



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 25, 2023 – 04:05 AM EDT

PDB ID : 5VI8
Title : Structure of a mycobacterium smegmatis transcription initiation complex with an upstream-fork promoter fragment
Authors : Hubin, E.A.; Campbell, E.A.; Darst, S.A.
Deposited on : 2017-04-14
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35.1

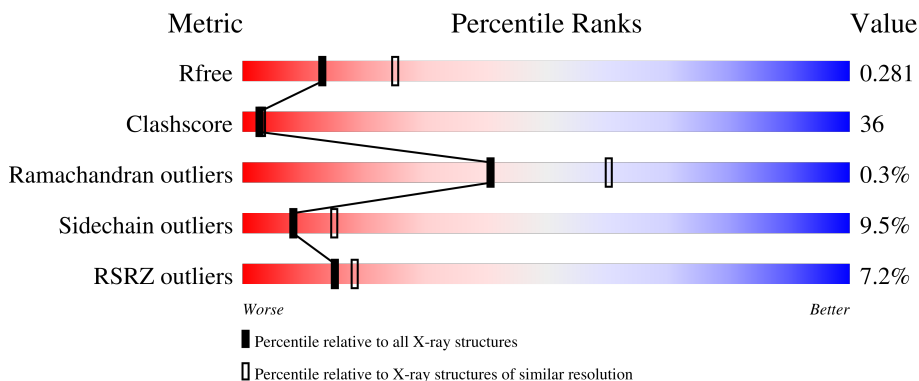
1 Overall quality at a glance

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}	130704	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	
2	A	350	
2	B	350	
3	C	1169	
4	D	1317	

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Mol	Chain	Length	Quality of chain
5	E	107	
6	F	466	
7	O	31	
8	P	26	
9	T	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	-

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 26631 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
			Total	C	N	O	S			
1	J	83	667	419	118	128	2	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	A	218	1617	1020	276	318	3	0	0	0
2	B	233	1667	1054	289	322	2	0	0	0

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	319	Total	C	N	O	S	0	0	0
			2481	1553	450	471	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			

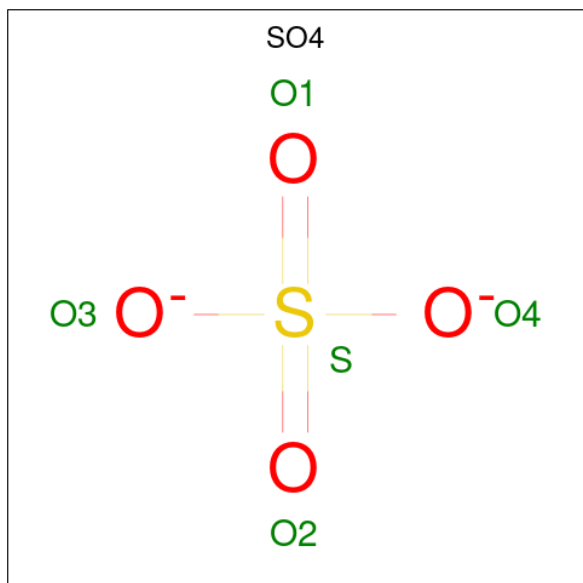
- Molecule 8 is a DNA chain called DNA (26-MER).

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 DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	T	53	Total	C	N	O	S	0	0	0
			377	237	66	73	1			

- Molecule 10 is SULFATE ION (three-letter code: SO₄) (formula: O₄S).



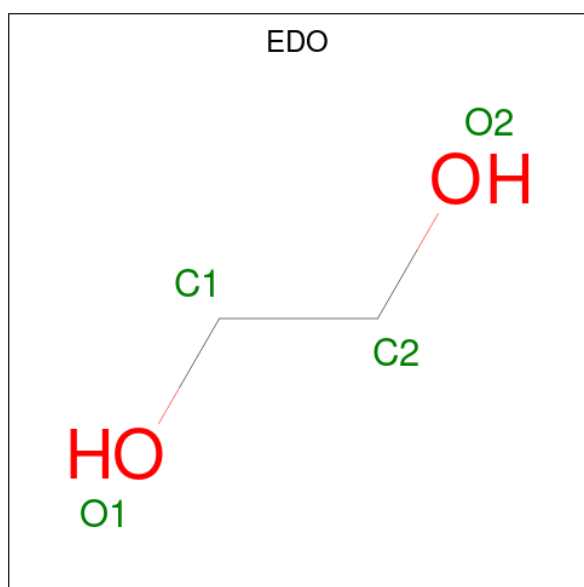
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	C	1	Total	O	S	0	0
			5	4	1		

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

- Molecule 11 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

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

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

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

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

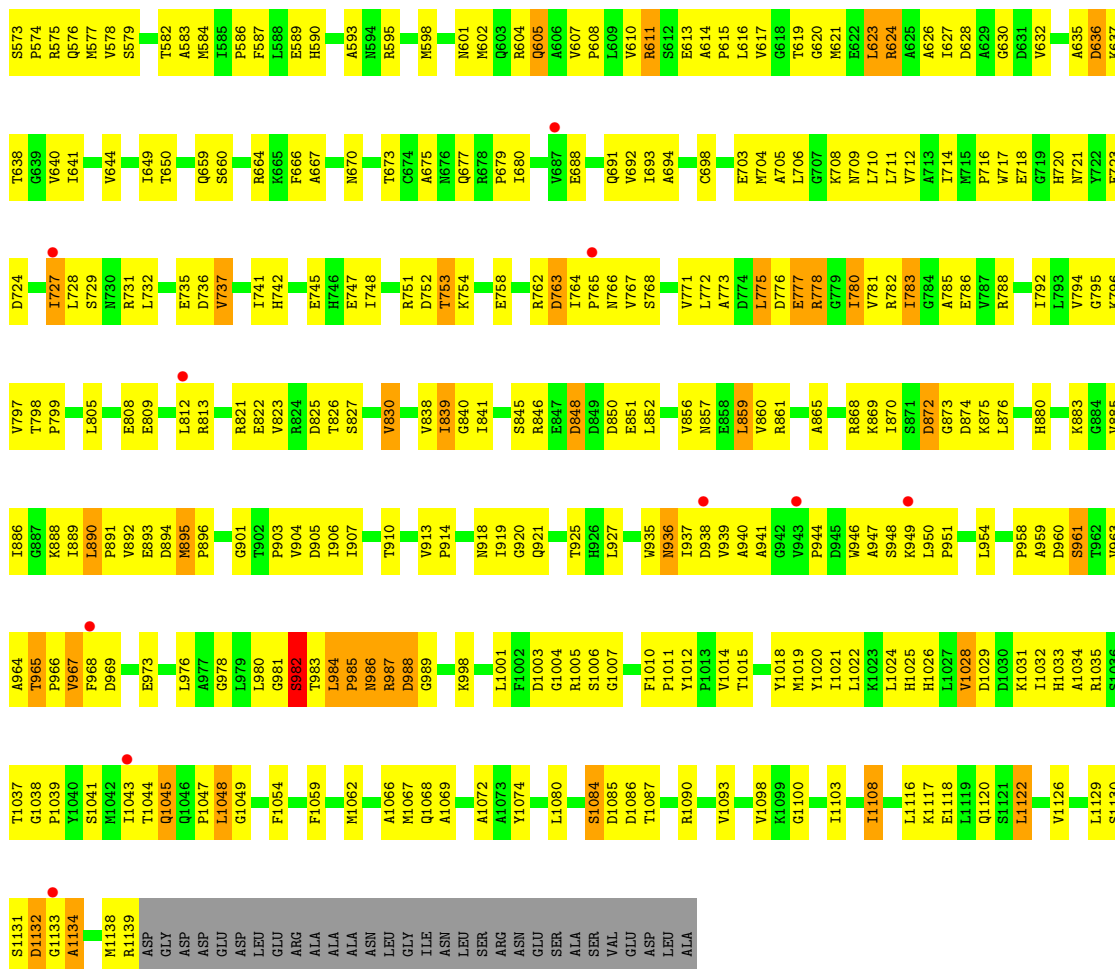
- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	J	1	Total	O	0	0
			1	1		
14	A	3	Total	O	0	0
			3	3		
14	B	1	Total	O	0	0
			1	1		
14	C	17	Total	O	0	0
			17	17		
14	D	51	Total	O	0	0
			51	51		
14	E	2	Total	O	0	0
			2	2		
14	F	16	Total	O	0	0
			16	16		

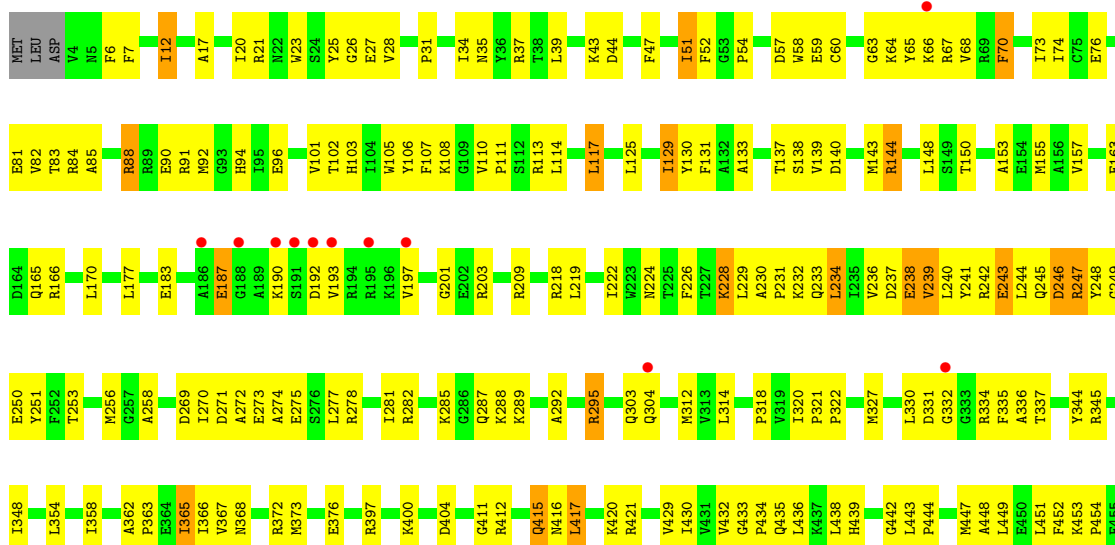
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	O	13	Total 13	O 13	0	0
14	P	4	Total 4	O 4	0	0
14	T	1	Total 1	O 1	0	0



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



4 Data and refinement statistics

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)	51.99 – 2.76 54.91 – 2.75	Depositor EDS
% Data completeness (in resolution range)	99.5 (51.99-2.76) 99.4 (54.91-2.75)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.16 (at 2.77Å)	Xtrriage
Refinement program	PHENIX (1.10.1_2155)	Depositor
R, R_{free}	0.240 , 0.281 0.241 , 0.281	Depositor DCC
R_{free} test set	1989 reflections (1.38%)	wwPDB-VP
Wilson B-factor (Å ²)	78.4	Xtrriage
Anisotropy	0.150	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 52.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtrriage
Estimated twinning fraction	0.003 for l,-k,h	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	26631	wwPDB-VP
Average B, all atoms (Å ²)	86.0	wwPDB-VP

Xtrriage'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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.24	0/681	0.45	0/923
2	A	0.24	0/1641	0.48	0/2236
2	B	0.24	0/1693	0.48	0/2316
3	C	0.25	0/8394	0.47	1/11410 (0.0%)
4	D	0.25	0/9742	0.45	0/13189
5	E	0.24	0/604	0.45	0/822
6	F	0.23	0/2510	0.42	1/3389 (0.0%)
7	O	0.54	0/710	0.96	0/1095
8	P	0.56	0/589	0.95	0/906
9	T	0.24	0/379	0.39	0/515
All	All	0.27	0/26943	0.50	2/36801 (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(°)	Ideal(°)
6	F	144	PRO	N-CA-CB	5.81	110.27	103.30
3	C	890	LEU	CA-CB-CG	5.20	127.26	115.30

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	48	0
2	A	1617	0	1636	178	0
2	B	1667	0	1636	198	0
3	C	8250	0	7989	690	1
4	D	9588	0	9552	634	1
5	E	592	0	583	54	0
6	F	2481	0	2481	137	0
7	O	634	0	350	34	0
8	P	526	0	296	16	0
9	T	377	0	348	30	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	3	0	0	1	0
14	B	1	0	0	1	0
14	C	17	0	0	8	0
14	D	51	0	0	7	0
14	E	2	0	0	0	0
14	F	16	0	0	2	0
14	J	1	0	0	0	0
14	O	13	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	P	4	0	0	0	0
14	T	1	0	0	1	0
All	All	26595	36	25556	1848	1

