	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:58:ASN:HD21	1:J:60:LEU:HD12	1.78	0.48
2:A:18:ARG:NH1	2:A:195:ASP:OD2	2.46	0.48
2:A:18:ARG:HB2	2:A:196:VAL:O	2.13	0.48
2:B:79:ASN:O	2:B:123:MET:HE2	2.13	0.48
3:C:174:PRO:HB2	3:C:303:GLY:CA	2.43	0.48
3:C:55:LEU:HD22	3:C:376:ILE:HB	1.95	0.48
3:C:29:ARG:HG2	3:C:964:ALA:HB2	1.96	0.48
4:D:1005:PRO:HG3	4:D:1150:ILE:HD11	1.95	0.48
4:D:190:LYS:HZ2	4:D:192:ASP:HB3	1.78	0.48
4:D:622:MET:HE1	4:D:629:VAL:HG13	1.94	0.48
4:D:665:THR:HG21	4:D:682:PHE:CE2	2.49	0.48
6:F:272:LYS:HE3	7:O:25:DC:P	2.53	0.48
7:O:6:DA:C1'	7:O:7:DC:H5'	2.44	0.48
4:D:1088:ARG:HD2	4:D:1111:GLN:HB3	1.95	0.48
3:C:1098:VAL:HG11	4:D:469:ILE:CD1	2.42	0.48
4:D:935:VAL:O	4:D:935:VAL:HG12	2.13	0.48
4:D:1276:THR:HG22	5:E:102:GLU:HG2	1.95	0.48
4:D:336:ALA:HA	6:F:359:ILE:O	2.14	0.48
2:B:65:THR:HG22	2:B:66:VAL:N	2.29	0.48
4:D:153:ALA:O	4:D:157:VAL:HG23	2.13	0.48
1:J:51:PRO:O	1:J:64:LEU:HD12	2.13	0.48
2:B:22:VAL:HG12	2:B:193:ILE:CD1	2.40	0.48
3:C:202:TRP:H	3:C:202:TRP:HD1	1.59	0.48
3:C:231:ALA:HB1	3:C:265:LEU:HD12	1.94	0.48
3:C:1080:LEU:HD12	4:D:1253:VAL:HG13	1.96	0.48
4:D:365:ILE:HD13	6:F:235:GLU:HG2	1.96	0.48
4:D:58:TRP:CE3	4:D:68:VAL:HG22	2.49	0.48
4:D:924:LEU:CD2	4:D:943:LEU:HD11	2.43	0.48
6:F:244:LEU:HD12	6:F:289:ILE:CG2	2.44	0.48
6:F:360:SER:HB3	6:F:363:GLN:HG3	1.95	0.48
7:O:28:DT:H2"	7:O:29:DA:C5'	2.40	0.48
2:A:152:ASN:HB3	2:A:157:ALA:HB3	1.93	0.48
3:C:1084:SER:OG	3:C:1085:ASP:N	2.45	0.48
1:J:53:THR:HA	1:J:62:GLY:O	2.13	0.48
2:A:112:PRO:HB2	2:A:116:VAL:CG2	2.43	0.47
2:B:64:THR:HA	2:B:73:VAL:HG21	1.95	0.47
3:C:1048:LEU:CD2	3:C:1048:LEU:H	2.17	0.47
3:C:203:LEU:HD13	3:C:217:ILE:CG2	2.42	0.47
3:C:203:LEU:HD22	3:C:217:ILE:CG2	2.44	0.47
3:C:215:VAL:O	3:C:223:GLN:HB2	2.14	0.47
3:C:265:LEU:CD1	3:C:287:LEU:HD12	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:1171:SER:O	4:D:1202:ALA:HB2	2.14	0.47
4:D:226:PHE:CE1	4:D:248:TYR:HB3	2.48	0.47
3:C:477:ILE:HD11	4:D:852:THR:HG21	1.95	0.47
2:A:55:ARG:HH12	2:A:161:ARG:CZ	2.26	0.47
2:B:52:THR:O	2:B:164:VAL:HG22	2.13	0.47
2:B:198:THR:HG21	2:B:202:ILE:O	2.14	0.47
3:C:178:PHE:CD1	3:C:193:VAL:HB	2.49	0.47
3:C:372:VAL:O	3:C:376:ILE:HG12	2.14	0.47
3:C:589:GLU:OE1	3:C:589:GLU:N	2.37	0.47
3:C:731:ARG:NH1	3:C:735:GLU:OE1	2.47	0.47
3:C:752:ASP:OD1	3:C:857:ASN:ND2	2.45	0.47
6:F:310:MET:O	6:F:313:VAL:HG13	2.14	0.47
2:A:40:ARG:HH21	2:B:32:TYR:HD2	1.62	0.47
3:C:523:THR:HG23	3:C:526:GLU:HG2	1.96	0.47
3:C:649:ILE:HG21	3:C:693:ILE:CG2	2.44	0.47
5:E:81:GLU:O	5:E:94:ARG:NH2	2.47	0.47
7:O:6:DA:H1'	7:O:7:DC:C5'	2.44	0.47
2:A:147:VAL:HG13	2:A:147:VAL:O	2.14	0.47
2:A:42:LEU:HD23	2:A:211:ALA:HB2	1.96	0.47
3:C:788:ARG:O	3:C:830:VAL:HG11	2.14	0.47
4:D:1119:PRO:HA	4:D:1122:VAL:HG12	1.95	0.47
4:D:246:ASP:OD1	4:D:246:ASP:N	2.46	0.47
3:C:716:PRO:O	4:D:724:THR:HB	2.14	0.47
8:P:11:DA:H2'	8:P:12:DA:C8	2.48	0.47
2:A:31:GLY:CA	2:A:192:LEU:HD23	2.32	0.47
2:A:9:LEU:HB2	2:A:23:ILE:HG12	1.96	0.47
2:B:18:ARG:HG3	2:B:197:GLU:CG	2.41	0.47
2:B:213:GLY:CA	2:B:216:VAL:HG12	2.43	0.47
3:C:203:LEU:HD22	3:C:217:ILE:HA	1.96	0.47
3:C:87:ILE:O	3:C:95:SER:HA	2.13	0.47
4:D:602:ALA:CB	4:D:607:PRO:O	2.62	0.47
6:F:279:TYR:CE1	7:O:28:DT:H5"	2.49	0.47
2:A:181:THR:H	2:A:189:PHE:C	2.15	0.47
2:A:78:LEU:HD12	3:C:611:ARG:HH11	1.79	0.47
2:B:63:PHE:CD1	2:B:63:PHE:N	2.81	0.47
3:C:560:GLU:HG3	3:C:562:VAL:HG23	1.97	0.47
4:D:240:LEU:C	4:D:240:LEU:HD23	2.35	0.47
4:D:66:LYS:O	4:D:66:LYS:HG2	2.13	0.47
4:D:869:SER:HB2	4:D:1029:LEU:HD21	1.97	0.47
4:D:948:ILE:O	4:D:952:LEU:HB2	2.14	0.47
5:E:57:ARG:HD3	5:E:57:ARG:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:257:THR:OG1	2:T:260:SER:OG	2.33	0.47
2:A:207:ALA:O	2:A:210:SER:OG	2.12	0.47
2:A:78:LEU:O	2:A:81:LYS:HB2	2.15	0.47
3:C:269:TYR:CD2	3:C:278:PRO:HB3	2.50	0.47
3:C:549:ARG:HB2	3:C:561:PHE:CZ	2.50	0.47
3:C:614:ALA:HA	3:C:705:ALA:HB2	1.97	0.47
4:D:846:LEU:HD12	4:D:846:LEU:N	2.29	0.47
3:C:124:LEU:HD23	3:C:125:PHE:H	1.80	0.47
3:C:128:ALA:CB	3:C:405:PRO:HB3	2.45	0.47
3:C:130:PHE:CZ	3:C:403:ILE:HG13	2.50	0.47
3:C:272:LEU:C	3:C:274:PRO:HD3	2.35	0.47
3:C:498:ASN:HB2	3:C:502:PHE:O	2.15	0.47
3:C:586:PRO:O	3:C:880:HIS:HE1	1.98	0.47
4:D:231:PRO:O	4:D:232:LYS:HB2	2.15	0.47
4:D:262:LYS:HG3	4:D:310:MET:HE3	1.97	0.47
4:D:320:ILE:HG12	4:D:321:PRO:CD	2.45	0.47
7:O:2:DC:H2"	7:O:3:DT:O5'	2.15	0.47
2:B:214:THR:O	2:B:218:LEU:HB2	2.13	0.47
3:C:896:PRO:HB2	3:C:1001:LEU:HD13	1.97	0.47
3:C:148:PHE:HD2	3:C:150:MET:HE3	1.78	0.47
3:C:794:VAL:HG11	3:C:860:VAL:HG11	1.96	0.47
2:A:107:ALA:HB3	2:A:121:PRO:HA	1.96	0.47
2:A:161:ARG:O	2:A:163:PRO:HD3	2.15	0.47
2:A:219:PHE:CE1	2:B:38:LEU:HD21	2.50	0.47
3:C:516:THR:CG2	3:C:518:GLN:HB2	2.45	0.47
3:C:728:LEU:HD23	3:C:906:ILE:HG22	1.97	0.47
4:D:823:VAL:HG12	4:D:824:THR:N	2.30	0.47
1:J:88:ARG:HG3	1:J:89:ARG:N	2.30	0.47
8:P:17:DT:H5"	2:T:290:GLY:N	2.30	0.47
2:T:264:LEU:HB3	2:T:269:VAL:HG21	1.93	0.47
2:B:153:LYS:N	2:B:154:ALA:CA	2.72	0.47
2:B:69:VAL:HG23	2:B:71:GLU:O	2.14	0.47
3:C:1093:VAL:HG13	3:C:1094:TYR:N	2.30	0.47
3:C:368:ARG:HA	3:C:369:LEU:HB3	1.97	0.47
3:C:460:GLY:HA3	3:C:462:GLU:OE1	2.15	0.47
3:C:587:PHE:HB3	3:C:590:HIS:HD2	1.80	0.47
3:C:664:ARG:HB2	3:C:677:GLN:OE1	2.15	0.47
3:C:792:ILE:HD12	3:C:792:ILE:N	2.28	0.47
4:D:287:GLN:HG3	4:D:288:LYS:HZ2	1.79	0.47
4:D:590:THR:CG2	4:D:630:ARG:HE	2.28	0.47
3:C:1103:ILE:HD12	4:D:548:SER:CA	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:426:GLN:CD	3:C:450:GLY:HA2	2.34	0.46
3:C:475:CYS:HA	3:C:577:MET:O	2.15	0.46
4:D:1056:LEU:HD23	4:D:1057:GLU:H	1.79	0.46
4:D:129:ILE:HD11	4:D:130:TYR:CE2	2.49	0.46
3:C:1103:ILE:CD1	4:D:547:LEU:HB3	2.44	0.46
4:D:656:LYS:CE	4:D:656:LYS:O	2.63	0.46
6:F:320:ILE:HG22	6:F:337:LEU:HD12	1.97	0.46
2:B:66:VAL:HG12	2:B:69:VAL:HG22	1.97	0.46
3:C:1031:LYS:NZ	10:C:1203:SO4:S	2.88	0.46
4:D:889:ASP:OD2	4:D:962:ARG:NH2	2.48	0.46
6:F:414:ARG:HG2	6:F:419:LEU:HD12	1.98	0.46
1:J:40:PHE:HZ	1:J:58:ASN:HB2	1.80	0.46
2:A:56:ILE:HG12	2:A:136:VAL:HB	1.98	0.46
3:C:1003:ASP:HB2	3:C:1010:PHE:CE1	2.50	0.46
3:C:477:ILE:HG22	3:C:477:ILE:O	2.16	0.46
3:C:508:ARG:HD2	3:C:570:MET:HE3	1.98	0.46
3:C:475:CYS:HB2	3:C:579:SER:HB3	1.96	0.46
3:C:643:GLU:OE2	14:C:1310:HOH:O	2.21	0.46
3:C:29:ARG:HD3	3:C:964:ALA:HB2	1.97	0.46
4:D:738:PRO:HA	4:D:791:PHE:HD2	1.80	0.46
2:A:108:GLY:CA	2:A:121:PRO:HB3	2.46	0.46
2:B:94:THR:HA	2:B:138:LEU:O	2.16	0.46
3:C:913:VAL:HB	3:C:914:PRO:HD3	1.96	0.46
5:E:80:VAL:CG1	5:E:94:ARG:HH21	2.29	0.46
2:A:54:ILE:C	2:A:54:ILE:HD12	2.36	0.46
2:A:68:GLY:CA	2:A:129:ASN:HD21	2.27	0.46
2:A:151:GLN:HB3	3:C:786:GLU:OE2	2.15	0.46
4:D:285:LYS:HA	4:D:289:LYS:HB2	1.96	0.46
4:D:397:ARG:O	4:D:397:ARG:HG3	2.15	0.46
4:D:720:PHE:O	4:D:724:THR:HG23	2.15	0.46
4:D:58:TRP:HH2	4:D:84:ARG:NH2	2.14	0.46
2:T:286:ILE:HG22	2:T:289:PHE:CB	2.45	0.46
3:C:71:GLU:OE2	3:C:71:GLU:HA	2.16	0.46
4:D:1152:ASP:O	4:D:1156:GLU:HG3	2.16	0.46
4:D:400:LYS:CE	4:D:404:ASP:HB3	2.44	0.46
4:D:517:VAL:HG12	4:D:518:GLU:O	2.15	0.46
4:D:765:ASN:ND2	4:D:767:THR:HG23	2.30	0.46
6:F:170:LEU:HA	6:F:173:ILE:HG12	1.97	0.46
8:P:4:DA:H2"	8:P:5:DC:C6	2.51	0.46
2:B:152:ASN:O	2:B:153:LYS:CB	2.64	0.46
2:B:196:VAL:O	2:B:196:VAL:HG13	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:230:GLU:OE1	2:B:230:GLU:HA	2.16	0.46
3:C:1066:ALA:HB1	4:D:506:ARG:HA	1.96	0.46
3:C:80:VAL:CG2	3:C:377:GLN:HG3	2.45	0.46
3:C:615:PRO:HB3	3:C:1020:TYR:CE2	2.50	0.46
3:C:780:ILE:HD12	3:C:781:VAL:O	2.15	0.46
3:C:850:ASP:HB3	3:C:851:GLU:H	1.55	0.46
4:D:1034:GLU:O	14:D:2107:HOH:O	2.20	0.46
4:D:129:ILE:HG12	4:D:130:TYR:CD2	2.51	0.46
4:D:676:LEU:HD12	4:D:676:LEU:H	1.79	0.46
4:D:991:GLY:HA2	4:D:1265:ILE:HD12	1.98	0.46
6:F:316:LYS:HD3	6:F:341:MET:HE3	1.98	0.46
2:A:63:PHE:O	3:C:666:PHE:CD2	2.69	0.46
2:B:28:PRO:HA	2:B:190:ASP:OD2	2.16	0.46
2:B:63:PHE:N	2:B:63:PHE:HD1	2.13	0.46
2:B:80:LEU:HG	2:B:125:ILE:HD13	1.97	0.46
3:C:1032:ILE:HG21	4:D:520:LYS:HD3	1.98	0.46