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 (1848) 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	1.16
3:C:940:ALA:HB1	3:C:941:ALA:HA	1.27	1.14
3:C:228:LEU:HD21	3:C:268:ILE:HG12	1.33	1.08
3:C:540:ASP:HB2	3:C:546:THR:HG23	1.30	1.08
3:C:176:VAL:HG12	3:C:195:VAL:HG22	1.36	1.06
4:D:641:ARG:HA	4:D:656:LYS:HE3	1.40	1.04
3:C:982:SER:HB3	3:C:983:THR:HG23	1.40	1.03
3:C:799:PRO:HA	3:C:823:VAL:HG12	1.36	1.03
4:D:1275:PRO:HG3	5:E:76:VAL:HG11	1.34	1.03
3:C:215:VAL:HG23	3:C:225:VAL:HA	1.39	1.02
3:C:710:LEU:HD22	3:C:1021:ILE:HD11	1.40	1.01
3:C:635:ALA:HB2	3:C:693:ILE:HD11	1.40	1.00
4:D:432:VAL:HG22	4:D:434:PRO:HD3	1.41	1.00
3:C:444:ARG:HH21	3:C:491:LEU:HD23	1.24	1.00
9:T:289:PHE:HE2	9:T:294:ILE:HG13	1.26	0.99
3:C:602:MET:HE1	3:C:883:LYS:HB3	1.39	0.98
2:A:31:GLY:HA2	2:A:192:LEU:HD23	1.46	0.97
4:D:1174:THR:HG23	4:D:1176:PHE:H	1.28	0.97
4:D:603:THR:HG22	4:D:604:LYS:HE2	1.49	0.95
3:C:478:GLU:OE2	3:C:604:ARG:NH2	1.98	0.94
2:A:1:MET:N	2:B:142:ARG:O	1.99	0.94
4:D:815:THR:HG22	4:D:820:LYS:HA	1.49	0.94
6:F:253:MET:HE3	6:F:297:MET:HA	1.50	0.94
4:D:951:LEU:HB3	4:D:956:ILE:HD11	1.50	0.93
3:C:191:HIS:HA	3:C:192:SER:HB3	1.47	0.93
3:C:41:VAL:O	3:C:624:ARG:NH2	2.01	0.92
6:F:308:VAL:HG21	7:O:23:DT:H71	1.49	0.92
3:C:217:ILE:HD11	3:C:272:LEU:HD11	1.52	0.92
3:C:338:ARG:HD2	3:C:346:MET:HG3	1.49	0.92
3:C:1132:ASP:HB3	3:C:1133:GLY:HA2	1.51	0.92
2:B:34:LEU:HD11	2:B:192:LEU:HD22	1.52	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:783:ILE:HD12	3:C:783:ILE:H	1.34	0.91
4:D:327:MET:HG3	4:D:337:THR:HB	1.51	0.91
2:B:63:PHE:CE2	4:D:603:THR:HG23	2.05	0.90
3:C:935:TRP:HA	3:C:983:THR:HG23	1.51	0.90
2:A:89:ASP:CB	2:A:90:ASP:HA	2.00	0.90
2:B:84:VAL:HB	2:B:199:LYS:HD3	1.53	0.90
3:C:92:GLY:O	3:C:133:ASN:ND2	2.06	0.89
5:E:86:GLU:OE2	5:E:94:ARG:NH1	2.06	0.89
6:F:211:LEU:HB2	6:F:216:ARG:HD2	1.54	0.89
3:C:454:LEU:HD22	3:C:459:ALA:HB2	1.55	0.89
3:C:508:ARG:HD3	3:C:515:VAL:HG11	1.54	0.88
6:F:324:LEU:HD23	6:F:328:LEU:HD13	1.54	0.88
2:A:98:ARG:HG2	2:A:135:GLU:HG2	1.54	0.88
2:B:153:LYS:N	2:B:154:ALA:HA	1.86	0.88
3:C:150:MET:HA	3:C:150:MET:HE2	1.55	0.88
3:C:77:LEU:HD11	3:C:124:LEU:HD11	1.54	0.88
3:C:159:ILE:HB	3:C:164:ARG:HD2	1.56	0.87
4:D:930:ASP:O	4:D:933:GLY:HA3	1.74	0.87
3:C:758:GLU:HG2	3:C:798:THR:HG22	1.54	0.87
3:C:510:VAL:N	3:C:568:ASP:O	2.08	0.87
2:A:152:ASN:HB2	2:A:157:ALA:HB3	1.57	0.87
2:B:152:ASN:C	2:B:154:ALA:HA	1.96	0.87
1:J:31:ARG:NH2	1:J:39:GLU:OE1	2.08	0.86
3:C:584:MET:HA	3:C:619:THR:HG21	1.55	0.86
4:D:668:GLY:HA2	4:D:671:MET:HE2	1.55	0.86
3:C:649:ILE:HD11	3:C:679:PRO:HB3	1.57	0.86
4:D:1174:THR:HG21	4:D:1176:PHE:HB2	1.58	0.86
4:D:1071:ASP:HB2	4:D:1073:GLY:N	1.91	0.86
4:D:269:ASP:HB3	4:D:272:ALA:HB3	1.58	0.86
4:D:442:GLY:HA3	4:D:523:GLN:HB2	1.56	0.86
4:D:740:GLN:HE21	4:D:740:GLN:H	1.22	0.86
3:C:938:ASP:O	3:C:944:PRO:HD3	1.76	0.85
4:D:365:ILE:H	4:D:365:ILE:HD12	1.40	0.85
4:D:655:TRP:HA	4:D:655:TRP:CE3	2.09	0.85
2:B:21:PHE:HB2	2:B:194:ILE:HG22	1.59	0.85
4:D:1088:ARG:HG2	4:D:1089:VAL:H	1.42	0.85
2:B:6:ARG:O	2:B:25:PRO:HD2	1.77	0.85
6:F:253:MET:CE	6:F:300:GLN:HB2	2.06	0.85
3:C:170:LEU:HA	3:C:369:LEU:H	1.42	0.84
2:B:32:TYR:HB3	3:C:1005:ARG:HG3	1.57	0.84
2:B:95:MET:HG2	2:B:113:PRO:HD2	1.60	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:157:ALA:HB1	2:A:161:ARG:HD2	1.57	0.84
6:F:280:LYS:HG2	7:O:30:DC:OP2	1.76	0.84
4:D:599:TYR:HB2	4:D:610:GLY:HA3	1.56	0.84
3:C:981:GLY:O	3:C:982:SER:OG	1.95	0.83
3:C:1048:LEU:HD23	3:C:1048:LEU:H	1.44	0.83
2:B:64:THR:O	2:B:65:THR:OG1	1.95	0.83
3:C:379:GLN:HG2	3:C:421:PHE:HB2	1.61	0.83
4:D:901:ALA:H	4:D:912:ASP:HB2	1.44	0.83
9:T:289:PHE:CE2	9:T:294:ILE:HG13	2.12	0.83
3:C:574:PRO:O	3:C:575:ARG:HG2	1.79	0.82
3:C:940:ALA:HB1	3:C:941:ALA:CA	2.09	0.82
4:D:1174:THR:HG23	4:D:1176:PHE:N	1.94	0.82
3:C:718:GLU:H	4:D:724:THR:HG21	1.45	0.82
4:D:612:TYR:HB2	4:D:635:VAL:HG12	1.59	0.82
3:C:1059:PHE:HZ	3:C:1067:MET:HE3	1.44	0.82
4:D:929:VAL:HG12	4:D:935:VAL:HG22	1.60	0.82
4:D:818:GLY:O	4:D:838:SER:HB3	1.79	0.81
2:B:151:GLN:HG2	2:B:154:ALA:HB1	1.63	0.81
4:D:12:ILE:HD11	4:D:1221:TRP:CD2	2.16	0.81
4:D:1275:PRO:HB3	5:E:79:LEU:HD11	1.62	0.81
2:B:100:GLN:HA	2:B:133:LYS:HA	1.62	0.81
7:O:28:DT:H2''	7:O:29:DA:H5'	1.62	0.81
4:D:573:PRO:HG2	4:D:576:MET:HE3	1.63	0.81
5:E:85:GLN:HE21	5:E:85:GLN:H	1.29	0.81
2:A:48:GLY:HA2	2:A:49:ALA:HB3	1.61	0.81
3:C:540:ASP:CB	3:C:546:THR:HG23	2.11	0.81
3:C:445:ARG:NH2	14:C:1304:HOH:O	2.13	0.80
4:D:643:PRO:O	4:D:647:GLU:HB3	1.80	0.80
6:F:253:MET:HE2	6:F:300:GLN:HB2	1.61	0.80
4:D:1248:GLY:O	4:D:1252:ASN:ND2	2.14	0.80
1:J:102:LEU:O	1:J:105:ILE:HG22	1.81	0.79
2:A:181:THR:N	2:A:189:PHE:O	2.15	0.79
3:C:148:PHE:HE1	3:C:380:ILE:HD11	1.46	0.79
4:D:642:PRO:HD3	4:D:656:LYS:HG2	1.63	0.79
4:D:1171:SER:CA	4:D:1174:THR:HG22	2.12	0.79
3:C:412:ARG:HD2	6:F:322:ARG:HE	1.47	0.79
7:O:11:DA:H2''	7:O:12:DG:H5''	1.64	0.79
2:B:18:ARG:HG3	2:B:197:GLU:HG3	1.64	0.79
4:D:47:PHE:O	4:D:88:ARG:NH2	2.15	0.79
2:A:152:ASN:CB	2:A:157:ALA:HB3	2.13	0.79
3:C:348:VAL:HB	3:C:351:GLY:HA3	1.65	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:84:LEU:H	5:E:84:LEU:HD12	1.46	0.78
4:D:599:TYR:CE1	4:D:601:ALA:HB2	2.18	0.78
2:A:40:ARG:HD3	2:B:33:THR:HG22	1.65	0.78
3:C:891:PRO:HB2	3:C:893:GLU:HG2	1.64	0.78
6:F:454:HIS:ND1	6:F:455:PRO:HD2	1.98	0.78
2:A:86:SER:OG	2:A:119:HIS:NE2	2.14	0.78
3:C:88:GLU:HG2	3:C:92:GLY:HA2	1.65	0.78
4:D:641:ARG:CA	4:D:656:LYS:HE3	2.13	0.78
3:C:51:SER:OG	3:C:373:GLY:N	2.14	0.78
4:D:12:ILE:HD11	4:D:1221:TRP:CE3	2.19	0.78
3:C:1138:MET:O	3:C:1139:ARG:HG3	1.84	0.78
4:D:937:ILE:HD12	4:D:951:LEU:HG	1.65	0.77
4:D:111:PRO:O	4:D:113:ARG:NH1	2.16	0.77
4:D:26:GLY:HA3	4:D:51:ILE:HG22	1.65	0.77
2:A:56:ILE:HB	2:A:59:VAL:HG22	1.67	0.77
2:A:86:SER:HG	2:A:119:HIS:HE2	1.29	0.77
2:B:170:PRO:HB2	2:B:202:ILE:HD11	1.66	0.77
3:C:593:ALA:HB2	4:D:852:THR:HG22	1.67	0.77
3:C:763:ASP:HB3	3:C:821:ARG:HH22	1.50	0.77
5:E:30:LEU:O	5:E:33:THR:HG22	1.85	0.77
3:C:637:LYS:HD2	3:C:659:GLN:HE22	1.49	0.77
9:T:279:THR:HG23	9:T:282:ASP:HB2	1.67	0.77
1:J:68:ASP:HA	1:J:69:VAL:HB	1.66	0.77
4:D:962:ARG:NH1	4:D:977:CYS:SG	2.58	0.77
3:C:1003:ASP:OD1	3:C:1006:SER:N	2.17	0.77
6:F:404:THR:O	6:F:457:ARG:NH2	2.18	0.77
4:D:444:PRO:HG3	4:D:521:ALA:O	1.84	0.76
3:C:940:ALA:CB	3:C:941:ALA:HA	2.11	0.76
4:D:573:PRO:HG2	4:D:576:MET:CE	2.15	0.76
4:D:735:VAL:HG12	4:D:840:ARG:HD2	1.66	0.76
7:O:14:DG:H2''	7:O:15:DT:OP2	1.84	0.76
4:D:1168:ILE:HD13	4:D:1176:PHE:HB3	1.65	0.76
4:D:901:ALA:HB2	4:D:911:ARG:HA	1.66	0.76
4:D:487:LEU:HG	4:D:491:ILE:HD12	1.67	0.76
6:F:201:LEU:HD11	6:F:219:MET:HB3	1.67	0.76
2:B:32:TYR:HE1	2:B:178:VAL:HG21	1.50	0.75
2:B:184:GLU:CA	2:B:187:THR:HG22	2.14	0.75
3:C:720:HIS:O	4:D:432:VAL:HG11	1.86	0.75
3:C:773:ALA:O	3:C:782:ARG:NH2	2.20	0.75
3:C:935:TRP:HA	3:C:983:THR:CG2	2.16	0.75
4:D:772:SER:O	4:D:776:ILE:HG13	1.87	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:822:LEU:HD23	4:D:834:PRO:HA	1.67	0.75
4:D:1009:LEU:HD12	4:D:1146:GLN:HG3	1.67	0.75
4:D:951:LEU:HB3	4:D:956:ILE:CD1	2.15	0.75
2:B:26:LEU:HD11	2:B:34:LEU:HD21	1.69	0.75
4:D:417:LEU:HG	4:D:1254:ILE:HG23	1.67	0.75
2:A:28:PRO:HA	2:A:190:ASP:OD2	1.87	0.74
3:C:215:VAL:HG12	3:C:217:ILE:CG2	2.16	0.74
4:D:277:LEU:HD11	4:D:295:ARG:HG2	1.67	0.74
3:C:509:LYS:O	3:C:516:THR:HG22	1.87	0.74
3:C:205:PHE:CE1	3:C:215:VAL:HG13	2.22	0.74
4:D:139:VAL:HG12	4:D:231:PRO:HD3	1.69	0.74
9:T:264:LEU:HB3	9:T:269:VAL:CG2	2.18	0.74
4:D:796:ASN:HD21	4:D:798:ILE:HB	1.53	0.74
3:C:204:GLU:OE1	3:C:216:ARG:NH1	2.19	0.74
4:D:721:TYR:O	4:D:725:ARG:HG2	1.86	0.74
4:D:644:THR:HA	4:D:647:GLU:OE1	1.88	0.74
7:O:6:DA:H2 ^{''}	7:O:7:DC:H5 [']	1.69	0.74
3:C:191:HIS:HA	3:C:192:SER:CB	2.17	0.74
3:C:720:HIS:CE1	3:C:888:LYS:HD3	2.23	0.74
2:A:66:VAL:O	2:A:69:VAL:HG22	1.87	0.74
2:B:24:GLU:OE2	2:B:191:LYS:HD3	1.87	0.74
3:C:235:THR:N	3:C:238:GLN:OE1	2.20	0.74
3:C:361:ILE:H	3:C:361:ILE:HD12	1.53	0.74
4:D:590:THR:HG21	4:D:630:ARG:HH21	1.53	0.74
4:D:859:LEU:O	4:D:862:THR:HG22	1.87	0.74
4:D:237:ASP:HB3	4:D:240:LEU:HB3	1.70	0.73
4:D:596:THR:HG22	4:D:626:ALA:O	1.88	0.73
8:P:11:DA:H2 ^{''}	8:P:12:DA:O5 [']	1.88	0.73
3:C:742:HIS:CD2	3:C:868:ARG:HG3	2.23	0.73
4:D:642:PRO:HG3	4:D:661:TRP:CE2	2.22	0.73
2:A:14:VAL:HG13	2:A:18:ARG:HG3	1.68	0.73
3:C:231:ALA:HB1	3:C:265:LEU:CD1	2.17	0.73
3:C:494:TYR:HB3	3:C:506:PRO:HG3	1.69	0.73
3:C:132:ASN:HB3	3:C:135:THR:HG22	1.68	0.73
2:B:22:VAL:HG12	2:B:193:ILE:HD12	1.70	0.73
2:B:158:GLU:HB3	2:B:161:ARG:HB2	1.70	0.73
3:C:728:LEU:CD2	3:C:906:ILE:HG22	2.19	0.73
2:A:14:VAL:HG12	2:A:19:SER:HA	1.69	0.73
2:B:181:THR:O	2:B:189:PHE:N	2.20	0.73
3:C:578:VAL:HG13	3:C:582:THR:HB	1.70	0.73
3:C:1018:TYR:O	14:C:1302:HOH:O	2.04	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:238:GLU:HA	4:D:241:TYR:HB3	1.69	0.73
4:D:26:GLY:HA3	4:D:51:ILE:CG2	2.19	0.73
4:D:1069:PRO:HG2	4:D:1073:GLY:H	1.54	0.73
8:P:13:DC:H2''	8:P:14:DA:C8	2.24	0.73
3:C:249:MET:O	3:C:253:LEU:HD23	1.89	0.72
3:C:939:VAL:CG2	3:C:940:ALA:HA	2.19	0.72
4:D:655:TRP:HA	4:D:655:TRP:HE3	1.52	0.72
6:F:253:MET:HE3	6:F:297:MET:CA	2.17	0.72
3:C:47:VAL:HG23	3:C:497:VAL:HG21	1.71	0.72
3:C:637:LYS:HD2	3:C:659:GLN:NE2	2.03	0.72
4:D:344:TYR:O	4:D:348:ILE:HG22	1.89	0.72
3:C:636:ASP:OD1	3:C:636:ASP:N	2.21	0.72
3:C:984:LEU:HB2	3:C:985:PRO:HA	1.70	0.72
4:D:106:TYR:HB3	4:D:312:MET:CE	2.20	0.72
2:B:2:LEU:CB	2:B:231:HIS:HA	2.19	0.72
2:A:48:GLY:CA	2:A:49:ALA:HB3	2.19	0.72
3:C:87:ILE:HD12	3:C:388:GLU:HG3	1.69	0.72
4:D:587:TYR:O	4:D:590:THR:HG22	1.89	0.72
3:C:426:GLN:HE21	3:C:451:PRO:HD3	1.55	0.72
4:D:527:LEU:HD22	4:D:575:ALA:O	1.89	0.72
7:O:19:DA:H2''	7:O:20:DT:O5'	1.88	0.72
3:C:205:PHE:HE1	3:C:215:VAL:HG13	1.55	0.72
3:C:982:SER:OG	14:C:1303:HOH:O	2.06	0.71
4:D:488:GLU:HG3	4:D:516:LEU:HD12	1.71	0.71
3:C:444:ARG:NH2	3:C:492:SER:O	2.23	0.71
3:C:1130:SER:HB3	3:C:1132:ASP:O	1.90	0.71
3:C:239:ILE:HG21	3:C:253:LEU:HD22	1.71	0.71
3:C:496:ARG:NH2	3:C:504:GLU:OE1	2.23	0.71
3:C:845:SER:N	3:C:850:ASP:OD2	2.21	0.71
7:O:15:DT:OP1	9:T:258:VAL:HG21	1.89	0.71
3:C:482:GLY:O	3:C:485:ILE:HG13	1.90	0.71
3:C:936:ASN:HD22	3:C:937:ILE:H	1.37	0.71
3:C:1086:ASP:O	3:C:1090:ARG:HG2	1.90	0.71
4:D:278:ARG:O	4:D:281:ILE:HG13	1.90	0.71
3:C:494:TYR:HD2	3:C:572:VAL:HG21	1.55	0.71
2:A:11:GLU:OE1	2:A:205:ARG:NE	2.22	0.71
3:C:780:ILE:HD11	3:C:841:ILE:HD13	1.73	0.71
4:D:138:SER:HB3	4:D:253:THR:OG1	1.90	0.71
4:D:527:LEU:HD21	4:D:581:MET:HE1	1.72	0.71
5:E:45:SER:OG	5:E:105:GLU:OE2	2.01	0.71
4:D:113:ARG:HB2	4:D:312:MET:HE3	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:155:MET:CE	4:D:219:LEU:HB3	2.20	0.71
6:F:308:VAL:HG22	14:F:607:HOH:O	1.91	0.71
6:F:320:ILE:HG23	6:F:340:GLU:HG2	1.72	0.71
3:C:250:MET:HA	3:C:253:LEU:HD21	1.73	0.70
6:F:397:GLN:O	6:F:401:VAL:HG23	1.90	0.70
3:C:508:ARG:HD3	3:C:515:VAL:CG1	2.21	0.70
3:C:613:GLU:HB3	3:C:708:LYS:HD3	1.71	0.70
1:J:91:VAL:HG22	1:J:92:GLU:OE1	1.92	0.70
3:C:711:LEU:HD23	3:C:904:VAL:HA	1.73	0.70
3:C:44:LEU:HD13	3:C:440:LEU:HD21	1.72	0.70
6:F:164:ASP:OD1	6:F:166:VAL:HG22	1.91	0.70
3:C:328:ASP:O	3:C:332:THR:HG23	1.92	0.70
3:C:1026:HIS:HB3	3:C:1031:LYS:HE3	1.74	0.70
3:C:102:ARG:NH2	3:C:127:THR:OG1	2.23	0.70
3:C:1045:GLN:HG2	3:C:1087:THR:HG22	1.73	0.70
3:C:1100:GLY:HA3	4:D:458:LYS:HE3	1.74	0.70
4:D:238:GLU:OE2	4:D:242:ARG:NH2	2.23	0.70
3:C:1068:GLN:NE2	4:D:1249:LEU:HD13	2.07	0.70
1:J:79:ARG:NH2	7:O:25:DC:OP1	2.25	0.70
3:C:265:LEU:HD11	3:C:287:LEU:HD12	1.73	0.70
3:C:728:LEU:HB2	3:C:889:ILE:HG12	1.73	0.69
3:C:982:SER:HB3	3:C:983:THR:CG2	2.21	0.69
4:D:1166:VAL:HA	4:D:1207:VAL:HG23	1.74	0.69
9:T:256:LEU:HD22	9:T:297:VAL:HG22	1.74	0.69
2:B:63:PHE:HE2	4:D:603:THR:HG23	1.53	0.69
3:C:390:VAL:O	3:C:394:ARG:HB2	1.92	0.69
3:C:1108:ILE:H	3:C:1108:ILE:HD12	1.55	0.69
4:D:951:LEU:C	4:D:956:ILE:HD11	2.13	0.69
4:D:1232:ARG:NH1	4:D:1236:ASP:OD2	2.24	0.69
2:A:38:LEU:HD13	2:A:208:LEU:HD11	1.75	0.69
2:B:30:PHE:HA	2:B:33:THR:HG23	1.72	0.69
5:E:26:TYR:HE1	5:E:29:PRO:HD3	1.57	0.69
3:C:299:LEU:HB3	3:C:323:THR:HA	1.74	0.69
3:C:531:VAL:HG13	3:C:552:VAL:CG2	2.22	0.69
4:D:668:GLY:HA2	4:D:671:MET:CE	2.22	0.69
6:F:399:GLN:O	6:F:403:GLU:HG2	1.92	0.69
3:C:246:SER:CB	3:C:337:VAL:HG11	2.22	0.69
3:C:52:PHE:HZ	3:C:150:MET:HE2	1.57	0.69
3:C:575:ARG:HE	3:C:967:VAL:HG22	1.57	0.69
3:C:754:LYS:HE2	3:C:754:LYS:H	1.58	0.69
2:B:47:PRO:HA	2:B:144:ARG:HG3	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:182:ARG:N	2:B:186:ARG:O	2.25	0.69
2:B:32:TYR:CB	3:C:1005:ARG:HG3	2.23	0.69
2:B:216:VAL:HG13	2:B:217:GLU:H	1.58	0.69
3:C:776:ASP:HB2	3:C:777:GLU:OE1	1.93	0.69
7:O:28:DT:OP1	14:O:101:HOH:O	2.11	0.69
2:A:94:THR:HG22	2:A:139:VAL:HG22	1.74	0.68
3:C:732:LEU:HA	3:C:737:VAL:CG1	2.23	0.68
4:D:1174:THR:HA	4:D:1175:GLU:CB	2.22	0.68
6:F:253:MET:CE	6:F:297:MET:HA	2.21	0.68
2:A:106:THR:HA	2:A:125:ILE:HD13	1.75	0.68
3:C:727:ILE:HG22	3:C:888:LYS:HB3	1.73	0.68
4:D:230:ALA:N	4:D:233:GLN:OE1	2.23	0.68
4:D:622:MET:CE	4:D:629:VAL:HG22	2.23	0.68
3:C:507:TYR:OH	3:C:527:GLU:OE2	2.10	0.68
3:C:910:THR:HG23	4:D:730:VAL:HG23	1.75	0.68
4:D:106:TYR:HB3	4:D:312:MET:HE3	1.74	0.68
4:D:647:GLU:HB2	4:D:655:TRP:CZ3	2.29	0.68
2:B:3:ILE:HA	2:B:232:ILE:CB	2.24	0.68
3:C:148:PHE:CE1	3:C:380:ILE:HD11	2.29	0.68
3:C:754:LYS:H	3:C:754:LYS:CE	2.07	0.68
5:E:35:PRO:HG2	5:E:40:LEU:HD11	1.76	0.68
2:A:158:GLU:H	2:A:161:ARG:HH11	1.42	0.68
4:D:708:VAL:O	4:D:712:VAL:HG23	1.93	0.68
3:C:650:THR:HG22	3:C:660:SER:OG	1.93	0.68
4:D:400:LYS:HE3	4:D:404:ASP:HB3	1.76	0.68
4:D:931:ALA:HB1	4:D:932:ASN:HD22	1.59	0.68
8:P:11:DA:H2''	8:P:12:DA:C5'	2.24	0.68
3:C:1098:VAL:HG11	4:D:469:ILE:HD12	1.75	0.67
4:D:73:ILE:O	4:D:82:VAL:HG12	1.94	0.67
1:J:42:VAL:HG13	4:D:74:ILE:HD12	1.75	0.67
3:C:191:HIS:HB2	3:C:336:LEU:HD21	1.76	0.67
3:C:239:ILE:CG2	3:C:253:LEU:HD22	2.24	0.67
3:C:851:GLU:O	3:C:852:LEU:HG	1.94	0.67
6:F:330:ARG:NH2	6:F:336:GLU:OE2	2.25	0.67
4:D:599:TYR:CB	4:D:610:GLY:HA3	2.25	0.67
4:D:648:ALA:O	4:D:652:GLU:HB2	1.93	0.67
3:C:613:GLU:O	3:C:705:ALA:HB1	1.94	0.67
4:D:603:THR:CG2	4:D:604:LYS:HE2	2.23	0.67
1:J:89:ARG:NH2	6:F:276:THR:HG23	2.09	0.67
2:B:74:THR:HG21	4:D:611:VAL:HG11	1.74	0.67
3:C:45:LEU:HD12	3:C:628:ASP:O	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:64:LEU:HD22	1:J:66:GLU:H	1.58	0.67
2:A:33:THR:HG21	2:B:37:SER:HA	1.76	0.67
3:C:426:GLN:NE2	3:C:450:GLY:HA2	2.09	0.67
3:C:1028:VAL:O	3:C:1032:ILE:HG22	1.94	0.67
6:F:254:ALA:HA	10:F:502:SO4:O3	1.95	0.67
4:D:588:LEU:HD22	4:D:668:GLY:HA3	1.77	0.67
4:D:878:ASP:OD2	4:D:1250:LYS:NZ	2.28	0.67
7:O:27:DA:OP1	14:O:102:HOH:O	2.13	0.67
3:C:467:HIS:CG	3:C:468:PRO:HD2	2.30	0.67
3:C:250:MET:HA	3:C:253:LEU:CD2	2.25	0.66
3:C:667:ALA:N	14:C:1301:HOH:O	2.03	0.66
3:C:710:LEU:HD13	3:C:1021:ILE:HG12	1.76	0.66
4:D:1168:ILE:O	4:D:1178:PRO:HA	1.95	0.66
5:E:57:ARG:NE	5:E:95:GLU:OE1	2.23	0.66
4:D:826:PRO:HD3	4:D:853:HIS:ND1	2.10	0.66
2:B:79:ASN:OD1	4:D:636:ARG:NH2	2.24	0.66
3:C:77:LEU:CD1	3:C:124:LEU:HD11	2.25	0.66
3:C:533:ALA:HB2	3:C:567:VAL:HG11	1.77	0.66
3:C:872:ASP:OD1	3:C:872:ASP:N	2.17	0.66
3:C:1059:PHE:CZ	3:C:1067:MET:HE3	2.30	0.66
3:C:1062:MET:HE3	14:C:1308:HOH:O	1.94	0.66
4:D:647:GLU:HG2	4:D:648:ALA:N	2.11	0.66
4:D:1174:THR:CG2	4:D:1176:PHE:HB2	2.25	0.66
2:B:105:VAL:HB	2:B:125:ILE:HG23	1.78	0.66
2:B:120:ASN:ND2	2:B:123:MET:SD	2.67	0.66
4:D:578:ARG:HB2	11:D:2008:EDO:C2	2.26	0.66
4:D:599:TYR:CZ	4:D:601:ALA:HB2	2.30	0.66
2:B:32:TYR:CG	3:C:1005:ARG:HG3	2.29	0.66
3:C:799:PRO:CA	3:C:823:VAL:HG12	2.21	0.66
4:D:780:ALA:O	4:D:784:VAL:HG22	1.95	0.66
6:F:219:MET:HA	6:F:219:MET:HE2	1.78	0.66
2:B:32:TYR:CE1	2:B:178:VAL:HG21	2.30	0.66
3:C:250:MET:O	3:C:253:LEU:HG	1.96	0.66
4:D:706:ILE:HD12	5:E:36:PRO:HB3	1.76	0.66
3:C:796:LYS:HB3	3:C:826:THR:O	1.95	0.66
4:D:1079:ASP:N	4:D:1079:ASP:OD1	2.28	0.66
3:C:454:LEU:HD22	3:C:459:ALA:CB	2.24	0.66
2:A:177:LYS:HE2	2:A:193:ILE:HD11	1.77	0.66
2:B:43:LEU:HD12	2:B:171:VAL:HG23	1.78	0.66
3:C:721:ASN:HD22	3:C:727:ILE:HD11	1.61	0.66
4:D:889:ASP:OD2	4:D:891:GLU:N	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:712:VAL:HB	3:C:906:ILE:HD11	1.76	0.65
3:C:44:LEU:CD1	3:C:440:LEU:HD21	2.25	0.65
3:C:1103:ILE:HD12	4:D:548:SER:HA	1.78	0.65
4:D:59:GLU:OE2	4:D:66:LYS:NZ	2.29	0.65
4:D:139:VAL:CG1	4:D:231:PRO:HD3	2.26	0.65
2:A:66:VAL:HB	2:A:69:VAL:HG21	1.77	0.65
2:B:143:GLY:HA3	2:B:168:TYR:CD1	2.31	0.65
4:D:881:GLN:HE22	4:D:1250:LYS:HE2	1.62	0.65
4:D:1074:GLU:O	14:D:2102:HOH:O	2.12	0.65
2:A:177:LYS:HE2	2:A:193:ILE:CD1	2.26	0.65
2:A:157:ALA:CB	2:A:161:ARG:HD2	2.25	0.65
3:C:176:VAL:HG12	3:C:195:VAL:CG2	2.23	0.65