3:C:1033:HIS:HB3	11:C:1205:EDO:O1	2.15	0.46
3:C:1084:SER:OG	4:D:420:LYS:HD3	2.16	0.46
3:C:38:PRO:CB	3:C:508:ARG:HH21	2.28	0.46
3:C:427:LEU:HD12	3:C:427:LEU:N	2.31	0.46
3:C:767:VAL:HB	3:C:771:VAL:HG21	1.97	0.46
3:C:984:LEU:CD1	3:C:989:GLY:HA2	2.46	0.46
4:D:125:LEU:O	4:D:129:ILE:HG23	2.16	0.46
4:D:924:LEU:HD22	4:D:959:VAL:HG11	1.95	0.46
5:E:80:VAL:HG12	5:E:94:ARG:HH21	1.81	0.46
6:F:201:LEU:HD11	6:F:219:MET:CB	2.40	0.46
1:J:73:LYS:O	1:J:74:LYS:HG3	2.16	0.46
3:C:193:VAL:HG22	3:C:194:LYS:N	2.31	0.46
3:C:848:ASP:OD1	3:C:848:ASP:N	2.49	0.46
4:D:1123:LEU:HB2	4:D:1131:VAL:HG21	1.97	0.46
4:D:735:VAL:CG1	4:D:840:ARG:HD2	2.40	0.46
5:E:37:ILE:H	5:E:37:ILE:HG13	1.26	0.46
3:C:766:ASN:HB3	6:F:465:LEU:HD21	1.98	0.46
2:B:202:ILE:HD13	2:B:207:ALA:HB2	1.97	0.46
2:B:26:LEU:HD13	2:B:30:PHE:HB3	1.98	0.46
2:B:9:LEU:HD21	2:B:208:LEU:HD21	1.98	0.46
3:C:447:SER:HB2	3:C:449:LEU:HD11	1.98	0.46
4:D:931:ALA:HA	4:D:932:ASN:HA	1.63	0.46
6:F:176:VAL:CG1	6:F:177:ALA:N	2.78	0.46
6:F:440:ARG:O	6:F:444:ILE:HG13	2.16	0.46
6:F:465:LEU:HD23	6:F:465:LEU:C	2.37	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:73:LYS:O	1:J:74:LYS:CG	2.63	0.46
2:B:105:VAL:HG23	2:B:128:LEU:HD11	1.97	0.45
2:B:150:VAL:O	2:B:150:VAL:HG13	2.16	0.45
3:C:601:ASN:O	3:C:604:ARG:HG2	2.16	0.45
3:C:632:VAL:CG1	3:C:692:VAL:HG13	2.46	0.45
3:C:727:ILE:HA	3:C:888:LYS:O	2.16	0.45
3:C:96:LEU:HD22	3:C:98:PHE:HE1	1.79	0.45
4:D:67:ARG:HH12	6:F:423:GLN:HA	1.81	0.45
2:B:43:LEU:HA	2:B:43:LEU:HD12	1.78	0.45
4:D:1086:ARG:O	4:D:1087:LEU:HD23	2.17	0.45
4:D:163:GLU:HG2	4:D:166:ARG:HH21	1.81	0.45
4:D:647:GLU:HB2	4:D:655:TRP:HZ3	1.76	0.45
4:D:85:ALA:O	4:D:88:ARG:HB2	2.17	0.45
2:A:125:ILE:N	2:A:125:ILE:HD12	2.31	0.45
2:A:48:GLY:O	2:A:142:ARG:HG2	2.15	0.45
2:B:28:PRO:HD3	2:B:189:PHE:CD1	2.51	0.45
3:C:361:ILE:HD12	3:C:361:ILE:N	2.25	0.45
3:C:405:PRO:O	3:C:409:ILE:HG13	2.16	0.45
3:C:638:THR:HG23	3:C:688:GLU:HA	1.97	0.45
3:C:797:VAL:HG11	3:C:823:VAL:CG2	2.46	0.45
3:C:888:LYS:HG2	3:C:890:LEU:HD13	1.99	0.45
3:C:935:TRP:HB2	3:C:982:SER:HB2	1.98	0.45
4:D:1009:LEU:CD1	4:D:1146:GLN:HG3	2.44	0.45
4:D:666:THR:HG23	4:D:669:ARG:HD2	1.98	0.45
5:E:29:PRO:CG	5:E:34:ASN:HB2	2.46	0.45
5:E:57:ARG:NH2	5:E:77:GLY:HA3	2.30	0.45
2:B:174:VAL:HA	2:B:195:ASP:O	2.16	0.45
3:C:1041:SER:HB3	3:C:1044:THR:O	2.16	0.45
3:C:767:VAL:HB	3:C:771:VAL:CG2	2.46	0.45
3:C:859:LEU:HD22	3:C:860:VAL:N	2.30	0.45
3:C:900:ASP:OD1	3:C:992:MET:SD	2.74	0.45
3:C:976:LEU:O	3:C:980:LEU:HD23	2.16	0.45
4:D:1032:VAL:HG23	4:D:1142:VAL:HG11	1.99	0.45
4:D:875:ARG:HH22	4:D:1033:GLN:CD	2.19	0.45
4:D:952:LEU:HA	4:D:952:LEU:HD12	1.85	0.45
2:T:257:THR:O	2:T:260:SER:N	2.50	0.45
2:B:181:THR:HB	2:B:182:ARG:CB	2.47	0.45
2:B:76:ILE:HG23	2:B:125:ILE:HD12	1.98	0.45
3:C:169:GLN:HB2	3:C:427:LEU:HD21	1.98	0.45
3:C:174:PRO:HB2	3:C:303:GLY:HA3	1.99	0.45
3:C:506:PRO:O	3:C:572:VAL:HG13	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:741:ILE:HG22	3:C:742:HIS:N	2.31	0.45
4:D:1106:VAL:HG13	4:D:1110:ASP:HB2	1.98	0.45
4:D:365:ILE:H	4:D:365:ILE:CD1	2.07	0.45
4:D:644:THR:HA	4:D:647:GLU:CD	2.35	0.45
2:B:95:MET:CE	2:B:110:ILE:HD11	2.46	0.45
3:C:1037:THR:HG22	3:C:1038:GLY:N	2.32	0.45
3:C:797:VAL:HG11	3:C:823:VAL:HG21	1.98	0.45
4:D:633:ILE:O	4:D:665:THR:O	2.35	0.45
4:D:929:VAL:O	4:D:929:VAL:HG23	2.16	0.45
7:O:1:DG:C4'	7:O:1:DG:O5'	2.65	0.45
2:B:65:THR:N	2:B:73:VAL:HG23	2.31	0.45
2:B:99:LYS:HB3	2:B:99:LYS:HE2	1.64	0.45
3:C:747:GLU:HG3	3:C:859:LEU:HD21	1.98	0.45
4:D:376:GLU:OE2	6:F:165:SER:OG	2.26	0.45
1:J:104:LEU:HD23	1:J:104:LEU:O	2.17	0.45
7:O:12:DG:H2'	7:O:13:DT:H71	1.98	0.45
3:C:1035:ARG:CZ	3:C:1047:PRO:HB3	2.46	0.45
4:D:1122:VAL:HG23	4:D:1126:GLN:HE21	1.80	0.45
4:D:285:LYS:HG3	4:D:289:LYS:CD	2.46	0.45
4:D:591:LEU:HD23	4:D:630:ARG:O	2.17	0.45
4:D:693:ALA:O	4:D:697:ASN:HB2	2.17	0.45
2:A:10:SER:OG	2:A:22:VAL:HG13	2.17	0.45
3:C:154:LYS:O	3:C:443:LYS:HE3	2.17	0.45
4:D:102:THR:OG1	4:D:129:ILE:HD12	2.16	0.45
4:D:1191:ASN:OD1	4:D:1202:ALA:HB3	2.16	0.45
4:D:814:ARG:O	4:D:817:ALA:O	2.35	0.45
4:D:920:PHE:CZ	4:D:948:ILE:HG13	2.52	0.45
6:F:321:GLN:NE2	6:F:331:GLU:OE2	2.50	0.45
2:B:147:VAL:CG1	2:B:166:SER:HB2	2.47	0.45
3:C:154:LYS:HE2	3:C:630:GLY:O	2.17	0.45
3:C:203:LEU:HD22	3:C:217:ILE:HB	1.99	0.45
3:C:203:LEU:C	3:C:204:GLU:HG3	2.37	0.45
4:D:1220:SER:HB3	4:D:1223:SER:HB3	1.99	0.45
4:D:269:ASP:OD2	4:D:272:ALA:N	2.50	0.45
4:D:956:ILE:CD1	4:D:956:ILE:O	2.65	0.45
7:O:2:DC:H2"	7:O:3:DT:C5'	2.47	0.45
3:C:103:PHE:CE2	3:C:124:LEU:HG	2.53	0.44
3:C:291:PHE:HA	3:C:297:TYR:HB2	1.98	0.44
3:C:390:VAL:HG11	3:C:394:ARG:HH21	1.83	0.44
3:C:723:GLU:OE1	3:C:723:GLU:HA	2.18	0.44
4:D:103:HIS:HB3	4:D:106:TYR:HD2	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:138:SER:HB3	4:D:253:THR:HG1	1.79	0.44
2:B:22:VAL:HG12	2:B:193:ILE:HG23	1.98	0.44
3:C:1126:VAL:HG23	3:C:1126:VAL:O	2.17	0.44
3:C:53:GLU:OE2	3:C:60:ARG:NH1	2.37	0.44
3:C:62:ARG:HG3	3:C:66:ILE:HD11	1.99	0.44
4:D:1110:ASP:OD1	4:D:1110:ASP:N	2.50	0.44
4:D:1129:ARG:O	4:D:1133:ILE:HG12	2.17	0.44
4:D:119:ASP:C	4:D:120:LEU:HD12	2.37	0.44
4:D:791:PHE:O	4:D:791:PHE:HD1	2.01	0.44
1:J:84:MET:HE2	6:F:272:LYS:HE2	1.99	0.44
2:B:176:TYR:HD1	2:B:176:TYR:H	1.65	0.44
3:C:1011:PRO:HB2	3:C:1012:TYR:CD2	2.53	0.44
3:C:1043:ILE:HD12	3:C:1043:ILE:H	1.82	0.44
3:C:62:ARG:HG3	3:C:66:ILE:CD1	2.47	0.44
3:C:659:GLN:N	3:C:659:GLN:OE1	2.50	0.44
3:C:680:ILE:HD11	3:C:692:VAL:HG12	1.99	0.44
4:D:656:LYS:HE2	4:D:656:LYS:O	2.17	0.44
4:D:911:ARG:HG2	4:D:952:LEU:HD21	2.00	0.44
4:D:929:VAL:HG22	14:D:2112:HOH:O	2.16	0.44
5:E:53:TYR:CE1	5:E:101:LEU:HD12	2.53	0.44
6:F:462:ARG:HD3	6:F:462:ARG:HA	1.79	0.44
3:C:197:PRO:HB3	3:C:297:TYR:OH	2.16	0.44
3:C:627:ILE:HD12	3:C:628:ASP:N	2.33	0.44
4:D:467:GLN:HA	4:D:467:GLN:NE2	2.32	0.44
4:D:686:GLN:O	4:D:686:GLN:HG3	2.18	0.44
3:C:1022:LEU:N	3:C:1022:LEU:HD23	2.32	0.44
3:C:1090:ARG:O	3:C:1093:VAL:HG12	2.18	0.44
3:C:43:GLY:O	3:C:46:ASP:HB2	2.17	0.44
4:D:1190:GLU:O	4:D:1190:GLU:HG3	2.16	0.44
4:D:525:HIS:O	4:D:528:VAL:HG22	2.17	0.44
4:D:599:TYR:CA	4:D:610:GLY:HA3	2.47	0.44
4:D:640:LEU:O	4:D:656:LYS:HE3	2.17	0.44
4:D:687:MET:CE	4:D:695:ILE:HD11	2.48	0.44
2:T:286:ILE:CG2	2:T:289:PHE:HB2	2.47	0.44
2:A:44:SER:HB3	3:C:893:GLU:OE1	2.17	0.44
2:A:64:THR:O	2:A:73:VAL:HG23	2.18	0.44
2:A:95:MET:HE2	2:A:110:ILE:HG22	2.00	0.44
2:A:40:ARG:CZ	2:B:33:THR:HG22	2.47	0.44
3:C:1003:ASP:OD1	3:C:1005:ARG:HB3	2.17	0.44
3:C:197:PRO:HB3	3:C:297:TYR:CZ	2.53	0.44
3:C:369:LEU:HD12	3:C:369:LEU:HA	1.56	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:102:THR:HG23	4:D:258:ALA:CB	2.48	0.44
4:D:444:PRO:HD2	4:D:447:MET:HE2	1.99	0.44
4:D:47:PHE:CD1	4:D:322:PRO:HB3	2.52	0.44
4:D:579:LEU:HD23	4:D:807:THR:HB	1.99	0.44
3:C:577:MET:CE	4:D:849:PHE:HD1	2.29	0.44
3:C:31:SER:O	3:C:954:LEU:HD11	2.18	0.44
3:C:71:GLU:C	3:C:73:PRO:HD3	2.38	0.44
4:D:1140:GLN:NE2	4:D:1155:ILE:HD12	2.33	0.44
4:D:91:ARG:O	4:D:321:PRO:HG3	2.18	0.44
5:E:76:VAL:CG1	5:E:77:GLY:N	2.81	0.44
8:P:11:DA:H2'	8:P:12:DA:H8	1.83	0.44
2:B:170:PRO:CB	2:B:202:ILE:HD11	2.42	0.44
3:C:1049:GLY:HA3	4:D:421:ARG:CZ	2.48	0.44
3:C:478:GLU:OE1	3:C:579:SER:OG	2.25	0.44
4:D:1034:GLU:OE2	4:D:1041:PRO:HA	2.17	0.44
4:D:740:GLN:H	4:D:740:GLN:NE2	2.01	0.44
4:D:878:ASP:OD1	14:D:2108:HOH:O	2.21	0.44
1:J:57:ARG:HG3	4:D:25:TYR:HA	2.00	0.44
8:P:4:DA:H2"	8:P:5:DC:H6	1.82	0.44
2:A:187:THR:HG23	2:A:187:THR:O	2.18	0.44
3:C:167:VAL:HG13	3:C:445:ARG:O	2.18	0.44
3:C:77:LEU:HA	3:C:77:LEU:HD23	1.76	0.44
4:D:1171:SER:O	4:D:1174:THR:HG22	2.18	0.44
4:D:1174:THR:OG1	4:D:1175:GLU:CB	2.66	0.44
4:D:781:THR:CG2	4:D:814:ARG:HD2	2.47	0.44
6:F:406:SER:HB3	6:F:409:GLU:HG3	2.00	0.44
6:F:465:LEU:HD23	6:F:466:ASP:HB2	2.00	0.44
2:A:175:THR:HG22	2:A:195:ASP:HB3	2.00	0.43
3:C:1118:GLU:OE1	4:D:412:ARG:HG3	2.19	0.43
3:C:346:MET:HB2	3:C:356:VAL:CG2	2.48	0.43
3:C:523:THR:HG22	3:C:526:GLU:OE2	2.18	0.43
3:C:616:LEU:HB2	3:C:709:ASN:CG	2.38	0.43
3:C:70:GLU:N	3:C:70:GLU:OE1	2.51	0.43