4:D:642:PRO:CD	4:D:656:LYS:HG2	2.27	0.65
4:D:218:ARG:O	4:D:222:ILE:HG13	1.96	0.65
4:D:924:LEU:HD21	4:D:943:LEU:HD11	1.78	0.65
5:E:40:LEU:HB3	5:E:50:LEU:HD11	1.79	0.65
2:A:89:ASP:CB	2:A:90:ASP:CA	2.75	0.65
3:C:772:LEU:HA	3:C:775:LEU:HD22	1.79	0.65
4:D:320:ILE:HG12	4:D:321:PRO:HD2	1.79	0.65
4:D:527:LEU:HD21	4:D:581:MET:CE	2.26	0.65
4:D:980:ARG:HD3	4:D:985:GLY:O	1.98	0.64
7:O:12:DG:N7	14:O:104:HOH:O	2.30	0.64
2:A:33:THR:CG2	2:B:37:SER:HA	2.28	0.64
3:C:338:ARG:HD3	3:C:343:GLN:NE2	2.11	0.64
3:C:434:ASN:O	3:C:608:PRO:HD3	1.97	0.64
3:C:480:PRO:O	3:C:485:ILE:HG12	1.97	0.64
3:C:710:LEU:CD2	3:C:1021:ILE:HD11	2.23	0.64
4:D:193:VAL:O	4:D:197:VAL:HG23	1.97	0.64
2:A:24:GLU:CD	2:A:191:LYS:HD3	2.18	0.64
3:C:236:ASN:OD1	3:C:253:LEU:HD13	1.97	0.64
7:O:19:DA:H4'	7:O:20:DT:OP1	1.96	0.64
3:C:1072:ALA:HB1	4:D:554:GLU:OE2	1.97	0.64
4:D:661:TRP:HZ3	4:D:663:ALA:HB2	1.62	0.64
4:D:956:ILE:HD12	4:D:956:ILE:O	1.98	0.64
4:D:1171:SER:HA	4:D:1174:THR:HG22	1.78	0.64
6:F:451:LYS:O	6:F:454:HIS:HB3	1.98	0.64
3:C:531:VAL:HG13	3:C:552:VAL:HG23	1.80	0.64
10:C:1203:SO4:O1	4:D:540:GLN:NE2	2.30	0.64
4:D:363:PRO:HB2	4:D:365:ILE:CD1	2.27	0.64
6:F:345:PRO:O	6:F:348:VAL:HG13	1.98	0.64
3:C:215:VAL:HG12	3:C:217:ILE:HG23	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:348:VAL:HB	3:C:351:GLY:CA	2.27	0.64
3:C:771:VAL:HG23	3:C:772:LEU:CD1	2.27	0.64
4:D:237:ASP:OD1	4:D:239:VAL:HG13	1.98	0.64
4:D:438:LEU:HA	4:D:525:HIS:CD2	2.33	0.64
4:D:614:SER:HB2	4:D:615:PRO:HD2	1.78	0.64
4:D:627:LEU:HD13	4:D:667:LEU:HD12	1.80	0.64
2:A:42:LEU:O	2:A:171:VAL:HG11	1.98	0.64
2:B:198:THR:HG21	2:B:202:ILE:HD12	1.80	0.64
2:A:40:ARG:NH1	2:B:33:THR:HG22	2.13	0.64
3:C:477:ILE:CD1	4:D:852:THR:HG21	2.28	0.64
3:C:846:ARG:N	3:C:857:ASN:O	2.28	0.64
2:B:30:PHE:HA	2:B:33:THR:CG2	2.28	0.63
3:C:981:GLY:O	14:C:1303:HOH:O	2.15	0.63
4:D:21:ARG:NE	4:D:96:GLU:OE2	2.26	0.63
4:D:642:PRO:HG3	4:D:661:TRP:CD2	2.32	0.63
4:D:846:LEU:O	4:D:850:ILE:HG12	1.98	0.63
3:C:729:SER:OG	3:C:905:ASP:HA	1.99	0.63
4:D:6:PHE:CD1	4:D:1257:LYS:HE3	2.34	0.63
6:F:338:ALA:HB1	6:F:343:ILE:O	1.98	0.63
3:C:135:THR:HG23	3:C:137:GLU:H	1.64	0.63
4:D:190:LYS:HE3	4:D:193:VAL:HG23	1.81	0.63
8:P:11:DA:H4'	8:P:12:DA:OP1	1.98	0.63
3:C:765:PRO:HD2	3:C:825:ASP:HB2	1.79	0.63
6:F:462:ARG:NH1	6:F:465:LEU:HD12	2.14	0.63
2:A:14:VAL:CG1	2:A:18:ARG:HG3	2.29	0.63
5:E:29:PRO:HG2	5:E:34:ASN:HB2	1.80	0.63
3:C:718:GLU:H	4:D:724:THR:CG2	2.11	0.63
4:D:31:PRO:HB2	4:D:345:ARG:HG2	1.81	0.63
6:F:253:MET:HE1	6:F:300:GLN:HB2	1.80	0.63
1:J:96:GLU:O	1:J:100:GLU:HG3	1.99	0.63
4:D:190:LYS:NZ	4:D:192:ASP:HB3	2.13	0.63
2:A:40:ARG:NH2	3:C:894:ASP:OD2	2.32	0.63
4:D:1119:PRO:HA	4:D:1122:VAL:CG1	2.28	0.63
6:F:181:ALA:O	6:F:185:VAL:HG23	1.99	0.63
2:B:95:MET:HG2	2:B:113:PRO:CD	2.29	0.62
3:C:203:LEU:HD13	3:C:217:ILE:HG22	1.80	0.62
3:C:876:LEU:HD13	3:C:886:ILE:HG13	1.81	0.62
4:D:435:GLN:OE1	4:D:435:GLN:N	2.26	0.62
2:B:50:ALA:HB3	2:B:168:TYR:HD2	1.63	0.62
2:B:85:VAL:HG23	2:B:117:THR:O	1.98	0.62
3:C:727:ILE:HG13	3:C:907:ILE:HB	1.79	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:665:THR:HG22	4:D:684:ASN:ND2	2.15	0.62
4:D:726:SER:OG	4:D:728:VAL:HG23	1.98	0.62
4:D:1168:ILE:HD13	4:D:1176:PHE:CB	2.29	0.62
4:D:1275:PRO:HG3	5:E:76:VAL:CG1	2.20	0.62
2:A:158:GLU:H	2:A:161:ARG:NH1	1.97	0.62
4:D:177:LEU:HD23	4:D:177:LEU:O	1.99	0.62
4:D:594:GLY:HA2	4:D:598:GLU:OE1	1.99	0.62
4:D:602:ALA:HB3	4:D:607:PRO:O	2.00	0.62
4:D:846:LEU:H	4:D:846:LEU:HD12	1.62	0.62
6:F:204:LEU:O	6:F:208:GLY:N	2.32	0.62
1:J:89:ARG:NH2	6:F:274:ASP:OD1	2.21	0.62
2:A:177:LYS:HG2	2:A:193:ILE:HD11	1.82	0.62
4:D:1100:LEU:HD23	4:D:1101:SER:N	2.13	0.62
4:D:1188:GLU:O	4:D:1192:ARG:HG3	1.99	0.62
2:A:3:ILE:O	2:A:3:ILE:HG13	1.98	0.62
3:C:937:ILE:CB	3:C:939:VAL:HG12	2.28	0.62
4:D:453:LYS:HB3	4:D:454:PRO:HD3	1.82	0.62
3:C:302:VAL:O	3:C:306:LYS:HG2	2.00	0.62
3:C:732:LEU:HD22	3:C:737:VAL:HG11	1.82	0.62
3:C:751:ARG:NH1	4:D:332:GLY:O	2.32	0.62
4:D:1054:VAL:HG12	4:D:1104:ASP:O	2.00	0.62
8:P:17:DT:O5'	9:T:290:GLY:HA3	1.99	0.62
4:D:275:GLU:HA	4:D:278:ARG:HB2	1.82	0.62
2:A:113:PRO:HD2	2:A:116:VAL:HG21	1.82	0.62
2:B:144:ARG:NH1	2:B:144:ARG:HB2	2.15	0.62
3:C:38:PRO:HB3	3:C:508:ARG:HH21	1.63	0.62
3:C:1045:GLN:HG3	3:C:1090:ARG:HH21	1.64	0.61
1:J:47:ASP:OD1	1:J:47:ASP:N	2.19	0.61
2:A:24:GLU:OE1	2:A:191:LYS:HD3	2.00	0.61
2:A:36:ASN:HB2	2:A:176:TYR:OH	2.00	0.61
2:B:21:PHE:HB2	2:B:194:ILE:CG2	2.29	0.61
3:C:302:VAL:HG11	3:C:368:ARG:HD3	1.82	0.61
3:C:363:HIS:NE2	3:C:528:ASP:OD2	2.32	0.61
3:C:45:LEU:HD21	3:C:443:LYS:HD2	1.81	0.61
3:C:221:ARG:O	3:C:223:GLN:NE2	2.29	0.61
3:C:783:ILE:HG13	3:C:841:ILE:HD12	1.81	0.61
4:D:436:LEU:O	4:D:716:LYS:NZ	2.32	0.61
3:C:584:MET:HA	3:C:619:THR:CG2	2.27	0.61
4:D:102:THR:HG23	4:D:258:ALA:HB2	1.82	0.61
4:D:137:THR:HG22	4:D:253:THR:O	1.98	0.61
3:C:1028:VAL:HG12	4:D:429:VAL:HG12	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:176:VAL:HG12	6:F:177:ALA:N	2.15	0.61
6:F:324:LEU:HD22	6:F:332:PRO:HB3	1.82	0.61
4:D:58:TRP:CD2	4:D:68:VAL:HG22	2.36	0.61
4:D:920:PHE:CE2	4:D:948:ILE:HG13	2.34	0.61
4:D:108:LYS:O	4:D:108:LYS:HG3	2.01	0.61
4:D:622:MET:CE	4:D:667:LEU:HD13	2.31	0.61
4:D:1089:VAL:HG13	4:D:1098:GLY:C	2.21	0.61
2:B:212:GLY:O	2:B:216:VAL:HG12	2.00	0.61
4:D:578:ARG:HB2	11:D:2008:EDO:H21	1.83	0.61
4:D:622:MET:HE3	4:D:667:LEU:HD13	1.83	0.61
6:F:444:ILE:O	6:F:448:THR:HG23	2.01	0.61
9:T:279:THR:HG23	9:T:282:ASP:CB	2.30	0.61
2:A:99:LYS:HE3	2:A:109:ASP:CG	2.21	0.61
6:F:321:GLN:O	6:F:325:LEU:HB2	2.00	0.61
1:J:98:LEU:O	1:J:102:LEU:HD13	2.00	0.60
3:C:421:PHE:O	3:C:425:SER:HB3	2.01	0.60
3:C:876:LEU:HD11	3:C:886:ILE:CD1	2.31	0.60
3:C:966:PRO:HG2	3:C:969:ASP:O	2.01	0.60
4:D:745:LEU:O	4:D:749:GLU:HG2	2.00	0.60
4:D:1171:SER:CB	4:D:1174:THR:HG22	2.31	0.60
6:F:345:PRO:HA	6:F:348:VAL:CG1	2.31	0.60
2:A:169:SER:OG	14:A:401:HOH:O	2.16	0.60
4:D:785:GLY:O	4:D:789:GLU:HG3	2.00	0.60
1:J:74:LYS:HG3	1:J:74:LYS:O	2.01	0.60
1:J:82:TRP:CE2	6:F:199:GLN:HG2	2.36	0.60
2:A:40:ARG:HD3	2:B:33:THR:CG2	2.30	0.60
3:C:394:ARG:HG3	3:C:398:GLN:HG3	1.83	0.60
3:C:522:LEU:HB3	3:C:526:GLU:HG3	1.83	0.60
3:C:795:GLY:HA2	3:C:827:SER:OG	2.01	0.60
2:B:74:THR:CG2	4:D:611:VAL:HG11	2.31	0.60
3:C:32:PHE:O	3:C:34:LYS:HD2	2.02	0.60
3:C:742:HIS:HD2	3:C:868:ARG:HG3	1.64	0.60
3:C:873:GLY:HA3	3:C:1028:VAL:HG11	1.82	0.60
4:D:735:VAL:HG22	4:D:798:ILE:HD11	1.83	0.60
5:E:85:GLN:H	5:E:85:GLN:NE2	1.96	0.60
2:B:146:TYR:OH	14:B:401:HOH:O	2.14	0.60
3:C:751:ARG:HG2	3:C:856:VAL:HG22	1.84	0.60
3:C:895:MET:HG3	3:C:896:PRO:HD2	1.83	0.60
4:D:622:MET:HE1	4:D:629:VAL:HG22	1.84	0.60
4:D:673:ASN:HA	4:D:676:LEU:HD13	1.82	0.60
6:F:219:MET:HA	6:F:219:MET:CE	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:272:LYS:HE3	7:O:25:DC:OP1	2.01	0.60
2:A:100:GLN:OE1	2:A:101:GLY:N	2.30	0.60
2:B:183:VAL:O	2:B:183:VAL:HG12	2.02	0.60
3:C:1045:GLN:HG3	3:C:1090:ARG:NH2	2.15	0.60
2:A:48:GLY:HA2	2:A:49:ALA:CB	2.32	0.60
2:B:52:THR:OG1	2:B:141:GLU:HG2	2.02	0.60
3:C:768:SER:O	3:C:771:VAL:HG22	2.02	0.60
4:D:144:ARG:NH2	4:D:229:LEU:O	2.35	0.60
2:A:210:SER:HB3	2:B:229:SER:HB2	1.83	0.60
2:B:41:THR:O	2:B:45:SER:HB3	2.02	0.60
3:C:712:VAL:HA	3:C:906:ILE:HG13	1.83	0.60
3:C:1034:ALA:HB2	4:D:447:MET:HG3	1.84	0.60
4:D:647:GLU:HB2	4:D:655:TRP:CH2	2.37	0.60
7:O:6:DA:C2'	7:O:7:DC:H5'	2.31	0.60
3:C:203:LEU:HD22	3:C:217:ILE:HG22	1.84	0.60
3:C:680:ILE:HD11	3:C:692:VAL:O	2.01	0.60
3:C:32:PHE:HE1	3:C:963:VAL:CG1	2.15	0.59
3:C:412:ARG:HD2	6:F:322:ARG:NE	2.16	0.59
3:C:714:ILE:O	3:C:714:ILE:HG22	2.02	0.59
3:C:973:GLU:CA	4:D:732:MET:HE1	2.31	0.59
3:C:1026:HIS:HB3	3:C:1031:LYS:CE	2.30	0.59
4:D:755:ILE:HD12	4:D:776:ILE:HD11	1.83	0.59
6:F:176:VAL:HG12	6:F:177:ALA:H	1.65	0.59
6:F:317:LEU:HD21	6:F:337:LEU:HG	1.84	0.59
2:B:101:GLY:N	2:B:132:GLY:O	2.35	0.59
2:B:198:THR:CG2	2:B:202:ILE:HD12	2.32	0.59
3:C:335:TYR:CE1	3:C:356:VAL:HG13	2.37	0.59
3:C:876:LEU:CD1	3:C:886:ILE:HG13	2.32	0.59
3:C:1116:LEU:O	3:C:1120:GLN:HG3	2.02	0.59
2:A:30:PHE:CE1	2:B:40:ARG:HG3	2.37	0.59
3:C:299:LEU:HD12	3:C:299:LEU:O	2.03	0.59
3:C:649:ILE:HD13	3:C:693:ILE:HG22	1.84	0.59
4:D:17:ALA:O	4:D:21:ARG:HG3	2.01	0.59
4:D:901:ALA:HB1	4:D:910:ILE:O	2.02	0.59
1:J:68:ASP:HA	1:J:69:VAL:CB	2.32	0.59
4:D:275:GLU:O	4:D:278:ARG:N	2.35	0.59
4:D:1041:PRO:HB3	4:D:1116:ALA:HB3	1.82	0.59
4:D:661:TRP:CZ3	4:D:663:ALA:HB2	2.36	0.59
5:E:80:VAL:HG12	5:E:81:GLU:N	2.17	0.59
3:C:721:ASN:HD22	3:C:727:ILE:CD1	2.14	0.59
4:D:240:LEU:HD23	4:D:244:LEU:HG	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:510:VAL:HG12	3:C:568:ASP:C	2.23	0.59
3:C:876:LEU:HD11	3:C:886:ILE:HD11	1.85	0.59
4:D:924:LEU:HD22	4:D:959:VAL:CG1	2.33	0.59
2:A:90:ASP:O	2:A:91:GLU:HG2	2.03	0.59
2:B:85:VAL:HG23	2:B:117:THR:C	2.23	0.59
3:C:176:VAL:HG22	3:C:307:VAL:HG12	1.85	0.59
3:C:766:ASN:O	3:C:767:VAL:HG13	2.03	0.59
3:C:171:VAL:N	3:C:368:ARG:O	2.35	0.59
3:C:348:VAL:HG13	3:C:349:PRO:HD2	1.85	0.59
3:C:578:VAL:HG12	3:C:579:SER:O	2.02	0.59
3:C:745:GLU:OE2	3:C:861:ARG:HD2	2.03	0.59
4:D:248:TYR:HA	4:D:251:TYR:CD2	2.38	0.59
4:D:982:MET:CE	4:D:1153:LYS:HE3	2.33	0.59
4:D:1071:ASP:HB2	4:D:1072:GLY:C	2.23	0.59
6:F:289:ILE:O	6:F:293:ILE:HG13	2.02	0.59
1:J:95:GLU:OE1	1:J:95:GLU:HA	2.03	0.59
2:B:76:ILE:HA	2:B:79:ASN:HB2	1.85	0.59
6:F:180:ASN:OD1	6:F:183:GLU:HG3	2.02	0.59
2:A:197:GLU:OE1	3:C:987:ARG:NH1	2.35	0.58
3:C:231:ALA:HB1	3:C:265:LEU:HD13	1.82	0.58
3:C:509:LYS:HA	3:C:569:TYR:HA	1.84	0.58
3:C:549:ARG:HA	3:C:563:SER:HA	1.85	0.58
4:D:850:ILE:O	4:D:853:HIS:HB2	2.02	0.58
4:D:957:THR:O	4:D:958:THR:HG23	2.03	0.58
1:J:44:PHE:HE2	4:D:76:GLU:HA	1.69	0.58
2:B:84:VAL:HB	2:B:199:LYS:CD	2.30	0.58
3:C:1045:GLN:HG2	3:C:1087:THR:CG2	2.32	0.58
6:F:462:ARG:HH12	6:F:465:LEU:HD12	1.68	0.58
2:A:85:VAL:HG22	2:A:86:SER:H	1.68	0.58
3:C:698:CYS:O	3:C:705:ALA:N	2.31	0.58
3:C:792:ILE:HD12	3:C:792:ILE:H	1.67	0.58
6:F:402:LEU:HD23	6:F:414:ARG:HE	1.67	0.58
2:A:8:THR:OG1	2:A:24:GLU:O	2.12	0.58
2:B:34:LEU:CD1	2:B:192:LEU:HD22	2.32	0.58
2:B:39:ARG:NH2	4:D:623:ASP:OD2	2.36	0.58
3:C:649:ILE:HG21	3:C:693:ILE:HG21	1.85	0.58
3:C:710:LEU:HD13	3:C:1021:ILE:CG1	2.33	0.58
4:D:6:PHE:HD1	4:D:1257:LYS:HE3	1.68	0.58
5:E:76:VAL:HG13	5:E:77:GLY:N	2.19	0.58
3:C:221:ARG:HG3	3:C:222:ARG:HG3	1.86	0.58
9:T:256:LEU:CD2	9:T:297:VAL:HG22	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:200:ASN:H	2:B:200:ASN:ND2	2.02	0.58
3:C:498:ASN:OD1	3:C:499:PRO:HD2	2.03	0.58
3:C:910:THR:CG2	4:D:730:VAL:HG23	2.34	0.58
3:C:998:LYS:NZ	4:D:734:ASP:OD2	2.32	0.58
4:D:982:MET:HE2	4:D:1153:LYS:HE3	1.84	0.58
2:B:34:LEU:HD12	2:B:35:GLY:N	2.18	0.58
2:B:180:ALA:HA	2:B:189:PHE:O	2.04	0.58
3:C:1029:ASP:OD1	4:D:520:LYS:HD2	2.04	0.58
4:D:1009:LEU:HB3	4:D:1029:LEU:HD13	1.86	0.58
4:D:1132:GLN:HE21	4:D:1163:LEU:HD12	1.69	0.58
4:D:1249:LEU:HD12	4:D:1250:LYS:N	2.19	0.58
3:C:166:VAL:HG11	3:C:372:VAL:HG23	1.86	0.58
2:A:93:VAL:HG22	2:A:113:PRO:HG3	1.86	0.58
2:A:152:ASN:HA	2:A:155:SER:OG	2.03	0.58
3:C:937:ILE:HA	3:C:938:ASP:CB	2.34	0.58
2:A:170:PRO:HB3	2:A:202:ILE:HG12	1.84	0.58
2:B:22:VAL:CG1	2:B:193:ILE:HD12	2.34	0.58
3:C:727:ILE:CG1	3:C:907:ILE:HB	2.34	0.58
2:B:151:GLN:CG	2:B:154:ALA:HB1	2.34	0.57
3:C:132:ASN:CB	3:C:135:THR:HG22	2.33	0.57
3:C:229:LEU:O	3:C:229:LEU:HD12	2.04	0.57
4:D:273:GLU:O	4:D:277:LEU:HB2	2.04	0.57
4:D:924:LEU:CD2	4:D:959:VAL:HG11	2.34	0.57
1:J:45:ALA:HB2	4:D:73:ILE:HD12	1.85	0.57
2:A:50:ALA:HB3	2:A:168:TYR:CD1	2.39	0.57
4:D:1231:THR:O	4:D:1235:THR:HG23	2.03	0.57
5:E:26:TYR:CE1	5:E:29:PRO:HD3	2.38	0.57
2:A:2:LEU:HD12	2:B:143:GLY:HA2	1.85	0.57
2:A:9:LEU:HD13	2:A:23:ILE:CG1	2.34	0.57
2:A:199:LYS:O	2:A:200:ASN:HB2	2.03	0.57
2:B:213:GLY:HA2	2:B:216:VAL:HG12	1.86	0.57
3:C:338:ARG:HB3	3:C:343:GLN:HE21	1.70	0.57
3:C:602:MET:HE1	3:C:883:LYS:CB	2.27	0.57
2:B:210:SER:O	2:B:214:THR:HG23	2.05	0.57
3:C:575:ARG:NH2	3:C:966:PRO:HB2	2.19	0.57
4:D:603:THR:HG22	4:D:604:LYS:CE	2.30	0.57
5:E:84:LEU:HB2	5:E:85:GLN:HE21	1.70	0.57
8:P:3:DC:H2"	8:P:4:DA:C8	2.40	0.57
2:B:167:ILE:HD11	4:D:617:GLU:HG3	1.85	0.57
3:C:38:PRO:HB3	3:C:508:ARG:NH2	2.19	0.57
3:C:476:PRO:O	4:D:856:ARG:NH2	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:506:PRO:HB2	3:C:572:VAL:HG11	1.86	0.57
4:D:137:THR:HG22	4:D:253:THR:C	2.25	0.57
2:A:112:PRO:HB2	2:A:116:VAL:HG23	1.86	0.57
2:B:66:VAL:O	2:B:69:VAL:HG22	2.04	0.57
2:B:105:VAL:HG23	2:B:128:LEU:CD1	2.34	0.57
3:C:216:ARG:HG2	3:C:221:ARG:HA	1.85	0.57
4:D:269:ASP:HB3	4:D:272:ALA:CB	2.33	0.57
6:F:293:ILE:O	6:F:297:MET:HG3	2.04	0.57
2:A:14:VAL:HG13	2:A:15:ALA:H	1.68	0.57
2:A:31:GLY:HA2	2:A:192:LEU:CD2	2.28	0.57
3:C:21:ASN:O	3:C:22:SER:OG	2.21	0.57
4:D:743:GLU:O	4:D:747:ARG:HG3	2.05	0.57
5:E:80:VAL:HG12	5:E:81:GLU:H	1.69	0.57
6:F:324:LEU:HD23	6:F:328:LEU:CD1	2.30	0.57
6:F:338:ALA:HB2	6:F:348:VAL:HG11	1.86	0.57
7:O:11:DA:C2'	7:O:12:DG:H5''	2.35	0.57
2:B:44:SER:HA	2:B:145:GLY:HA2	1.86	0.57
3:C:224:PRO:HB2	3:C:227:VAL:HG13	1.87	0.57
3:C:721:ASN:ND2	3:C:727:ILE:HD11	2.20	0.57
4:D:460:LEU:HD11	4:D:472:ALA:HB1	1.87	0.57
4:D:1128:PRO:HG3	4:D:1206:PRO:CB	2.35	0.57
1:J:92:GLU:OE1	1:J:92:GLU:N	2.37	0.56
3:C:203:LEU:HD22	3:C:217:ILE:CB	2.35	0.56
3:C:338:ARG:CD	3:C:346:MET:HG3	2.31	0.56
4:D:585:LEU:HD12	4:D:692:GLN:NE2	2.19	0.56
2:A:106:THR:CA	2:A:125:ILE:HD13	2.34	0.56
2:A:210:SER:CB	2:B:229:SER:HB2	2.35	0.56
3:C:540:ASP:O	3:C:543:GLY:N	2.32	0.56
2:A:85:VAL:HG22	2:A:86:SER:N	2.19	0.56
2:A:89:ASP:CB	2:A:142:ARG:HD2	2.35	0.56
2:A:211:ALA:O	2:A:215:LEU:N	2.36	0.56
2:B:76:ILE:HG23	2:B:125:ILE:CD1	2.35	0.56
2:B:97:LEU:HB3	2:B:136:VAL:CG1	2.36	0.56
3:C:508:ARG:HH11	3:C:570:MET:HE2	1.69	0.56
3:C:763:ASP:CB	3:C:821:ARG:HH22	2.17	0.56
3:C:885:VAL:CG1	4:D:538:GLY:HA2	2.35	0.56
4:D:468:ASN:ND2	6:F:463:ASP:OD2	2.33	0.56
4:D:607:PRO:O	4:D:609:GLN:HG2	2.04	0.56
4:D:641:ARG:NE	4:D:655:TRP:HZ2	2.04	0.56
4:D:901:ALA:HB2	4:D:911:ARG:CA	2.35	0.56
4:D:1088:ARG:HG2	4:D:1089:VAL:N	2.17	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:81:GLU:OE1	5:E:81:GLU:HA	2.06	0.56
3:C:572:VAL:HG22	3:C:576:GLN:CD	2.25	0.56
6:F:253:MET:HE3	6:F:297:MET:N	2.20	0.56
6:F:364:THR:O	6:F:364:THR:HG23	2.05	0.56
2:A:9:LEU:HD23	2:B:221:LEU:O	2.05	0.56
2:A:82:GLY:HA3	2:A:123:MET:HE1	1.88	0.56
2:A:207:ALA:O	2:A:210:SER:OG	2.10	0.56
3:C:299:LEU:HD12	3:C:299:LEU:C	2.26	0.56
3:C:510:VAL:HG11	3:C:567:VAL:HB	1.87	0.56
4:D:203:ARG:NE	4:D:203:ARG:HA	2.20	0.56
2:A:43:LEU:HD11	2:A:174:VAL:HB	1.88	0.56
3:C:431:MET:O	3:C:670:ASN:ND2	2.38	0.56
3:C:939:VAL:HG23	3:C:940:ALA:HA	1.86	0.56
4:D:354:LEU:O	4:D:358:ILE:HG12	2.06	0.56
4:D:930:ASP:HB3	4:D:954:ALA:HB1	1.87	0.56
4:D:1062:PHE:CD2	4:D:1080:LYS:HD2	2.41	0.56
4:D:1275:PRO:CG	5:E:76:VAL:HG11	2.24	0.56
6:F:449:MET:O	6:F:453:ARG:HG3	2.06	0.56
2:A:197:GLU:OE1	3:C:987:ARG:NH2	2.39	0.56
3:C:602:MET:HE2	3:C:1024:LEU:HD21	1.87	0.56
3:C:736:ASP:OD1	3:C:869:LYS:HE2	2.06	0.56
3:C:805:LEU:HD12	3:C:809:GLU:CD	2.26	0.56
3:C:973:GLU:HA	4:D:732:MET:HE1	1.86	0.56
4:D:687:MET:HE2	4:D:695:ILE:CD1	2.36	0.56
4:D:890:CYS:SG	4:D:892:THR:HG22	2.45	0.56
4:D:631:ALA:O	4:D:666:THR:HA	2.05	0.56
4:D:937:ILE:CD1	4:D:951:LEU:HG	2.33	0.56
3:C:641:ILE:HG21	3:C:644:VAL:HG13	1.87	0.56
4:D:706:ILE:HD11	5:E:36:PRO:HA	1.87	0.56
4:D:753:ASP:O	4:D:757:ARG:N	2.38	0.56
4:D:932:ASN:N	4:D:933:GLY:HA2	2.21	0.56
4:D:1081:LEU:CB	4:D:1113:MET:HE3	2.35	0.56
6:F:360:SER:HB3	6:F:363:GLN:HG3	1.87	0.56
3:C:380:ILE:HG12	3:C:418:ILE:HD11	1.87	0.56
3:C:717:TRP:HH2	3:C:1005:ARG:NH2	2.04	0.56
3:C:984:LEU:HD13	3:C:989:GLY:O	2.06	0.56
3:C:988:ASP:OD1	3:C:988:ASP:N	2.38	0.56
3:C:534:GLN:NE2	4:D:846:LEU:HD11	2.20	0.55
3:C:556:GLY:N	3:C:557:GLY:HA2	2.21	0.55
4:D:653:ASN:HB2	4:D:654:GLY:CA	2.35	0.55
6:F:465:LEU:HD23	6:F:466:ASP:N	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:99:LYS:HE3	2:A:109:ASP:OD1	2.06	0.55
2:B:177:LYS:HG3	2:B:193:ILE:HB	1.89	0.55
4:D:170:LEU:HD13	4:D:209:ARG:NH2	2.21	0.55
4:D:1121:GLU:OE2	4:D:1124:ARG:NH2	2.31	0.55
4:D:1168:ILE:CD1	4:D:1176:PHE:HB3	2.36	0.55
2:A:82:GLY:HA3	2:A:123:MET:CE	2.37	0.55
3:C:269:TYR:CE2	3:C:278:PRO:HB3	2.40	0.55
3:C:549:ARG:HB2	3:C:561:PHE:CE2	2.41	0.55
3:C:808:GLU:O	3:C:812:LEU:HD13	2.07	0.55
4:D:183:GLU:O	4:D:187:GLU:HG2	2.07	0.55
3:C:62:ARG:O	3:C:66:ILE:HG13	2.06	0.55
6:F:291:GLN:HG3	6:F:292:ALA:N	2.21	0.55
7:O:28:DT:H2''	7:O:29:DA:C5'	2.33	0.55
2:A:40:ARG:HD3	2:B:33:THR:CB	2.37	0.55
2:B:50:ALA:HB3	2:B:168:TYR:CD2	2.42	0.55
3:C:891:PRO:HB2	3:C:893:GLU:CG	2.35	0.55
3:C:892:VAL:CG2	3:C:903:PRO:HG2	2.37	0.55
3:C:973:GLU:OE1	4:D:840:ARG:NH2	2.40	0.55
3:C:986:ASN:OD1	3:C:986:ASN:N	2.34	0.55