3:C:89:ASP:N	3:C:89:ASP:OD1	2.51	0.43
4:D:1036:PHE:HD2	4:D:1162:MET:HE1	1.83	0.43
4:D:113:ARG:HB2	4:D:312:MET:CE	2.43	0.43
6:F:394:LEU:HB2	6:F:464:TYR:CE1	2.53	0.43
2:A:78:LEU:CD1	3:C:611:ARG:HH11	2.31	0.43
3:C:873:GLY:HA3	3:C:1028:VAL:CG1	2.47	0.43
3:C:1074:TYR:CZ	4:D:1258:LEU:HD21	2.53	0.43
3:C:174:PRO:O	3:C:303:GLY:HA2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:365:GLY:HA3	3:C:525:ASP:OD1	2.18	0.43
4:D:1041:PRO:HB3	4:D:1116:ALA:CB	2.48	0.43
4:D:1056:LEU:HD23	4:D:1057:GLU:N	2.33	0.43
4:D:447:MET:HE3	4:D:543:VAL:HG21	2.00	0.43
3:C:973:GLU:CB	4:D:732:MET:HE1	2.48	0.43
4:D:739:PRO:HD3	4:D:791:PHE:CE2	2.53	0.43
6:F:359:ILE:HG22	6:F:360:SER:N	2.32	0.43
1:J:58:ASN:HD21	1:J:60:LEU:CG	2.31	0.43
2:A:48:GLY:HA3	2:A:168:TYR:HB3	2.01	0.43
3:C:221:ARG:O	3:C:223:GLN:NE2	2.34	0.43
3:C:215:VAL:CG2	3:C:225:VAL:HA	2.30	0.43
3:C:291:PHE:O	3:C:297:TYR:HB3	2.18	0.43
3:C:529:ARG:CZ	3:C:529:ARG:HB3	2.48	0.43
3:C:494:TYR:CD2	3:C:572:VAL:HG21	2.46	0.43
3:C:619:THR:OG1	3:C:620:GLY:N	2.50	0.43
3:C:809:GLU:O	3:C:813:ARG:HG2	2.18	0.43
4:D:1081:LEU:HB3	4:D:1113:MET:SD	2.58	0.43
4:D:131:PHE:HA	4:D:256:MET:HE2	2.01	0.43
4:D:277:LEU:HD21	4:D:292:ALA:O	2.18	0.43
6:F:171:LYS:HE2	6:F:171:LYS:HB3	1.77	0.43
6:F:173:ILE:HG22	6:F:238:LEU:HD13	2.00	0.43
6:F:263:ASN:O	6:F:267:ILE:HG13	2.18	0.43
3:C:45:LEU:CD2	3:C:443:LYS:HD2	2.48	0.43
3:C:562:VAL:HG12	3:C:563:SER:N	2.33	0.43
3:C:706:LEU:N	14:C:1311:HOH:O	2.23	0.43
3:C:710:LEU:HD23	3:C:732:LEU:HD11	2.01	0.43
3:C:751:ARG:CD	3:C:856:VAL:HG22	2.48	0.43
4:D:493:GLU:HA	4:D:513:GLU:OE1	2.18	0.43
4:D:67:ARG:NH1	6:F:423:GLN:HA	2.33	0.43
2:B:147:VAL:HG13	2:B:147:VAL:O	2.19	0.43
3:C:510:VAL:HG12	3:C:568:ASP:O	2.19	0.43
2:A:63:PHE:HE1	3:C:741:ILE:HD13	1.83	0.43
2:A:146:TYR:OH	3:C:869:LYS:NZ	2.52	0.43
4:D:452:PHE:CE1	4:D:491:ILE:HG12	2.53	0.43
3:C:1103:ILE:HD13	4:D:547:LEU:HB3	2.00	0.43
4:D:740:GLN:O	4:D:744:ILE:HG13	2.18	0.43
4:D:859:LEU:HD12	4:D:862:THR:HG21	2.01	0.43
2:T:254:LEU:HB2	2:T:256:LEU:HG	2.01	0.43
2:A:18:ARG:HA	2:A:204:PRO:CG	2.49	0.43
2:B:28:PRO:HA	2:B:29:GLY:HA2	1.79	0.43
2:A:219:PHE:HE1	2:B:38:LEU:HD21	1.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:1036:PHE:O	4:D:1211:ILE:HG23	2.18	0.43
4:D:788:LEU:HD21	4:D:792:TYR:CE2	2.53	0.43
4:D:863:ALA:O	4:D:866:THR:HG22	2.18	0.43
4:D:900:LEU:HD11	4:D:948:ILE:HD12	2.01	0.43
1:J:69:VAL:N	1:J:70:PRO:HD3	2.34	0.43
2:A:11:GLU:OE2	2:B:225:LEU:HD22	2.18	0.43
2:A:214:THR:HG23	2:B:231:HIS:CG	2.54	0.43
3:C:228:LEU:HA	3:C:228:LEU:HD23	1.70	0.43
3:C:623:LEU:HD12	3:C:703:GLU:OE1	2.19	0.43
3:C:780:ILE:HG13	3:C:780:ILE:O	2.18	0.43
3:C:984:LEU:HD13	3:C:989:GLY:HA2	2.00	0.43
4:D:910:ILE:HG12	4:D:910:ILE:O	2.19	0.43
1:J:85:LEU:HD21	6:F:192:GLU:HB3	2.01	0.43
6:F:394:LEU:HD13	6:F:464:TYR:CG	2.54	0.43
1:J:48:ALA:HB2	4:D:65:TYR:OH	2.18	0.43
2:A:11:GLU:CD	2:A:205:ARG:HG2	2.38	0.43
3:C:591:ASP:OD2	3:C:880:HIS:ND1	2.41	0.43
4:D:633:ILE:HD13	4:D:635:VAL:HG13	2.00	0.43
4:D:796:ASN:ND2	4:D:798:ILE:HB	2.28	0.43
4:D:799:ILE:HD13	4:D:799:ILE:HA	1.73	0.43
7:O:6:DA:H2"	7:O:7:DC:OP2	2.17	0.43
2:A:93:VAL:CG2	2:A:113:PRO:HG3	2.48	0.43
2:B:111:VAL:HG13	2:B:111:VAL:O	2.18	0.43
3:C:178:PHE:CE1	3:C:193:VAL:HG21	2.54	0.43
3:C:394:ARG:HG3	3:C:398:GLN:CG	2.48	0.43
3:C:404:THR:HG23	3:C:407:THR:HG23	1.99	0.43
4:D:110:VAL:HG13	4:D:110:VAL:O	2.19	0.43
4:D:1258:LEU:HD12	4:D:1258:LEU:HA	1.90	0.43
4:D:590:THR:HG23	4:D:630:ARG:HE	1.84	0.43
4:D:676:LEU:CD1	4:D:676:LEU:N	2.81	0.43
4:D:813:THR:HG22	4:D:813:THR:O	2.18	0.43
2:A:34:LEU:HD23	2:A:34:LEU:HA	1.77	0.43
2:A:82:GLY:CA	2:A:123:MET:HE1	2.49	0.43
2:A:98:ARG:O	2:A:99:LYS:HD2	2.18	0.43
2:B:191:LYS:HG2	2:B:193:ILE:HD11	2.01	0.43
2:B:34:LEU:CD1	2:B:192:LEU:HD22	2.37	0.43
3:C:1025:HIS:O	3:C:1025:HIS:CD2	2.72	0.43
3:C:239:ILE:HG22	3:C:253:LEU:HD22	1.99	0.43
3:C:265:LEU:HD21	3:C:284:GLN:HA	2.01	0.43
4:D:1272:GLN:HA	4:D:1272:GLN:OE1	2.19	0.43
4:D:51:ILE:HG12	4:D:51:ILE:H	1.64	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:612:TYR:OH	4:D:627:LEU:HG	2.19	0.43
6:F:320:ILE:O	6:F:324:LEU:HB2	2.18	0.43
6:F:373:LEU:HD23	6:F:373:LEU:O	2.18	0.43
1:J:28:GLN:N	1:J:44:PHE:O	2.50	0.43
2:B:226:ASN:O	2:B:227:ALA:HB3	2.19	0.42
3:C:1105:GLU:HG3	3:C:1106:PRO:HD2	2.00	0.42
3:C:454:LEU:O	3:C:454:LEU:HD12	2.19	0.42
3:C:51:SER:HB2	3:C:371:THR:OG1	2.19	0.42
2:A:197:GLU:CD	3:C:987:ARG:HH22	2.20	0.42
4:D:114:LEU:HG	4:D:312:MET:CE	2.48	0.42
4:D:1247:ASN:O	4:D:1260:PRO:HG3	2.19	0.42
4:D:155:MET:HE3	4:D:219:LEU:HD22	2.00	0.42
4:D:735:VAL:CG1	4:D:816:LEU:HD22	2.49	0.42
4:D:58:TRP:HA	4:D:82:VAL:HG23	2.01	0.42
4:D:1279:ALA:HB1	5:E:79:LEU:HD13	2.00	0.42
8:P:3:DC:H2"	8:P:4:DA:H8	1.82	0.42
3:C:114:LYS:HG2	3:C:161:GLY:O	2.19	0.42
3:C:344:THR:HG22	3:C:344:THR:O	2.19	0.42
3:C:698:CYS:O	3:C:705:ALA:N	2.49	0.42
3:C:781:VAL:CG2	3:C:838:VAL:HG21	2.48	0.42
3:C:31:SER:HA	3:C:964:ALA:O	2.19	0.42
4:D:1165:ARG:HG2	4:D:1183:GLU:HA	2.01	0.42
4:D:237:ASP:O	4:D:238:GLU:HB3	2.18	0.42
5:E:28:THR:HG23	5:E:28:THR:O	2.19	0.42
2:T:269:VAL:HG23	2:T:269:VAL:O	2.19	0.42
2:A:96:TYR:O	2:A:111:VAL:HG13	2.18	0.42
2:A:46:ILE:HA	2:A:47:PRO:HD3	1.89	0.42
2:B:68:GLY:O	2:B:129:ASN:N	2.41	0.42
3:C:640:VAL:CG2	3:C:641:ILE:N	2.82	0.42
3:C:728:LEU:HD22	3:C:906:ILE:HG22	1.97	0.42
3:C:946:TRP:CE2	3:C:978:GLY:HA3	2.55	0.42
4:D:934:ASN:OD1	4:D:934:ASN:N	2.53	0.42
5:E:80:VAL:CG1	5:E:81:GLU:N	2.82	0.42
6:F:186:GLU:OE1	6:F:186:GLU:HA	2.20	0.42
6:F:306:ILE:CG2	6:F:310:MET:HB3	2.49	0.42
6:F:345:PRO:HA	6:F:348:VAL:HG13	2.00	0.42
1:J:106:LYS:HB3	1:J:106:LYS:HE2	1.77	0.42
1:J:69:VAL:N	1:J:70:PRO:CD	2.83	0.42
3:C:602:MET:HE1	3:C:883:LYS:CB	2.30	0.42
4:D:1174:THR:CG2	4:D:1176:PHE:N	2.76	0.42
4:D:262:LYS:HG3	4:D:310:MET:CE	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:901:ALA:HB2	4:D:912:ASP:N	2.35	0.42
5:E:53:TYR:HE1	5:E:101:LEU:HD12	1.84	0.42
3:C:963:VAL:HG12	3:C:964:ALA:N	2.35	0.42
4:D:143:MET:HE1	4:D:250:GLU:O	2.19	0.42
4:D:23:TRP:HB3	4:D:92:MET:HE3	2.01	0.42
4:D:653:ASN:HB2	4:D:654:GLY:HA2	1.99	0.42
6:F:447:LYS:N	6:F:447:LYS:HD3	2.35	0.42
6:F:454:HIS:CD2	6:F:456:SER:OG	2.73	0.42
1:J:85:LEU:O	1:J:85:LEU:HD12	2.19	0.42
2:T:286:ILE:HG23	2:T:289:PHE:HB2	2.01	0.42
3:C:467:HIS:HD2	3:C:469:SER:OG	2.02	0.42
3:C:510:VAL:HG11	3:C:567:VAL:CB	2.50	0.42
3:C:691:GLN:HG2	3:C:692:VAL:H	1.84	0.42
3:C:875:LYS:C	3:C:876:LEU:HD12	2.39	0.42
2:A:174:VAL:O	3:C:901:GLY:HA3	2.20	0.42
3:C:919:ILE:HD12	3:C:920:GLY:H	1.84	0.42
4:D:214:ARG:NH1	14:D:2118:HOH:O	2.47	0.42
4:D:584:GLY:HA3	4:D:719:GLY:O	2.19	0.42
6:F:408:ARG:HH21	11:F:506:EDO:H22	1.85	0.42
2:B:104:VAL:O	2:B:104:VAL:HG13	2.20	0.42
2:B:97:LEU:HD23	2:B:136:VAL:CG1	2.50	0.42
3:C:279:THR:H	3:C:282:SER:HG	1.66	0.42
3:C:85:SER:HA	3:C:86:PRO:HA	1.69	0.42
4:D:1171:SER:O	4:D:1174:THR:CG2	2.67	0.42
4:D:412:ARG:HA	4:D:416:ASN:HD22	1.85	0.42
4:D:735:VAL:HG11	4:D:816:LEU:CD2	2.50	0.42
4:D:64:LYS:NZ	4:D:76:GLU:OE2	2.47	0.42
7:O:2:DC:H2"	7:O:3:DT:H5'	2.02	0.42
2:T:256:LEU:HB3	2:T:260:SER:HB2	2.00	0.42
2:A:42:LEU:O	2:A:46:ILE:HG12	2.20	0.42
3:C:595:ARG:HD2	3:C:595:ARG:HA	1.91	0.42
3:C:33:ALA:HB2	3:C:966:PRO:CG	2.49	0.42
3:C:98:PHE:HE2	3:C:387:MET:HE1	1.85	0.42
4:D:1165:ARG:HE	4:D:1209:MET:HE1	1.84	0.42
4:D:788:LEU:C	4:D:788:LEU:HD23	2.40	0.42
4:D:799:ILE:CG2	4:D:803:LYS:HE2	2.50	0.42
5:E:80:VAL:CG2	5:E:100:LEU:HD22	2.50	0.42
6:F:332:PRO:HA	6:F:336:GLU:OE1	2.20	0.42
6:F:349:LEU:HA	6:F:349:LEU:HD12	1.79	0.42
2:A:193:ILE:C	2:A:193:ILE:HD12	2.40	0.42
2:B:4:SER:OG	2:B:27:GLU:OE2	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:40:ARG:HH11	2:B:33:THR:HG22	1.81	0.42
3:C:180:GLU:HB3	3:C:191:HIS:CD2	2.55	0.42
3:C:310:LYS:O	3:C:354:VAL:HG21	2.20	0.42
4:D:448:ALA:HB1	4:D:491:ILE:HD11	2.01	0.42
4:D:831:ILE:HA	4:D:831:ILE:HD12	1.74	0.42
3:C:583:ALA:HB3	3:C:621:MET:HG3	2.00	0.42
3:C:788:ARG:O	3:C:830:VAL:CG1	2.68	0.42
4:D:250:GLU:HG3	4:D:251:TYR:CE2	2.55	0.42