4:D:39:LEU:HD13	4:D:335:PHE:HZ	1.71	0.55
4:D:334:ARG:HD3	6:F:356:ARG:HH21	1.71	0.55
4:D:641:ARG:CZ	4:D:655:TRP:HZ2	2.19	0.55
4:D:901:ALA:HB2	4:D:912:ASP:N	2.22	0.55
2:B:162:ILE:HG23	4:D:607:PRO:HG2	1.88	0.55
3:C:346:MET:HB2	3:C:356:VAL:HG21	1.88	0.55
3:C:937:ILE:CA	3:C:938:ASP:CB	2.85	0.55
4:D:676:LEU:HD12	4:D:676:LEU:N	2.22	0.55
4:D:781:THR:HG22	4:D:814:ARG:HD2	1.89	0.55
4:D:1229:GLU:O	4:D:1233:VAL:HG23	2.05	0.55
2:A:192:LEU:HD12	2:A:192:LEU:O	2.06	0.55
3:C:268:ILE:O	3:C:272:LEU:HD13	2.06	0.55
3:C:578:VAL:HG13	3:C:582:THR:CB	2.36	0.55
3:C:771:VAL:HG23	3:C:772:LEU:HD12	1.87	0.55
4:D:143:MET:CE	4:D:251:TYR:HA	2.36	0.55
4:D:962:ARG:HB3	4:D:977:CYS:HA	1.88	0.55
2:A:48:GLY:HA3	2:A:168:TYR:HB3	1.89	0.55
3:C:712:VAL:HG11	3:C:925:THR:HG23	1.89	0.55
3:C:680:ILE:HG12	3:C:693:ILE:O	2.07	0.55
3:C:935:TRP:HB2	3:C:982:SER:CB	2.37	0.55
4:D:155:MET:HE3	4:D:219:LEU:HB3	1.87	0.55
4:D:706:ILE:O	4:D:710:GLN:HG3	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:O:15:DT:H2''	7:O:16:DT:OP2	2.07	0.55
1:J:40:PHE:CZ	1:J:58:ASN:HB2	2.42	0.55
4:D:1037:GLU:HG2	4:D:1039:ARG:NH1	2.22	0.55
6:F:394:LEU:HB2	6:F:464:TYR:CD1	2.42	0.55
2:B:213:GLY:HA2	2:B:216:VAL:CG1	2.38	0.54
3:C:635:ALA:CB	3:C:693:ILE:HD11	2.28	0.54
5:E:29:PRO:HB2	5:E:33:THR:HG23	1.88	0.54
6:F:272:LYS:HE3	7:O:25:DC:P	2.47	0.54
3:C:523:THR:HG22	3:C:526:GLU:CD	2.28	0.54
3:C:839:ILE:HG22	3:C:840:GLY:N	2.21	0.54
3:C:984:LEU:HB2	3:C:985:PRO:CA	2.36	0.54
4:D:951:LEU:CB	4:D:956:ILE:HD11	2.31	0.54
4:D:1276:THR:HG22	5:E:102:GLU:CG	2.37	0.54
9:T:251:ILE:HG21	9:T:270:HIS:O	2.06	0.54
2:A:50:ALA:HB3	2:A:168:TYR:CE1	2.43	0.54
4:D:901:ALA:N	4:D:912:ASP:HB2	2.20	0.54
6:F:254:ALA:HB3	6:F:257:ASP:OD2	2.08	0.54
1:J:82:TRP:CZ2	6:F:199:GLN:HG2	2.42	0.54
2:B:97:LEU:HB3	2:B:136:VAL:HG13	1.90	0.54
2:B:99:LYS:O	2:B:133:LYS:HG3	2.07	0.54
3:C:215:VAL:CG2	3:C:225:VAL:HA	2.27	0.54
3:C:729:SER:OG	3:C:904:VAL:O	2.25	0.54
4:D:988:VAL:HG23	4:D:992:GLU:HG3	1.88	0.54
4:D:1056:LEU:HD21	4:D:1063:PHE:HD1	1.72	0.54
6:F:438:ARG:NH1	8:P:20:DG:N7	2.54	0.54
1:J:64:LEU:HD22	1:J:66:GLU:HB2	1.89	0.54
3:C:876:LEU:N	3:C:876:LEU:HD12	2.23	0.54
4:D:885:VAL:O	4:D:990:ILE:O	2.25	0.54
4:D:1071:ASP:N	4:D:1072:GLY:HA2	2.22	0.54
3:C:193:VAL:HG12	3:C:205:PHE:HB2	1.89	0.54
4:D:576:MET:HE1	4:D:693:ALA:HB2	1.90	0.54
2:A:33:THR:HG22	2:B:37:SER:OG	2.08	0.54
2:A:129:ASN:H	2:A:129:ASN:HD22	1.55	0.54
2:B:143:GLY:HA3	2:B:168:TYR:CE1	2.43	0.54
2:B:144:ARG:HB2	2:B:144:ARG:HH11	1.73	0.54
3:C:45:LEU:HD21	3:C:443:LYS:CD	2.38	0.54
3:C:275:GLY:O	6:F:171:LYS:HD2	2.07	0.54
3:C:852:LEU:CD2	3:C:856:VAL:HG12	2.37	0.54
4:D:602:ALA:HB3	4:D:607:PRO:C	2.28	0.54
4:D:706:ILE:CD1	5:E:36:PRO:HB3	2.37	0.54
6:F:335:GLU:OE1	6:F:335:GLU:N	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:T:251:ILE:O	9:T:254:LEU:HG	2.07	0.54
2:A:79:ASN:O	2:A:123:MET:HE1	2.06	0.54
3:C:368:ARG:HA	3:C:369:LEU:CB	2.38	0.54
3:C:369:LEU:HB3	3:C:501:GLY:O	2.07	0.54
3:C:577:MET:HE3	4:D:849:PHE:HD1	1.72	0.54
3:C:723:GLU:O	3:C:724:ASP:HB2	2.08	0.54
3:C:141:GLN:OE1	3:C:404:THR:OG1	2.26	0.54
3:C:568:ASP:OD1	3:C:568:ASP:N	2.41	0.54
3:C:967:VAL:HG23	3:C:968:PHE:H	1.72	0.54
4:D:248:TYR:HA	4:D:251:TYR:HD2	1.73	0.54
4:D:460:LEU:HD11	4:D:472:ALA:CB	2.38	0.54
4:D:936:ILE:CG2	4:D:951:LEU:HD23	2.37	0.54
2:A:66:VAL:HB	2:A:69:VAL:CG2	2.38	0.54
2:B:24:GLU:HG3	2:B:191:LYS:HG3	1.88	0.54
3:C:148:PHE:HD2	3:C:150:MET:HE3	1.73	0.54
3:C:393:GLU:OE2	6:F:247:ARG:HD3	2.08	0.54
3:C:479:THR:OG1	3:C:480:PRO:HD2	2.08	0.54
3:C:1132:ASP:HB3	3:C:1133:GLY:CA	2.32	0.54
4:D:368:ASN:ND2	14:D:2111:HOH:O	2.41	0.54
7:O:6:DA:H1'	7:O:7:DC:H5'	1.90	0.54
4:D:363:PRO:HB2	4:D:365:ILE:HD12	1.90	0.53
6:F:194:GLY:HA2	6:F:222:ILE:HG22	1.91	0.53
3:C:874:ASP:OD1	3:C:1028:VAL:HG22	2.07	0.53
4:D:270:ILE:O	4:D:274:ALA:N	2.39	0.53
5:E:62:ASN:O	5:E:66:ASN:ND2	2.41	0.53
6:F:215:GLN:O	6:F:219:MET:HG2	2.08	0.53
6:F:309:HIS:O	6:F:313:VAL:HG12	2.07	0.53
4:D:129:ILE:HD11	4:D:130:TYR:CZ	2.42	0.53
4:D:443:LEU:HD22	4:D:514:PRO:HB3	1.91	0.53
2:A:21:PHE:HB2	2:A:194:ILE:HG12	1.89	0.53
2:B:216:VAL:HG13	2:B:217:GLU:N	2.23	0.53
3:C:338:ARG:HD3	3:C:343:GLN:HE22	1.73	0.53
4:D:231:PRO:O	4:D:232:LYS:HB2	2.07	0.53
4:D:285:LYS:HA	4:D:289:LYS:HD2	1.91	0.53
4:D:1034:GLU:OE2	4:D:1042:ARG:HG2	2.09	0.53
2:A:8:THR:O	2:A:23:ILE:HA	2.09	0.53
2:A:36:ASN:CB	3:C:1007:GLY:HA3	2.39	0.53
6:F:304:ILE:HB	14:F:604:HOH:O	2.07	0.53
1:J:89:ARG:HH22	6:F:274:ASP:CG	2.11	0.53
2:A:56:ILE:HG12	2:A:136:VAL:HB	1.91	0.53
3:C:51:SER:OG	3:C:371:THR:HG23	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:338:ARG:HB3	3:C:343:GLN:NE2	2.23	0.53
3:C:590:HIS:O	3:C:919:ILE:HD11	2.09	0.53
2:B:60:LEU:HD22	2:B:60:LEU:N	2.24	0.53
3:C:52:PHE:CZ	3:C:150:MET:HE2	2.41	0.53
3:C:530:HIS:HB3	3:C:568:ASP:CG	2.29	0.53
3:C:624:ARG:NH1	3:C:628:ASP:OD2	2.41	0.53
3:C:939:VAL:HG22	3:C:940:ALA:HA	1.90	0.53
4:D:12:ILE:HG12	4:D:1221:TRP:CZ2	2.44	0.53
6:F:164:ASP:OD1	6:F:166:VAL:N	2.41	0.53
3:C:822:GLU:HG2	3:C:823:VAL:HG22	1.91	0.53
4:D:844:THR:H	4:D:847:GLU:HB2	1.73	0.53
4:D:848:TYR:O	4:D:852:THR:HG23	2.09	0.53
4:D:872:LEU:HG	4:D:876:LEU:CD2	2.39	0.53
4:D:992:GLU:OE1	5:E:48:TYR:OH	2.27	0.53
2:B:205:ARG:CZ	2:B:205:ARG:HB2	2.38	0.53
3:C:76:GLY:O	3:C:80:VAL:HG23	2.08	0.53
3:C:538:PRO:HB2	3:C:546:THR:OG1	2.09	0.53
4:D:602:ALA:HB1	4:D:606:ALA:HB3	1.90	0.53
9:T:260:SER:O	9:T:264:LEU:HG	2.08	0.53
2:A:192:LEU:HD12	2:A:192:LEU:C	2.30	0.53
2:B:198:THR:HG22	2:B:199:LYS:O	2.08	0.53
3:C:41:VAL:HG13	3:C:493:VAL:HG12	1.91	0.53
3:C:176:VAL:HG13	3:C:307:VAL:HG11	1.90	0.53
3:C:444:ARG:NH2	3:C:491:LEU:HD23	2.08	0.53
3:C:478:GLU:OE1	3:C:579:SER:OG	2.20	0.53
3:C:505:THR:CG2	3:C:506:PRO:HD2	2.39	0.53
3:C:1003:ASP:HB2	3:C:1010:PHE:CZ	2.44	0.53
4:D:579:LEU:HG	11:D:2008:EDO:H22	1.90	0.53
4:D:1123:LEU:HA	4:D:1131:VAL:CG2	2.39	0.53
2:A:138:LEU:HD12	2:A:138:LEU:N	2.24	0.52
3:C:712:VAL:CG1	3:C:925:THR:HG23	2.39	0.52
3:C:1039:PRO:HB2	3:C:1048:LEU:HD21	1.90	0.52
3:C:1069:ALA:HB3	4:D:506:ARG:HB3	1.91	0.52
3:C:1117:LYS:HD2	3:C:1120:GLN:NE2	2.24	0.52
4:D:106:TYR:HB3	4:D:312:MET:HE2	1.90	0.52
5:E:98:GLY:O	5:E:100:LEU:HD12	2.09	0.52
3:C:368:ARG:HB3	3:C:501:GLY:O	2.09	0.52
4:D:85:ALA:N	14:D:2108:HOH:O	2.41	0.52
3:C:106:VAL:HG11	3:C:120:TYR:CE1	2.44	0.52
3:C:228:LEU:HD21	3:C:268:ILE:CG1	2.22	0.52
3:C:1084:SER:HB2	4:D:421:ARG:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:744:ILE:O	4:D:748:HIS:HD2	1.93	0.52
3:C:132:ASN:HB3	3:C:135:THR:CG2	2.38	0.52
3:C:171:VAL:HG12	3:C:172:ARG:N	2.24	0.52
3:C:493:VAL:HG12	3:C:494:TYR:CD1	2.44	0.52
3:C:573:SER:HB2	3:C:574:PRO:HD2	1.92	0.52
2:A:111:VAL:O	2:A:111:VAL:HG22	2.08	0.52
3:C:549:ARG:HD3	3:C:561:PHE:CE2	2.44	0.52
3:C:852:LEU:HD22	3:C:856:VAL:HG12	1.90	0.52
3:C:921:GLN:HB2	3:C:1019:MET:HE1	1.92	0.52
4:D:1054:VAL:HG11	4:D:1100:LEU:HD21	1.92	0.52
5:E:56:LYS:HA	5:E:59:ARG:HG3	1.91	0.52
2:A:113:PRO:HD2	2:A:116:VAL:CG2	2.39	0.52
3:C:102:ARG:O	3:C:124:LEU:HD23	2.09	0.52
3:C:921:GLN:HB2	3:C:1019:MET:CE	2.39	0.52
4:D:1174:THR:CA	4:D:1175:GLU:CB	2.87	0.52
6:F:462:ARG:NH1	6:F:465:LEU:HB2	2.24	0.52
3:C:1084:SER:OG	3:C:1085:ASP:N	2.40	0.52
3:C:1126:VAL:HG12	4:D:12:ILE:HG23	1.91	0.52
4:D:932:ASN:N	4:D:933:GLY:CA	2.73	0.52
3:C:29:ARG:CD	3:C:964:ALA:HB2	2.39	0.52
3:C:33:ALA:HB2	3:C:966:PRO:HG3	1.90	0.52
3:C:584:MET:CA	3:C:619:THR:HG21	2.35	0.52
4:D:103:HIS:CE1	4:D:105:TRP:HB2	2.45	0.52
4:D:362:ALA:HB3	4:D:367:VAL:HG23	1.91	0.52
4:D:767:THR:O	4:D:771:GLU:HB2	2.10	0.52
4:D:815:THR:HG22	4:D:820:LYS:CA	2.33	0.52
8:P:17:DT:P	9:T:290:GLY:HA3	2.49	0.52
4:D:1132:GLN:CG	4:D:1163:LEU:HD12	2.40	0.52
2:A:78:LEU:O	2:A:81:LYS:HB2	2.10	0.52
2:B:183:VAL:O	2:B:184:GLU:CB	2.58	0.52
3:C:508:ARG:HD2	3:C:570:MET:CE	2.39	0.52
3:C:516:THR:HG21	3:C:518:GLN:HB2	1.91	0.52
3:C:614:ALA:HB1	3:C:615:PRO:HD2	1.90	0.52
4:D:54:PRO:HG3	4:D:81:GLU:O	2.10	0.52
4:D:365:ILE:HD13	6:F:235:GLU:HG2	1.92	0.52
3:C:174:PRO:HD2	3:C:302:VAL:HB	1.91	0.51
4:D:76:GLU:CD	4:D:76:GLU:H	2.12	0.51
4:D:1088:ARG:HD2	4:D:1111:GLN:HB3	1.92	0.51
3:C:329:VAL:O	3:C:332:THR:OG1	2.27	0.51
4:D:85:ALA:O	4:D:88:ARG:HB2	2.11	0.51
4:D:872:LEU:HG	4:D:876:LEU:HD22	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:878:ASP:OD1	14:D:2103:HOH:O	2.19	0.51