4:D:647:GLU:OE1	4:D:655:TRP:HH2	2.03	0.42
4:D:83:THR:OG1	4:D:84:ARG:N	2.53	0.42
2:B:38:LEU:HA	2:B:38:LEU:HD22	1.79	0.41
3:C:1015:THR:OG1	4:D:731:SER:OG	2.39	0.41
3:C:1130:SER:HB3	3:C:1132:ASP:C	2.41	0.41
3:C:193:VAL:CG1	3:C:205:PHE:HB2	2.50	0.41
3:C:649:ILE:CD1	3:C:693:ILE:HG22	2.50	0.41
4:D:1132:GLN:HG3	4:D:1163:LEU:CD1	2.50	0.41
4:D:130:TYR:O	4:D:372:ARG:HD3	2.20	0.41
4:D:229:LEU:HA	4:D:233:GLN:OE1	2.20	0.41
4:D:278:ARG:HH11	4:D:278:ARG:HG3	1.85	0.41
4:D:676:LEU:H	4:D:676:LEU:CD1	2.33	0.41
4:D:742:GLN:O	4:D:746:GLU:HG2	2.19	0.41
4:D:755:ILE:HD13	4:D:772:SER:OG	2.19	0.41
4:D:884:ILE:HD11	4:D:886:ARG:NE	2.35	0.41
1:J:71:GLU:HG2	1:J:72:PRO:HD2	2.01	0.41
3:C:400:VAL:C	3:C:402:ALA:H	2.23	0.41
3:C:602:MET:HA	3:C:605:GLN:HB2	2.03	0.41
3:C:704:MET:HE1	3:C:706:LEU:HD21	2.01	0.41
3:C:885:VAL:HG22	4:D:536:PHE:O	2.20	0.41
3:C:947:ALA:O	3:C:951:PRO:HD2	2.21	0.41
4:D:1165:ARG:HD2	4:D:1209:MET:CE	2.50	0.41
4:D:1181:LEU:CD1	4:D:1213:LYS:HE2	2.50	0.41
3:C:1100:GLY:CA	4:D:458:LYS:HE3	2.45	0.41
4:D:683:VAL:N	14:D:2103:HOH:O	2.53	0.41
4:D:860:ALA:O	4:D:863:ALA:HB3	2.20	0.41
4:D:901:ALA:O	4:D:902:GLU:CB	2.68	0.41
1:J:89:ARG:HH21	6:F:276:THR:HG23	1.83	0.41
6:F:465:LEU:O	6:F:466:ASP:HB2	2.19	0.41
2:A:212:GLY:O	2:A:216:VAL:N	2.34	0.41
3:C:1117:LYS:NZ	3:C:1120:GLN:HE22	2.18	0.41
3:C:361:ILE:CD1	3:C:361:ILE:H	2.30	0.41
3:C:165:VAL:HG23	3:C:431:MET:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:479:THR:OG1	3:C:480:PRO:CD	2.68	0.41
3:C:575:ARG:HE	3:C:967:VAL:CG2	2.28	0.41
3:C:614:ALA:HA	3:C:705:ALA:CB	2.50	0.41
4:D:224:ASN:O	4:D:228:LYS:HG3	2.19	0.41
4:D:815:THR:CG2	4:D:820:LYS:HA	2.34	0.41
3:C:466:VAL:HG12	4:D:856:ARG:CZ	2.51	0.41
4:D:52:PHE:O	4:D:91:ARG:HD2	2.20	0.41
1:J:58:ASN:HD21	1:J:60:LEU:HG	1.84	0.41
2:A:147:VAL:CG1	2:A:166:SER:HB2	2.50	0.41
2:B:152:ASN:CA	2:B:154:ALA:HA	2.49	0.41
3:C:263:GLU:HA	3:C:266:LEU:HD12	2.02	0.41
3:C:400:VAL:O	3:C:401:GLU:HB3	2.20	0.41
3:C:570:MET:HG2	3:C:571:ASP:N	2.36	0.41
3:C:895:MET:HB2	3:C:895:MET:HE2	1.74	0.41
4:D:1168:ILE:HD13	4:D:1176:PHE:CG	2.54	0.41
4:D:20:ILE:HD13	4:D:318:PRO:HD3	2.03	0.41
4:D:433:GLY:HA3	4:D:436:LEU:HD12	2.02	0.41
6:F:179:LEU:CD1	6:F:187:LEU:HD12	2.51	0.41
6:F:337:LEU:HD12	6:F:337:LEU:HA	1.80	0.41
7:O:31:DT:C6	7:O:31:DT:H5'	2.55	0.41
2:B:151:GLN:HG2	2:B:151:GLN:O	2.19	0.41
2:B:182:ARG:C	2:B:184:GLU:H	2.22	0.41
3:C:265:LEU:HD11	3:C:287:LEU:CD1	2.45	0.41
3:C:572:VAL:HG22	3:C:576:GLN:NE2	2.35	0.41
3:C:154:LYS:NZ	3:C:664:ARG:HH12	2.18	0.41
3:C:632:VAL:HG13	3:C:694:ALA:O	2.20	0.41
3:C:783:ILE:H	3:C:783:ILE:CD1	2.06	0.41
4:D:173:ARG:NH2	4:D:201:GLY:HA2	2.35	0.41
6:F:173:ILE:HG22	6:F:238:LEU:HD12	2.01	0.41
6:F:310:MET:O	6:F:314:ILE:HG13	2.21	0.41
2:T:279:THR:CG2	2:T:282:ASP:HB2	2.44	0.41
2:T:283:LEU:HA	2:T:283:LEU:HD23	1.85	0.41
2:A:84:VAL:HG13	2:A:84:VAL:O	2.21	0.41
3:C:574:PRO:HB2	3:C:968:PHE:HB2	2.03	0.41
3:C:764:ILE:HB	3:C:767:VAL:CG2	2.50	0.41
3:C:918:ASN:O	3:C:920:GLY:N	2.54	0.41
4:D:1044:LYS:HE3	4:D:1118:ASP:HB2	2.02	0.41
4:D:1165:ARG:HB2	4:D:1209:MET:HE2	2.02	0.41
1:J:108:LYS:HB3	1:J:108:LYS:HE2	1.88	0.41
2:A:62:GLU:OE2	3:C:867:LYS:HE3	2.21	0.41
3:C:523:THR:OG1	3:C:524:ALA:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:754:LYS:HD3	4:D:39:LEU:HD12	2.01	0.41
3:C:1066:ALA:CB	4:D:506:ARG:HA	2.51	0.41
5:E:84:LEU:HB2	5:E:85:GLN:NE2	2.36	0.41
6:F:344:THR:O	6:F:348:VAL:HG12	2.21	0.41
2:A:147:VAL:CG1	2:A:168:TYR:HE2	2.33	0.41
2:B:64:THR:C	2:B:65:THR:HG1	2.05	0.41
2:B:71:GLU:OE2	2:B:127:THR:HG23	2.20	0.41
2:B:89:ASP:O	2:B:90:ASP:HB2	2.20	0.41
3:C:590:HIS:O	3:C:919:ILE:CD1	2.68	0.41
3:C:758:GLU:CG	3:C:798:THR:HG22	2.38	0.41
4:D:1171:SER:HA	4:D:1174:THR:CG2	2.48	0.41
4:D:245:GLN:O	4:D:249:GLY:HA3	2.21	0.41
4:D:277:LEU:HD23	4:D:277:LEU:O	2.21	0.41
4:D:31:PRO:HB3	4:D:348:ILE:HG23	2.03	0.41
6:F:176:VAL:HG21	6:F:235:GLU:HB3	2.02	0.41
2:A:106:THR:HB	2:A:123:MET:O	2.21	0.41
3:C:1048:LEU:CD2	3:C:1048:LEU:N	2.81	0.41
3:C:228:LEU:O	3:C:231:ALA:N	2.54	0.41
3:C:270:ARG:O	3:C:274:PRO:HG3	2.20	0.41
3:C:41:VAL:HG22	3:C:494:TYR:HE1	1.86	0.41
3:C:610:VAL:HG23	3:C:611:ARG:N	2.36	0.41
4:D:1069:PRO:HB2	4:D:1071:ASP:OD1	2.21	0.41
4:D:507:LEU:HA	4:D:507:LEU:HD12	1.84	0.41
4:D:52:PHE:CD2	4:D:322:PRO:HD3	2.55	0.41
4:D:640:LEU:O	4:D:656:LYS:CE	2.69	0.41
6:F:452:LEU:HD12	6:F:452:LEU:HA	1.86	0.41
1:J:58:ASN:HD21	1:J:60:LEU:CD1	2.32	0.41
2:A:12:GLU:HB2	2:A:20:ARG:O	2.20	0.41
2:A:137:GLU:C	2:A:138:LEU:HD12	2.41	0.41
2:B:125:ILE:HG23	2:B:126:ALA:H	1.85	0.41
2:B:30:PHE:CA	2:B:33:THR:HG23	2.47	0.41
2:B:54:ILE:HG13	2:B:54:ILE:O	2.20	0.41
3:C:169:GLN:HB2	3:C:427:LEU:CD2	2.51	0.41
3:C:447:SER:HB3	3:C:488:ILE:HG12	2.02	0.41
4:D:365:ILE:HD11	6:F:235:GLU:OE2	2.21	0.41
5:E:29:PRO:CB	5:E:33:THR:HG23	2.50	0.41
5:E:86:GLU:OE1	5:E:91:ILE:HG12	2.20	0.41
6:F:244:LEU:HD12	6:F:289:ILE:HG21	2.03	0.41
2:B:139:VAL:CG2	2:B:161:ARG:HH21	2.35	0.41
2:A:40:ARG:NH2	2:B:32:TYR:HD2	2.19	0.41
2:A:40:ARG:CD	2:B:33:THR:HG22	2.43	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:556:GLY:N	3:C:557:GLY:CA	2.83	0.41
4:D:26:GLY:HA3	4:D:51:ILE:HG21	1.98	0.41
4:D:271:ASP:HA	4:D:303:GLN:NE2	2.36	0.41
4:D:527:LEU:HD21	4:D:581:MET:HE3	2.00	0.41
4:D:826:PRO:HD3	4:D:853:HIS:CE1	2.54	0.41
4:D:938:GLU:OE1	4:D:938:GLU:N	2.36	0.41
4:D:34:ILE:O	6:F:304:ILE:HG23	2.21	0.41
2:B:151:GLN:C	2:B:154:ALA:HB1	2.42	0.40
2:A:216:VAL:HG13	2:B:216:VAL:HG23	2.02	0.40
2:B:95:MET:HE3	2:B:110:ILE:CD1	2.51	0.40
3:C:1001:LEU:HB2	3:C:1010:PHE:HD2	1.86	0.40
3:C:166:VAL:CG1	3:C:372:VAL:HG23	2.49	0.40
3:C:538:PRO:O	3:C:546:THR:OG1	2.38	0.40
2:A:146:TYR:CE2	3:C:734:GLU:HA	2.57	0.40
4:D:1004:GLU:HB3	4:D:1005:PRO:HD3	2.04	0.40
4:D:117:LEU:O	4:D:117:LEU:HD22	2.19	0.40
4:D:1208:LEU:HD23	4:D:1208:LEU:HA	1.87	0.40
4:D:157:VAL:HG12	14:D:2114:HOH:O	2.22	0.40
4:D:899:THR:O	4:D:957:THR:O	2.39	0.40
2:T:279:THR:O	2:T:282:ASP:N	2.50	0.40
2:B:161:ARG:HD3	2:B:161:ARG:HA	1.53	0.40
3:C:132:ASN:O	3:C:136:GLY:N	2.52	0.40
3:C:273:ARG:N	3:C:274:PRO:HD3	2.35	0.40
3:C:614:ALA:HB2	3:C:700:GLN:HB3	2.03	0.40
4:D:119:ASP:O	4:D:120:LEU:HD12	2.22	0.40
4:D:228:LYS:H	4:D:228:LYS:HG3	1.75	0.40
4:D:243:GLU:HG2	4:D:247:ARG:HH21	1.85	0.40
4:D:556:ARG:O	4:D:560:LEU:HB2	2.20	0.40
4:D:566:LEU:N	4:D:566:LEU:HD23	2.37	0.40
4:D:920:PHE:HE1	4:D:945:ASP:HA	1.85	0.40
6:F:188:ALA:O	6:F:192:GLU:HG3	2.20	0.40
3:C:493:VAL:HG23	3:C:578:VAL:O	2.21	0.40
4:D:1004:GLU:N	4:D:1005:PRO:HD2	2.35	0.40
4:D:1090:ILE:N	4:D:1098:GLY:O	2.30	0.40
6:F:324:LEU:CD2	6:F:328:LEU:HD22	2.52	0.40
6:F:437:THR:OG1	7:O:3:DT:OP2	2.40	0.40
2:A:18:ARG:CB	2:A:197:GLU:HA	2.51	0.40
2:B:151:GLN:CG	2:B:151:GLN:O	2.69	0.40
3:C:602:MET:CE	3:C:1024:LEU:HD21	2.51	0.40
3:C:598:MET:O	3:C:602:MET:HG3	2.22	0.40
3:C:644:VAL:O	3:C:644:VAL:HG23	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:754:LYS:HD3	4:D:39:LEU:CD1	2.52	0.40
3:C:967:VAL:HG23	3:C:968:PHE:N	2.34	0.40
4:D:12:ILE:HG21	4:D:12:ILE:HD13	1.79	0.40
4:D:776:ILE:HG13	4:D:776:ILE:H	1.70	0.40
4:D:81:GLU:HG2	4:D:83:THR:HG22	2.04	0.40
6:F:310:MET:HA	6:F:313:VAL:CG1	2.51	0.40
2:A:2:LEU:HD12	2:B:143:GLY:CA	2.52	0.40
2:A:2:LEU:CD1	2:B:142:ARG:HB3	2.51	0.40
2:B:192:LEU:C	2:B:193:ILE:HD13	2.41	0.40
3:C:54:TRP:HD1	3:C:61:TRP:CZ2	2.39	0.40
3:C:943:VAL:HA	3:C:944:PRO:HD3	1.98	0.40
4:D:1004:GLU:HB3	4:D:1005:PRO:CD	2.52	0.40
4:D:35:ASN:OD1	4:D:37:ARG:N	2.48	0.40
4:D:444:PRO:HD2	4:D:447:MET:CE	2.50	0.40
4:D:972:GLY:HA2	10:D:2005:SO4:O2	2.21	0.40
6:F:359:ILE:HG22	6:F:360:SER:H	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	J	81/114 (71%)	75 (93%)	6 (7%)	0	100 100
2	A	214/350 (61%)	202 (94%)	12 (6%)	0	100 100
2	B	231/350 (66%)	216 (94%)	14 (6%)	1 (0%)	39 72
2	T	51/350 (15%)	51 (100%)	0	0	100 100
3	C	1093/1169 (94%)	1038 (95%)	51 (5%)	4 (0%)	39 72
4	D	1238/1317 (94%)	1189 (96%)	46 (4%)	3 (0%)	52 83
5	E	72/107 (67%)	65 (90%)	5 (7%)	2 (3%)	6 18