4:D:1034:GLU:OE2	4:D:1042:ARG:N	2.43	0.51
1:J:102:LEU:HA	1:J:105:ILE:HG22	1.92	0.51
2:A:70:LYS:HB3	2:A:71:GLU:OE1	2.11	0.51
3:C:894:ASP:HA	3:C:1004:GLY:HA3	1.92	0.51
4:D:243:GLU:O	4:D:247:ARG:HG3	2.11	0.51
4:D:363:PRO:HG2	4:D:366:ILE:HD12	1.92	0.51
9:T:286:ILE:HG22	9:T:289:PHE:CB	2.40	0.51
1:J:88:ARG:HG3	1:J:89:ARG:H	1.75	0.51
3:C:96:LEU:HD22	3:C:98:PHE:CE1	2.46	0.51
3:C:959:ALA:O	3:C:960:ASP:HB2	2.09	0.51
3:C:1043:ILE:HD12	3:C:1043:ILE:N	2.24	0.51
4:D:1171:SER:C	4:D:1174:THR:HG22	2.30	0.51
4:D:653:ASN:CB	4:D:654:GLY:CA	2.89	0.51
4:D:915:VAL:HG23	4:D:920:PHE:CE2	2.46	0.51
6:F:140:ALA:HA	6:F:143:ALA:HB3	1.91	0.51
6:F:308:VAL:HG21	7:O:23:DT:C7	2.31	0.51
3:C:150:MET:HA	3:C:150:MET:CE	2.33	0.51
3:C:202:TRP:C	3:C:203:LEU:HD23	2.30	0.51
3:C:446:LEU:N	3:C:446:LEU:HD23	2.26	0.51
4:D:924:LEU:CD2	4:D:943:LEU:HD11	2.40	0.51
4:D:1164:ARG:NH1	10:D:2005:SO4:O1	2.44	0.51
2:A:130:ASP:N	2:A:130:ASP:OD1	2.42	0.51
2:A:172:LEU:HD13	2:A:197:GLU:OE2	2.11	0.51
3:C:335:TYR:O	3:C:335:TYR:HD1	1.93	0.51
3:C:748:ILE:O	3:C:859:LEU:HD23	2.10	0.51
4:D:517:VAL:HG12	4:D:518:GLU:O	2.10	0.51
4:D:1275:PRO:CB	5:E:79:LEU:HD11	2.36	0.51
3:C:299:LEU:HD23	3:C:323:THR:N	2.25	0.51
3:C:404:THR:CG2	3:C:407:THR:HG23	2.41	0.51
3:C:626:ALA:HB2	3:C:704:MET:HG2	1.93	0.51
3:C:680:ILE:HD11	3:C:692:VAL:HG12	1.93	0.51
4:D:285:LYS:HG3	4:D:289:LYS:HD2	1.93	0.51
3:C:94:MET:CE	3:C:395:MET:HB3	2.40	0.51
3:C:494:TYR:HB3	3:C:506:PRO:CG	2.38	0.51
3:C:727:ILE:HG13	3:C:907:ILE:HD12	1.93	0.51
4:D:432:VAL:HG22	4:D:434:PRO:CD	2.27	0.51
4:D:936:ILE:HG23	4:D:951:LEU:HD23	1.93	0.51
9:T:259:ARG:NH2	14:T:401:HOH:O	2.44	0.51
2:B:103:GLY:O	2:B:128:LEU:HB2	2.10	0.51
3:C:280:LYS:O	3:C:284:GLN:HG2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1014:VAL:HG13	4:D:729:THR:HG21	1.93	0.51
4:D:937:ILE:HD12	4:D:951:LEU:CG	2.37	0.51
2:B:97:LEU:HD21	2:B:105:VAL:HG11	1.92	0.50
2:B:162:ILE:CG2	4:D:607:PRO:HG2	2.41	0.50
3:C:132:ASN:CG	3:C:135:THR:HG22	2.32	0.50
3:C:370:ARG:HH22	3:C:452:GLY:HA3	1.76	0.50
3:C:910:THR:O	3:C:914:PRO:HD3	2.11	0.50
3:C:1045:GLN:CG	3:C:1090:ARG:HH21	2.24	0.50
3:C:1098:VAL:HG11	4:D:469:ILE:CD1	2.40	0.50
4:D:612:TYR:HB2	4:D:635:VAL:CG1	2.34	0.50
4:D:735:VAL:HG22	4:D:798:ILE:CD1	2.40	0.50
3:C:936:ASN:HD22	3:C:937:ILE:N	2.05	0.50
4:D:67:ARG:HH12	6:F:423:GLN:HA	1.76	0.50
4:D:103:HIS:HB3	4:D:106:TYR:HD2	1.75	0.50
4:D:781:THR:O	4:D:784:VAL:HG23	2.11	0.50
6:F:279:TYR:CE1	7:O:28:DT:H5''	2.46	0.50
2:A:31:GLY:O	2:A:35:GLY:N	2.32	0.50
2:B:172:LEU:O	4:D:616:ALA:HB1	2.10	0.50
4:D:826:PRO:HG3	4:D:853:HIS:CE1	2.46	0.50
4:D:1272:GLN:OE1	4:D:1272:GLN:HA	2.12	0.50
6:F:317:LEU:CD2	6:F:337:LEU:HG	2.41	0.50
6:F:385:ALA:O	6:F:389:VAL:HG23	2.12	0.50
2:A:68:GLY:HA3	2:A:129:ASN:HD21	1.76	0.50
2:A:147:VAL:HG13	2:A:147:VAL:O	2.12	0.50
3:C:148:PHE:HD2	3:C:150:MET:CE	2.25	0.50
3:C:586:PRO:O	3:C:880:HIS:HE1	1.95	0.50
3:C:946:TRP:CZ2	3:C:978:GLY:HA3	2.46	0.50
3:C:1032:ILE:HG21	4:D:520:LYS:HD3	1.93	0.50
3:C:1133:GLY:O	3:C:1134:ALA:HB3	2.11	0.50
4:D:612:TYR:OH	4:D:627:LEU:HG	2.12	0.50
4:D:736:LEU:N	4:D:792:TYR:OH	2.34	0.50
4:D:991:GLY:HA2	4:D:1265:ILE:HD12	1.92	0.50
1:J:76:LYS:HG3	1:J:76:LYS:O	2.10	0.50
2:A:211:ALA:O	2:A:215:LEU:HB2	2.11	0.50
3:C:87:ILE:CD1	3:C:388:GLU:HG3	2.40	0.50
3:C:762:ARG:HG3	3:C:762:ARG:O	2.11	0.50
3:C:797:VAL:CG1	3:C:823:VAL:HB	2.41	0.50
3:C:965:THR:O	3:C:965:THR:OG1	2.24	0.50
4:D:981:SER:HB3	4:D:984:THR:OG1	2.10	0.50
4:D:1056:LEU:HD21	4:D:1063:PHE:CD1	2.47	0.50
4:D:1069:PRO:O	4:D:1072:GLY:HA2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:48:GLY:CA	2:A:49:ALA:CB	2.88	0.50
2:A:177:LYS:HG2	2:A:193:ILE:CD1	2.42	0.50
2:B:105:VAL:HG23	2:B:128:LEU:HD13	1.94	0.50
3:C:44:LEU:HG	3:C:628:ASP:OD2	2.12	0.50
3:C:126:VAL:HB	3:C:145:MET:HE2	1.93	0.50
3:C:578:VAL:HG13	3:C:582:THR:CG2	2.42	0.50
3:C:797:VAL:HG12	3:C:823:VAL:HB	1.94	0.50
4:D:935:VAL:O	4:D:935:VAL:HG12	2.11	0.50
4:D:1081:LEU:HB3	4:D:1113:MET:HE3	1.93	0.50
2:A:1:MET:O	2:A:1:MET:HG2	2.12	0.50
2:A:193:ILE:HD12	2:A:193:ILE:O	2.11	0.50
3:C:180:GLU:HG3	3:C:180:GLU:O	2.11	0.50
3:C:404:THR:HG23	3:C:407:THR:H	1.76	0.50
4:D:1106:VAL:HG13	4:D:1110:ASP:HB2	1.93	0.50
6:F:313:VAL:CG2	6:F:351:ILE:HD13	2.42	0.50
3:C:32:PHE:HE1	3:C:963:VAL:HG13	1.77	0.50
3:C:123:PRO:HB3	3:C:144:PHE:HE1	1.76	0.50
3:C:614:ALA:HA	3:C:705:ALA:HB2	1.94	0.50
4:D:585:LEU:HD12	4:D:692:GLN:HE21	1.75	0.50
4:D:653:ASN:CB	4:D:654:GLY:HA3	2.41	0.50
2:A:9:LEU:HD13	2:A:23:ILE:HG13	1.94	0.50
2:B:93:VAL:HG11	2:B:116:VAL:HG11	1.92	0.50
2:B:171:VAL:HG23	2:B:171:VAL:O	2.12	0.50
3:C:174:PRO:HB2	3:C:303:GLY:CA	2.42	0.50
3:C:269:TYR:CD2	3:C:278:PRO:HB3	2.47	0.50
4:D:43:LYS:O	4:D:44:ASP:HB2	2.12	0.50
4:D:599:TYR:HA	4:D:610:GLY:HA3	1.94	0.50
5:E:95:GLU:HB3	5:E:101:LEU:CD2	2.42	0.50
6:F:244:LEU:HD12	6:F:289:ILE:CG2	2.42	0.50
2:A:78:LEU:HD12	3:C:611:ARG:HH11	1.77	0.49
2:B:170:PRO:O	2:B:199:LYS:HB2	2.12	0.49
3:C:41:VAL:HG13	3:C:493:VAL:CG1	2.42	0.49
3:C:601:ASN:O	3:C:604:ARG:HG2	2.12	0.49
3:C:1103:ILE:CD1	4:D:547:LEU:HB3	2.41	0.49
4:D:336:ALA:HA	6:F:359:ILE:O	2.12	0.49
4:D:432:VAL:CG2	4:D:434:PRO:HD3	2.28	0.49
4:D:638:THR:HA	4:D:659:ASP:O	2.12	0.49
2:A:106:THR:C	2:A:125:ILE:HD13	2.32	0.49
2:A:107:ALA:HB3	2:A:121:PRO:HA	1.94	0.49
2:B:22:VAL:HA	2:B:192:LEU:O	2.13	0.49
3:C:284:GLN:HG3	3:C:285:THR:N	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:729:SER:HA	3:C:895:MET:HE1	1.94	0.49
3:C:788:ARG:O	3:C:830:VAL:HG11	2.11	0.49
3:C:873:GLY:HA3	3:C:1028:VAL:CG1	2.42	0.49
7:O:2:DC:H2''	7:O:3:DT:H5'	1.94	0.49
1:J:53:THR:HA	1:J:62:GLY:O	2.11	0.49
2:A:159:ILE:HD11	3:C:785:ALA:HA	1.93	0.49
3:C:467:HIS:ND1	3:C:468:PRO:HD2	2.27	0.49
3:C:728:LEU:HD23	3:C:906:ILE:HG22	1.94	0.49
3:C:888:LYS:HG2	3:C:890:LEU:HD13	1.95	0.49
3:C:1103:ILE:HD13	4:D:547:LEU:HB3	1.94	0.49
4:D:58:TRP:CE3	4:D:68:VAL:HG22	2.47	0.49
4:D:581:MET:HE3	4:D:716:LYS:HB2	1.95	0.49
5:E:57:ARG:O	5:E:57:ARG:HD3	2.12	0.49
3:C:368:ARG:HA	3:C:369:LEU:HB3	1.94	0.49
3:C:984:LEU:HD13	3:C:989:GLY:CA	2.43	0.49
3:C:1080:LEU:HD12	4:D:1253:VAL:HG13	1.95	0.49
4:D:114:LEU:HG	4:D:312:MET:HE2	1.94	0.49
4:D:1165:ARG:HE	4:D:1209:MET:HE1	1.78	0.49
6:F:166:VAL:O	6:F:170:LEU:HG	2.11	0.49
6:F:176:VAL:CG1	6:F:177:ALA:H	2.25	0.49
3:C:215:VAL:O	3:C:223:GLN:HB2	2.12	0.49
3:C:410:ASN:ND2	3:C:412:ARG:HG3	2.28	0.49
3:C:1074:TYR:CE1	4:D:1258:LEU:HD21	2.47	0.49
4:D:27:GLU:HB2	4:D:94:HIS:CE1	2.47	0.49
4:D:1009:LEU:HD23	4:D:1029:LEU:HD12	1.93	0.49
6:F:173:ILE:HG22	6:F:238:LEU:CD1	2.43	0.49
2:A:18:ARG:NH1	2:A:195:ASP:OD2	2.45	0.49
2:A:147:VAL:HG12	2:A:168:TYR:HE2	1.77	0.49
2:A:212:GLY:O	2:A:216:VAL:N	2.34	0.49
2:B:102:PRO:HB3	2:B:130:ASP:HA	1.94	0.49
3:C:632:VAL:CG1	3:C:692:VAL:HG13	2.43	0.49
4:D:67:ARG:NH1	6:F:423:GLN:HA	2.27	0.49
4:D:190:LYS:HZ2	4:D:192:ASP:HB3	1.77	0.49
4:D:411:GLY:O	4:D:415:GLN:HB3	2.13	0.49
4:D:898:VAL:HG11	4:D:919:ALA:HB2	1.93	0.49
4:D:1086:ARG:O	4:D:1087:LEU:HD23	2.13	0.49
4:D:1276:THR:HG22	5:E:102:GLU:HG3	1.95	0.49
6:F:310:MET:O	6:F:313:VAL:HG13	2.13	0.49
3:C:741:ILE:HG22	3:C:742:HIS:N	2.27	0.49
4:D:177:LEU:HD12	4:D:201:GLY:HA3	1.94	0.49
4:D:602:ALA:CB	4:D:607:PRO:O	2.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:1032:VAL:HG23	4:D:1142:VAL:HG11	1.95	0.49
3:C:176:VAL:O	3:C:176:VAL:HG23	2.11	0.49
3:C:199:ARG:HG2	3:C:200:GLY:N	2.27	0.49
3:C:704:MET:CE	3:C:706:LEU:HD21	2.43	0.49
3:C:848:ASP:OD1	3:C:848:ASP:N	2.46	0.49
4:D:656:LYS:HD3	4:D:656:LYS:H	1.77	0.49
4:D:846:LEU:HD12	4:D:846:LEU:N	2.27	0.49
4:D:1222:LEU:HD23	4:D:1244:ASP:OD2	2.12	0.49
5:E:80:VAL:HG12	5:E:94:ARG:HH21	1.78	0.49
3:C:36:ARG:O	3:C:38:PRO:HD3	2.11	0.49
3:C:196:ILE:HG23	3:C:196:ILE:O	2.13	0.49
3:C:203:LEU:HD22	3:C:217:ILE:CG2	2.43	0.49
4:D:125:LEU:O	4:D:129:ILE:HG23	2.13	0.49
4:D:915:VAL:O	4:D:920:PHE:HD2	1.96	0.49
6:F:414:ARG:HG2	6:F:419:LEU:HD12	1.95	0.49
9:T:257:THR:OG1	9:T:260:SER:OG	2.31	0.49
1:J:40:PHE:HZ	1:J:58:ASN:HB2	1.78	0.49
2:A:18:ARG:HA	2:A:204:PRO:HG3	1.95	0.49
2:A:18:ARG:HB2	2:A:196:VAL:O	2.12	0.49
2:B:69:VAL:HG23	2:B:71:GLU:O	2.12	0.49
3:C:649:ILE:HG21	3:C:693:ILE:CG2	2.43	0.49
4:D:20:ILE:HD13	4:D:318:PRO:HD3	1.95	0.49
4:D:363:PRO:HB2	4:D:365:ILE:HD13	1.95	0.49
4:D:716:LYS:HE3	4:D:717:ASP:OD1	2.13	0.49