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
6	F	298/466 (64%)	294 (99%)	4 (1%)	0	100 100
All	All	3278/4223 (78%)	3130 (96%)	138 (4%)	10 (0%)	46 77

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	E	76	VAL
3	C	982	SER
3	C	1134	ALA
4	D	902	GLU
4	D	1194	VAL
3	C	544	ARG
5	E	78	PRO
2	B	183	VAL
4	D	935	VAL
3	C	967	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
1	J	71/98 (72%)	65 (92%)	6 (8%)	13 34
2	A	178/297 (60%)	162 (91%)	16 (9%)	12 31
2	B	171/297 (58%)	152 (89%)	19 (11%)	8 20
2	T	35/297 (12%)	29 (83%)	6 (17%)	2 6
3	C	857/984 (87%)	777 (91%)	80 (9%)	11 29
4	D	994/1095 (91%)	904 (91%)	90 (9%)	12 30
5	E	62/86 (72%)	50 (81%)	12 (19%)	2 4
6	F	252/379 (66%)	232 (92%)	20 (8%)	15 37
All	All	2620/3533 (74%)	2371 (90%)	249 (10%)	11 27

All (249) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	47	ASP
1	J	55	LEU
1	J	58	ASN
1	J	64	LEU
1	J	91	VAL
1	J	105	ILE
2	A	14	VAL
2	A	40	ARG
2	A	71	GLU
2	A	74	THR
2	A	111	VAL
2	A	117	THR
2	A	127	THR
2	A	129	ASN
2	A	130	ASP
2	A	135	GLU
2	A	136	VAL
2	A	150	VAL
2	A	159	ILE
2	A	168	TYR
2	A	171	VAL
2	A	187	THR
2	B	17	ASN
2	B	33	THR
2	B	38	LEU
2	B	43	LEU
2	B	60	LEU
2	B	63	PHE
2	B	84	VAL
2	B	85	VAL
2	B	99	LYS
2	B	144	ARG
2	B	161	ARG
2	B	176	TYR
2	B	178	VAL
2	B	200	ASN
2	B	205	ARG
2	B	215	LEU
2	B	218	LEU
2	B	230	GLU
2	B	231	HIS
3	C	44	LEU
3	C	45	LEU

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Mol	Chain	Res	Type
3	C	46	ASP
3	C	58	SER
3	C	70	GLU
3	C	71	GLU
3	C	77	LEU
3	C	81	LEU
3	C	94	MET
3	C	96	LEU
3	C	119	THR
3	C	124	LEU
3	C	202	TRP
3	C	204	GLU
3	C	268	ILE
3	C	273	ARG
3	C	280	LYS
3	C	299	LEU
3	C	301	ARG
3	C	335	TYR
3	C	336	LEU
3	C	346	MET
3	C	347	THR
3	C	364	PHE
3	C	404	THR
3	C	434	ASN
3	C	436	PRO
3	C	437	LEU
3	C	443	LYS
3	C	446	LEU
3	C	449	LEU
3	C	454	LEU
3	C	491	LEU
3	C	520	ASP
3	C	546	THR
3	C	552	VAL
3	C	568	ASP
3	C	605	GLN
3	C	607	VAL
3	C	611	ARG
3	C	617	VAL
3	C	624	ARG
3	C	636	ASP
3	C	640	VAL

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Mol	Chain	Res	Type
3	C	703	GLU
3	C	727	ILE
3	C	737	VAL
3	C	753	THR
3	C	754	LYS
3	C	763	ASP
3	C	775	LEU
3	C	777	GLU
3	C	778	ARG
3	C	780	ILE
3	C	783	ILE
3	C	810	ARG
3	C	830	VAL
3	C	839	ILE
3	C	848	ASP
3	C	859	LEU
3	C	872	ASP
3	C	895	MET
3	C	927	LEU
3	C	936	ASN
3	C	961	SER
3	C	965	THR
3	C	984	LEU
3	C	986	ASN
3	C	987	ARG
3	C	988	ASP
3	C	1022	LEU
3	C	1028	VAL
3	C	1045	GLN
3	C	1048	LEU
3	C	1054	PHE
3	C	1084	SER
3	C	1108	ILE
3	C	1122	LEU
3	C	1129	LEU
3	C	1132	ASP
4	D	7	PHE
4	D	12	ILE
4	D	28	VAL
4	D	51	ILE
4	D	57	ASP
4	D	70	PHE

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Mol	Chain	Res	Type
4	D	84	ARG
4	D	107	PHE
4	D	117	LEU
4	D	129	ILE
4	D	144	ARG
4	D	148	LEU
4	D	150	THR
4	D	165	GLN
4	D	187	GLU
4	D	228	LYS
4	D	234	LEU
4	D	238	GLU
4	D	239	VAL
4	D	243	GLU
4	D	246	ASP
4	D	247	ARG
4	D	295	ARG
4	D	304	GLN
4	D	314	LEU
4	D	365	ILE
4	D	415	GLN
4	D	417	LEU
4	D	449	LEU
4	D	451	LEU
4	D	456	VAL
4	D	467	GLN
4	D	489	GLU
4	D	504	LEU
4	D	507	LEU
4	D	518	GLU
4	D	558	LEU
4	D	562	SER
4	D	566	LEU
4	D	567	SER
4	D	574	LEU
4	D	588	LEU
4	D	591	LEU
4	D	599	TYR
4	D	600	GLN
4	D	627	LEU
4	D	635	VAL
4	D	653	ASN

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Mol	Chain	Res	Type
4	D	655	TRP
4	D	656	LYS
4	D	666	THR
4	D	667	LEU
4	D	675	LEU
4	D	687	MET
4	D	706	ILE
4	D	713	ASP
4	D	724	THR
4	D	740	GLN
4	D	743	GLU
4	D	767	THR
4	D	769	ARG
4	D	784	VAL
4	D	799	ILE
4	D	830	PHE
4	D	831	ILE
4	D	853	HIS
4	D	876	LEU
4	D	900	LEU
4	D	914	HIS
4	D	923	THR
4	D	934	ASN
4	D	939	ARG
4	D	945	ASP
4	D	1039	ARG
4	D	1042	ARG
4	D	1049	ASP
4	D	1056	LEU
4	D	1079	ASP
4	D	1086	ARG
4	D	1110	ASP
4	D	1112	LEU
4	D	1150	ILE
4	D	1183	GLU
4	D	1186	GLU
4	D	1208	LEU
4	D	1215	SER
4	D	1222	LEU
4	D	1234	LEU
4	D	1241	CYS
4	D	1258	LEU

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Mol	Chain	Res	Type
5	E	37	ILE
5	E	50	LEU
5	E	53	TYR
5	E	57	ARG
5	E	59	ARG
5	E	75	TYR
5	E	76	VAL
5	E	84	LEU
5	E	85	GLN
5	E	101	LEU
5	E	102	GLU
5	E	104	THR
6	F	182	GLU
6	F	216	ARG
6	F	291	GLN
6	F	310	MET
6	F	313	VAL
6	F	317	LEU
6	F	324	LEU
6	F	325	LEU
6	F	337	LEU
6	F	348	VAL
6	F	349	LEU
6	F	373	LEU
6	F	402	LEU
6	F	420	THR
6	F	433	VAL
6	F	437	THR
6	F	452	LEU
6	F	462	ARG
6	F	465	LEU
6	F	466	ASP
2	T	252	ASP
2	T	254	LEU
2	T	255	ASP
2	T	260	SER
2	T	279	THR
2	T	284	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	J	58	ASN
2	A	129	ASN
3	C	48	GLN
3	C	160	ASN
3	C	343	GLN
3	C	398	GLN
3	C	410	ASN
3	C	426	GLN
3	C	433	GLN
3	C	467	HIS
3	C	576	GLN
3	C	590	HIS
3	C	603	GLN
3	C	685	GLN
3	C	700	GLN
3	C	720	HIS
3	C	742	HIS
3	C	936	ASN
3	C	1025	HIS
3	C	1068	GLN
3	C	1120	GLN
4	D	165	GLN
4	D	287	GLN
4	D	368	ASN
4	D	416	ASN
4	D	465	HIS
4	D	515	GLN
4	D	600	GLN
4	D	684	ASN
4	D	740	GLN
4	D	748	HIS
4	D	778	GLN
4	D	796	ASN
4	D	881	GLN
4	D	932	ASN
4	D	1085	GLN
4	D	1126	GLN
4	D	1140	GLN
4	D	1146	GLN
5	E	62	ASN
5	E	66	ASN
5	E	85	GLN
5	E	103	HIS

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Mol	Chain	Res	Type
6	F	214	GLN

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 21 ligands modelled in this entry, 3 are monoatomic - leaving 18 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	$\#\|Z\| > 2$
10	SO4	C	1201	-	4,4,4	0.26	0	6,6,6	0.12	0
10	SO4	C	1202	-	4,4,4	0.24	0	6,6,6	0.13	0
10	SO4	C	1203	-	4,4,4	0.24	0	6,6,6	0.28	0
11	EDO	C	1204	-	3,3,3	0.42	0	2,2,2	0.48	0
11	EDO	C	1205	-	3,3,3	0.50	0	2,2,2	0.28	0
10	SO4	D	2004	-	4,4,4	0.26	0	6,6,6	0.32	0
10	SO4	D	2005	-	4,4,4	0.24	0	6,6,6	0.25	0
10	SO4	D	2006	-	4,4,4	0.24	0	6,6,6	0.25	0
10	SO4	D	2007	-	4,4,4	0.23	0	6,6,6	0.13	0
11	EDO	D	2008	-	3,3,3	0.47	0	2,2,2	0.31	0
11	EDO	D	2009	-	3,3,3	0.44	0	2,2,2	0.36	0
11	EDO	D	2010	-	3,3,3	0.49	0	2,2,2	0.18	0
10	SO4	F	501	6	4,4,4	0.21	0	6,6,6	0.11	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
10	SO4	F	502	-	4,4,4	0.22	0	6,6,6	0.17	0
10	SO4	F	503	-	4,4,4	0.19	0	6,6,6	0.14	0
10	SO4	F	504	-	4,4,4	0.23	0	6,6,6	0.09	0
10	SO4	F	505	-	4,4,4	0.22	0	6,6,6	0.13	0
11	EDO	F	506	-	3,3,3	0.48	0	2,2,2	0.30	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	SO4	C	1201	-	-	0/0/0/0	0/0/0/0
10	SO4	C	1202	-	-	0/0/0/0	0/0/0/0
10	SO4	C	1203	-	-	0/0/0/0	0/0/0/0
11	EDO	C	1204	-	-	0/1/1/1	0/0/0/0
11	EDO	C	1205	-	-	0/1/1/1	0/0/0/0
10	SO4	D	2004	-	-	0/0/0/0	0/0/0/0
10	SO4	D	2005	-	-	0/0/0/0	0/0/0/0
10	SO4	D	2006	-	-	0/0/0/0	0/0/0/0
10	SO4	D	2007	-	-	0/0/0/0	0/0/0/0
11	EDO	D	2008	-	-	0/1/1/1	0/0/0/0
11	EDO	D	2009	-	-	0/1/1/1	0/0/0/0
11	EDO	D	2010	-	-	0/1/1/1	0/0/0/0
10	SO4	F	501	6	-	0/0/0/0	0/0/0/0
10	SO4	F	502	-	-	0/0/0/0	0/0/0/0
10	SO4	F	503	-	-	0/0/0/0	0/0/0/0
10	SO4	F	504	-	-	0/0/0/0	0/0/0/0
10	SO4	F	505	-	-	0/0/0/0	0/0/0/0
11	EDO	F	506	-	-	0/1/1/1	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	C	1203	SO4	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	C	1205	EDO	1	0
10	D	2005	SO4	2	0
11	D	2008	EDO	3	0
10	F	502	SO4	1	0
11	F	506	EDO	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	J	83/114 (72%)	0.43	10 (12%) 6 4	64, 97, 141, 158	0
2	A	218/350 (62%)	0.18	5 (2%) 64 57	59, 86, 118, 137	0
2	B	233/350 (66%)	0.87	36 (15%) 3 2	80, 110, 134, 148	0
2	T	53/350 (15%)	3.60	44 (83%) 0 0	113, 149, 165, 169	0
3	C	1099/1169 (94%)	0.60	98 (8%) 12 8	42, 85, 147, 163	0
4	D	1248/1317 (94%)	0.33	38 (3%) 54 47	39, 73, 125, 156	0
5	E	76/107 (71%)	0.35	4 (5%) 30 23	51, 78, 113, 117	0
6	F	302/466 (64%)	0.06	4 (1%) 79 75	38, 72, 122, 137	0
7	O	31/31 (100%)	-0.68	0 100 100	51, 64, 83, 89	0
8	P	26/26 (100%)	-0.78	0 100 100	59, 68, 83, 93	0
9	G	0/17	-	-	-	-
All	All	3369/4297 (78%)	0.46	239 (7%) 19 13	38, 82, 141, 169	0

All (239) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	228	LEU	8.6
2	T	275	LEU	8.0
2	T	269	VAL	7.3
3	C	215	VAL	6.5
2	T	256	LEU	6.4
2	T	261	TYR	6.3
3	C	330	VAL	6.2
2	T	297	VAL	6.1
2	B	183	VAL	6.1
3	C	354	VAL	6.0
3	C	239	ILE	5.9
2	T	298	LYS	5.7

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Mol	Chain	Res	Type	RSRZ
2	B	157	ALA	5.4
2	T	293	SER	5.4
3	C	287	LEU	5.3
2	T	299	ILE	5.3
2	T	281	SER	5.2
2	T	264	LEU	5.1
2	T	289	PHE	5.1
3	C	243	PHE	5.1
2	T	283	LEU	5.0
2	T	253	ASP	5.0
2	A	218	LEU	5.0
2	T	291	GLN	4.9
2	T	254	LEU	4.9
3	C	459	ALA	4.8
2	T	279	THR	4.6
3	C	182	ILE	4.6
3	C	349	PRO	4.4
3	C	252	THR	4.4
3	C	242	ARG	4.4
3	C	254	GLU	4.4
3	C	189	THR	4.4
2	T	268	GLY	4.3
2	B	140	VAL	4.3
2	T	259	ARG	4.2
2	T	273	GLY	4.2
3	C	203	LEU	4.2
3	C	550	VAL	4.2
2	T	296	GLU	4.1
3	C	225	VAL	4.1
3	C	131	ILE	4.0
3	C	244	GLY	4.0
3	C	227	VAL	4.0
2	B	21	PHE	3.9
2	T	278	ARG	3.9
3	C	205	PHE	3.9
3	C	455	SER	3.9
3	C	240	VAL	3.8
3	C	335	TYR	3.8
3	C	333	ILE	3.8
2	B	66	VAL	3.8
3	C	352	VAL	3.7
3	C	337	VAL	3.7

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Mol	Chain	Res	Type	RSRZ
3	C	185	SER	3.7
3	C	235	THR	3.7
2	B	134	LEU	3.7
2	T	294	ILE	3.7
3	C	191	HIS	3.6
3	C	226	THR	3.6
3	C	181	THR	3.6
3	C	351	GLY	3.6
3	C	66	ILE	3.6
2	T	272	VAL	3.5
2	B	110	ILE	3.5
1	J	105	ILE	3.5
3	C	943	VAL	3.5
2	T	263	CYS	3.5
4	D	1178	PRO	3.5
2	T	265	LYS	3.4
3	C	765	PRO	3.4
2	T	280	GLU	3.4
3	C	938	ASP	3.4
2	A	26	LEU	3.4
2	T	267	GLU	3.4
3	C	190	LEU	3.4
4	D	193	VAL	3.4
2	T	301	LEU	3.3
2	T	255	ASP	3.3
3	C	336	LEU	3.3
4	D	1009	LEU	3.3
3	C	70	GLU	3.3
4	D	66	LYS	3.3
3	C	234	TRP	3.3
2	B	128	LEU	3.3
3	C	353	GLU	3.3
3	C	271	LYS	3.3
1	J	74	LYS	3.3
2	B	138	LEU	3.2
3	C	229	LEU	3.2
3	C	186	THR	3.2
3	C	561	PHE	3.2
3	C	248	ILE	3.2
2	B	107	ALA	3.2
2	B	152	ASN	3.2
2	B	1	MET	3.2

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Mol	Chain	Res	Type	RSRZ
4	D	655	TRP	3.2
2	T	274	GLU	3.2
3	C	350	GLY	3.2
2	T	276	VAL	3.1
4	D	197	VAL	3.1
3	C	192	SER	3.1
3	C	968	PHE	3.1
3	C	348	VAL	3.1
2	T	295	ASP	3.1
2	T	270	HIS	3.1
3	C	1133	GLY	3.1
2	T	286	ILE	3.1
2	T	251	ILE	3.1
4	D	769	ARG	3.0
3	C	358	VAL	3.0
3	C	250	MET	3.0
3	C	346	MET	3.0
3	C	286	LEU	3.0
2	A	2	LEU	2.9
3	C	355	PRO	2.9
6	F	213	VAL	2.9
2	T	277	ALA	2.9
2	B	56	ILE	2.9
3	C	259	SER	2.9
4	D	849	PHE	2.9
4	D	1173	SER	2.9
2	B	104	VAL	2.9
2	B	164	VAL	2.9
2	B	59	VAL	2.9
4	D	190	LYS	2.9
2	B	154	ALA	2.9
3	C	456	ARG	2.8
1	J	69	VAL	2.8
2	T	257	THR	2.8
4	D	191	SER	2.8
3	C	71	GLU	2.8
4	D	1191	ASN	2.7
2	A	181	THR	2.7
3	C	687	VAL	2.7
4	D	762	GLY	2.7
1	J	73	LYS	2.7
2	B	64	THR	2.7

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Mol	Chain	Res	Type	RSRZ
4	D	192	ASP	2.7
3	C	302	VAL	2.7
1	J	97	LEU	2.7
3	C	98	PHE	2.7
3	C	196	ILE	2.7
3	C	949	LYS	2.7
3	C	253	LEU	2.6
1	J	103	ASP	2.6
3	C	260	GLY	2.6
4	D	1067	ILE	2.6
3	C	87	ILE	2.5
2	B	32	TYR	2.5
2	T	302	HIS	2.5
2	B	3	ILE	2.5
3	C	180	GLU	2.5
4	D	901	ALA	2.5
4	D	932	ASN	2.5
2	B	184	GLU	2.5
1	J	68	ASP	2.5
3	C	96	LEU	2.5
2	T	266	ARG	2.5
3	C	202	TRP	2.5
4	D	920	PHE	2.5
3	C	488	ILE	2.5
2	T	252	ASP	2.5
3	C	237	GLU	2.4
2	B	208	LEU	2.4
1	J	31	ARG	2.4
2	T	300	LYS	2.4
4	D	186	ALA	2.4
2	B	108	GLY	2.4
6	F	460	VAL	2.4
2	B	130	ASP	2.3
3	C	339	LEU	2.3
3	C	184	LYS	2.3
2	B	172	LEU	2.3
3	C	542	ASN	2.3
1	J	76	LYS	2.3
3	C	812	LEU	2.3
2	B	65	THR	2.3
3	C	522	LEU	2.3
3	C	268	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
3	C	519	ILE	2.3
4	D	1063	PHE	2.3
4	D	832	PRO	2.3
6	F	215	GLN	2.3
4	D	761	ARG	2.3
4	D	1112	LEU	2.3
4	D	467	GLN	2.2
4	D	611	VAL	2.2
3	C	341	GLU	2.2
4	D	1190	GLU	2.2
2	B	58	GLY	2.2
3	C	572	VAL	2.2
3	C	270	ARG	2.2
4	D	195	ARG	2.2
3	C	84	LEU	2.2
4	D	640	LEU	2.2
3	C	564	ALA	2.2
4	D	768	GLU	2.2
4	D	1179	GLY	2.2
3	C	727	ILE	2.2
4	D	822	LEU	2.2
3	C	291	PHE	2.2
4	D	1187	PHE	2.2
2	B	143	GLY	2.2
2	B	69	VAL	2.1
3	C	233	GLY	2.1
5	E	74	GLU	2.1
2	B	194	ILE	2.1
3	C	487	LEU	2.1
4	D	188	GLY	2.1
3	C	201	ALA	2.1
2	B	63	PHE	2.1
3	C	95	SER	2.1
2	T	292	LYS	2.1
3	C	560	GLU	2.1
3	C	32	PHE	2.1
3	C	1043	ILE	2.1
4	D	469	ILE	2.1
6	F	217	ARG	2.1
4	D	779	ASP	2.1
4	D	1027	GLY	2.1
2	B	118	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
5	E	50	LEU	2.1
2	B	15	ALA	2.1
5	E	79	LEU	2.1
5	E	75	TYR	2.1
4	D	934	ASN	2.1
2	T	284	LEU	2.0
2	A	194	ILE	2.0
4	D	607	PRO	2.0
2	B	62	GLU	2.0
2	B	95	MET	2.0
2	B	109	ASP	2.0
2	T	282	ASP	2.0
3	C	963	VAL	2.0
3	C	503	ILE	2.0
3	C	249	MET	2.0
1	J	82	TRP	2.0
3	C	552	VAL	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
10	SO4	F	505	5/5	0.84	0.43	8.69	80,84,117,167	0
12	ZN	D	2001	1/1	0.99	0.22	2.97	66,66,66,66	0
11	EDO	D	2010	4/4	0.87	0.28	1.86	62,75,77,89	0
12	ZN	D	2002	1/1	0.79	0.33	1.80	222,222,222,222	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
11	EDO	C	1204	4/4	0.90	0.23	1.22	53,63,75,77	0
10	SO4	D	2006	5/5	0.88	0.21	0.85	80,103,121,126	0
11	EDO	D	2008	4/4	0.79	0.21	0.36	74,89,105,105	0
11	EDO	F	506	4/4	0.87	0.21	0.32	73,88,95,95	0
11	EDO	C	1205	4/4	0.92	0.19	0.02	74,93,101,112	0
10	SO4	C	1202	5/5	0.84	0.19	-0.13	105,111,115,178	0
10	SO4	D	2005	5/5	0.94	0.17	-0.64	80,85,97,125	0
11	EDO	D	2009	4/4	0.87	0.15	-0.77	71,86,103,103	0
10	SO4	D	2007	5/5	0.92	0.13	-1.12	93,98,113,141	0
10	SO4	D	2004	5/5	0.96	0.16	-	69,72,83,87	0
10	SO4	C	1201	5/5	0.90	0.17	-	111,114,124,138	0
10	SO4	F	501	5/5	0.97	0.06	-	97,98,116,122	0
10	SO4	C	1203	5/5	0.75	0.27	-	103,113,139,197	0
10	SO4	F	503	5/5	0.95	0.08	-	85,92,98,113	0
10	SO4	F	502	5/5	0.95	0.11	-	84,86,102,108	0
13	MG	D	2003	1/1	0.94	0.28	-	82,82,82,82	0
10	SO4	F	504	5/5	0.90	0.24	-	112,114,117,128	0

6.5 Other polymers

There are no such residues in this entry.