9:T:286:ILE:CG2	9:T:289:PHE:HB2	2.42	0.49
3:C:55:LEU:HD22	3:C:376:ILE:HB	1.95	0.48
3:C:589:GLU:OE1	3:C:589:GLU:N	2.36	0.48
4:D:331:ASP:N	4:D:331:ASP:OD1	2.45	0.48
7:O:2:DC:H2'	7:O:3:DT:C5'	2.43	0.48
2:A:31:GLY:CA	2:A:192:LEU:HD23	2.32	0.48
2:B:214:THR:O	2:B:218:LEU:HB2	2.12	0.48
3:C:202:TRP:HD1	3:C:202:TRP:H	1.59	0.48
4:D:1171:SER:O	4:D:1202:ALA:HB2	2.13	0.48
2:A:181:THR:H	2:A:189:PHE:C	2.13	0.48
2:B:26:LEU:CD1	2:B:34:LEU:HD21	2.40	0.48
3:C:326:GLU:O	3:C:330:VAL:HG23	2.14	0.48
3:C:475:CYS:CB	3:C:579:SER:HB3	2.43	0.48
4:D:224:ASN:O	4:D:228:LYS:HG3	2.12	0.48
4:D:1069:PRO:HG2	4:D:1073:GLY:N	2.24	0.48
5:E:80:VAL:CG1	5:E:94:ARG:HH21	2.26	0.48
5:E:92:ALA:O	5:E:96:ILE:HG13	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:306:ILE:CG2	6:F:310:MET:HB3	2.43	0.48
2:A:49:ALA:HB1	2:A:85:VAL:O	2.12	0.48
2:A:186:ARG:O	2:A:187:THR:HG22	2.13	0.48
3:C:35:LEU:N	3:C:35:LEU:HD12	2.28	0.48
3:C:346:MET:HE2	3:C:348:VAL:HA	1.94	0.48
3:C:510:VAL:HG11	3:C:567:VAL:CG1	2.44	0.48
3:C:710:LEU:O	3:C:1018:TYR:HA	2.13	0.48
3:C:859:LEU:HD22	3:C:860:VAL:N	2.28	0.48
4:D:889:ASP:OD2	4:D:962:ARG:NH2	2.46	0.48
2:A:32:TYR:CE1	2:A:178:VAL:HG22	2.48	0.48
2:A:112:PRO:HB2	2:A:116:VAL:CG2	2.43	0.48
2:B:105:VAL:HG12	2:B:125:ILE:HG21	1.94	0.48
2:B:152:ASN:O	2:B:153:LYS:CB	2.62	0.48
4:D:373:MET:SD	6:F:256:LEU:HB3	2.54	0.48
4:D:884:ILE:HD12	4:D:885:VAL:O	2.13	0.48
4:D:1005:PRO:HG3	4:D:1150:ILE:HD11	1.95	0.48
4:D:1271:ILE:HG12	5:E:105:GLU:HA	1.95	0.48
2:A:44:SER:HB3	3:C:893:GLU:OE1	2.13	0.48
2:A:71:GLU:OE2	2:A:126:ALA:HA	2.12	0.48
2:B:172:LEU:HD12	4:D:620:MET:SD	2.54	0.48
3:C:268:ILE:HG23	3:C:272:LEU:HD22	1.96	0.48
3:C:516:THR:CG2	3:C:518:GLN:HB2	2.43	0.48
3:C:958:PRO:O	3:C:961:SER:OG	2.31	0.48
4:D:576:MET:HE1	4:D:693:ALA:CB	2.43	0.48
4:D:622:MET:HE1	4:D:629:VAL:HG13	1.94	0.48
4:D:924:LEU:HD22	4:D:959:VAL:HG11	1.92	0.48
2:B:52:THR:O	2:B:164:VAL:HG22	2.13	0.48
2:B:76:ILE:HG23	2:B:125:ILE:HD11	1.94	0.48
3:C:124:LEU:HD23	3:C:125:PHE:H	1.79	0.48
3:C:169:GLN:OE1	3:C:370:ARG:NH2	2.44	0.48
3:C:753:THR:HG21	3:C:799:PRO:HD2	1.96	0.48
3:C:754:LYS:HD3	4:D:39:LEU:HD12	1.94	0.48
4:D:330:LEU:HD22	4:D:330:LEU:H	1.77	0.48
4:D:1062:PHE:CE2	4:D:1080:LYS:HD2	2.49	0.48
6:F:465:LEU:HD23	6:F:465:LEU:C	2.34	0.48
2:A:40:ARG:HH21	2:B:32:TYR:HD2	1.62	0.48
2:A:177:LYS:HE2	2:A:193:ILE:HG12	1.96	0.48
3:C:572:VAL:O	3:C:573:SER:HB3	2.13	0.48
4:D:70:PHE:O	4:D:82:VAL:HG11	2.13	0.48
4:D:129:ILE:HD11	4:D:130:TYR:CE2	2.49	0.48
4:D:400:LYS:CE	4:D:404:ASP:HB3	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:81:HIS:CG	6:F:195:LEU:HD21	2.49	0.48
2:A:86:SER:CB	2:A:119:HIS:HE2	2.24	0.48
3:C:45:LEU:CD2	3:C:443:LYS:HD2	2.43	0.48
3:C:794:VAL:HG11	3:C:860:VAL:HG11	1.95	0.48
4:D:988:VAL:CG2	4:D:992:GLU:HG3	2.44	0.48
2:A:152:ASN:HB3	2:A:157:ALA:HB3	1.93	0.48
3:C:771:VAL:HG23	3:C:772:LEU:HD13	1.94	0.48
3:C:777:GLU:CD	3:C:777:GLU:H	2.15	0.48
9:T:283:LEU:O	9:T:286:ILE:HG22	2.14	0.48
2:B:94:THR:HA	2:B:138:LEU:O	2.14	0.47
3:C:29:ARG:HG2	3:C:964:ALA:HB2	1.96	0.47
3:C:664:ARG:HB2	3:C:677:GLN:OE1	2.14	0.47
3:C:797:VAL:HG11	3:C:823:VAL:HG21	1.96	0.47
3:C:948:SER:C	3:C:950:LEU:CB	2.83	0.47
2:B:79:ASN:O	2:B:123:MET:CE	2.62	0.47
3:C:38:PRO:CB	3:C:508:ARG:HH21	2.26	0.47
3:C:87:ILE:O	3:C:95:SER:HA	2.13	0.47
3:C:154:LYS:HE2	3:C:630:GLY:O	2.14	0.47
4:D:285:LYS:HA	4:D:289:LYS:HB2	1.94	0.47
6:F:253:MET:HE3	6:F:296:ALA:C	2.34	0.47
9:T:251:ILE:HD12	9:T:254:LEU:HD11	1.96	0.47
2:B:9:LEU:HD21	2:B:208:LEU:HD21	1.96	0.47
3:C:202:TRP:O	3:C:203:LEU:HD23	2.13	0.47
3:C:572:VAL:H	3:C:576:GLN:NE2	2.12	0.47
3:C:716:PRO:O	4:D:724:THR:HB	2.14	0.47
3:C:792:ILE:HD12	3:C:792:ILE:N	2.29	0.47
4:D:1279:ALA:HB1	5:E:79:LEU:HD13	1.95	0.47
6:F:416:ARG:HA	6:F:430:ILE:HD11	1.96	0.47
2:A:82:GLY:CA	2:A:123:MET:HE1	2.44	0.47
3:C:477:ILE:HD11	4:D:852:THR:HG21	1.96	0.47
4:D:137:THR:HG23	4:D:253:THR:OG1	2.15	0.47
4:D:665:THR:HG21	4:D:682:PHE:CE2	2.50	0.47
4:D:723:ALA:O	4:D:726:SER:HB3	2.14	0.47
9:T:264:LEU:HB3	9:T:269:VAL:HG21	1.92	0.47
1:J:58:ASN:HD21	1:J:60:LEU:HD12	1.80	0.47
2:B:198:THR:HG21	2:B:202:ILE:O	2.15	0.47
3:C:752:ASP:OD1	3:C:857:ASN:ND2	2.47	0.47
3:C:919:ILE:HD12	3:C:920:GLY:N	2.30	0.47
3:C:976:LEU:O	3:C:980:LEU:HD23	2.14	0.47
4:D:467:GLN:HA	4:D:467:GLN:NE2	2.29	0.47
4:D:1081:LEU:HB3	4:D:1113:MET:SD	2.54	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:1153:LYS:O	4:D:1157:VAL:HG23	2.14	0.47
1:J:84:MET:HE2	6:F:272:LYS:HE2	1.97	0.47
2:A:9:LEU:HB2	2:A:23:ILE:HG12	1.97	0.47
2:A:108:GLY:HA2	2:A:121:PRO:HB3	1.96	0.47
2:B:85:VAL:HB	2:B:118:VAL:HA	1.96	0.47
3:C:174:PRO:HB2	3:C:303:GLY:HA3	1.97	0.47
3:C:203:LEU:HD13	3:C:217:ILE:CG2	2.43	0.47
3:C:475:CYS:HA	3:C:577:MET:O	2.15	0.47
4:D:880:SER:O	4:D:995:GLY:HA3	2.13	0.47
4:D:1119:PRO:HA	4:D:1122:VAL:HG12	1.94	0.47
6:F:316:LYS:HD3	6:F:341:MET:HE3	1.97	0.47
6:F:462:ARG:HH11	6:F:465:LEU:HB2	1.78	0.47
7:O:15:DT:H1'	7:O:16:DT:H5''	1.97	0.47
2:B:18:ARG:HG3	2:B:197:GLU:CG	2.41	0.47
2:B:63:PHE:N	2:B:63:PHE:CD1	2.81	0.47
2:B:80:LEU:HG	2:B:125:ILE:HD13	1.96	0.47
2:B:139:VAL:HG21	2:B:161:ARG:HH21	1.79	0.47
2:B:147:VAL:HG13	2:B:166:SER:HB2	1.95	0.47
2:B:202:ILE:HD13	2:B:207:ALA:HB2	1.96	0.47
3:C:272:LEU:C	3:C:274:PRO:HD3	2.35	0.47
3:C:741:ILE:HG22	3:C:742:HIS:H	1.80	0.47
3:C:1033:HIS:HB3	11:C:1205:EDO:O1	2.13	0.47
3:C:1126:VAL:HG23	3:C:1126:VAL:O	2.15	0.47
4:D:91:ARG:O	4:D:321:PRO:HG3	2.15	0.47
4:D:105:TRP:CE2	4:D:1231:THR:HG23	2.49	0.47
4:D:590:THR:CG2	4:D:630:ARG:HE	2.27	0.47
4:D:653:ASN:N	4:D:654:GLY:HA3	2.30	0.47
4:D:799:ILE:HD13	4:D:799:ILE:HA	1.69	0.47
4:D:869:SER:HB2	4:D:1029:LEU:HD21	1.97	0.47
4:D:1247:ASN:O	4:D:1260:PRO:HG3	2.15	0.47
4:D:1276:THR:HG22	5:E:102:GLU:HG2	1.96	0.47
2:A:9:LEU:HD23	2:B:221:LEU:C	2.35	0.47
3:C:896:PRO:HB2	3:C:1001:LEU:HD13	1.97	0.47
4:D:52:PHE:O	4:D:91:ARG:HD2	2.15	0.47
4:D:430:ILE:HD13	4:D:541:MET:HG3	1.96	0.47
1:J:73:LYS:O	1:J:74:LYS:HG3	2.15	0.47
3:C:265:LEU:CD1	3:C:287:LEU:HD12	2.45	0.47
4:D:1117:ALA:O	4:D:1119:PRO:HD3	2.15	0.47
8:P:11:DA:H2'	8:P:12:DA:C8	2.48	0.47
9:T:257:THR:O	9:T:260:SER:N	2.48	0.47
2:A:11:GLU:CD	2:A:205:ARG:HG2	2.35	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:43:LEU:HD12	2:B:43:LEU:HA	1.77	0.47
3:C:361:ILE:HD12	3:C:361:ILE:N	2.24	0.47
3:C:598:MET:O	3:C:602:MET:HG3	2.15	0.47
3:C:764:ILE:HB	3:C:767:VAL:HG21	1.96	0.47
3:C:1084:SER:OG	4:D:420:LYS:HD3	2.15	0.47
3:C:1117:LYS:HE2	4:D:90:GLU:O	2.15	0.47
4:D:687:MET:CE	4:D:695:ILE:HD11	2.45	0.47
3:C:460:GLY:HA3	3:C:462:GLU:OE1	2.15	0.46
3:C:508:ARG:HD2	3:C:570:MET:HE3	1.97	0.46
3:C:731:ARG:NH1	3:C:735:GLU:OE1	2.48	0.46
3:C:885:VAL:HG22	4:D:536:PHE:O	2.14	0.46
4:D:704:PRO:HD2	4:D:707:VAL:HG21	1.97	0.46
3:C:70:GLU:N	3:C:70:GLU:OE1	2.48	0.46
3:C:167:VAL:HG13	3:C:445:ARG:O	2.16	0.46
4:D:236:VAL:O	4:D:236:VAL:HG12	2.15	0.46
4:D:285:LYS:HG3	4:D:289:LYS:CD	2.45	0.46
4:D:915:VAL:HG23	4:D:920:PHE:HE2	1.80	0.46
4:D:1056:LEU:HD23	4:D:1057:GLU:H	1.79	0.46
2:A:197:GLU:CD	3:C:987:ARG:HH22	2.17	0.46
3:C:372:VAL:O	3:C:376:ILE:HG12	2.15	0.46
3:C:549:ARG:HB2	3:C:561:PHE:CZ	2.50	0.46
3:C:754:LYS:HE2	3:C:754:LYS:N	2.26	0.46
3:C:767:VAL:HB	3:C:771:VAL:HG21	1.96	0.46
4:D:66:LYS:HG2	4:D:66:LYS:O	2.14	0.46
4:D:493:GLU:HA	4:D:513:GLU:OE1	2.14	0.46
4:D:920:PHE:CZ	4:D:948:ILE:HG13	2.50	0.46
2:A:177:LYS:HE2	2:A:193:ILE:CG1	2.46	0.46
2:A:210:SER:HB3	2:B:229:SER:CB	2.44	0.46
2:B:22:VAL:HG12	2:B:193:ILE:CD1	2.42	0.46
3:C:494:TYR:CD2	3:C:572:VAL:HG21	2.44	0.46
3:C:754:LYS:HD3	4:D:39:LEU:CD1	2.46	0.46
3:C:797:VAL:HG11	3:C:823:VAL:CG2	2.45	0.46
3:C:845:SER:O	3:C:850:ASP:HB2	2.16	0.46
3:C:935:TRP:HB2	3:C:982:SER:HB2	1.97	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
2:B:34:LEU:O	2:B:37:SER:N	2.49	0.46
2:B:181:THR:HB	2:B:182:ARG:CB	2.46	0.46
3:C:523:THR:CG2	3:C:526:GLU:HG2	2.46	0.46
3:C:560:GLU:HG3	3:C:562:VAL:HG23	1.98	0.46
3:C:714:ILE:O	3:C:910:THR:OG1	2.23	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:447:MET:HE3	4:D:543:VAL:HG21	1.98	0.46
8:P:4:DA:H2''	8:P:5:DC:C6	2.50	0.46
2:B:63:PHE:N	2:B:63:PHE:HD1	2.13	0.46
2:B:105:VAL:HG23	2:B:128:LEU:HD11	1.96	0.46
3:C:26:ALA:HB1	3:C:623:LEU:HD21	1.97	0.46
3:C:477:ILE:O	3:C:477:ILE:HG22	2.16	0.46
3:C:584:MET:O	14:C:1305:HOH:O	2.21	0.46
3:C:727:ILE:HA	3:C:888:LYS:O	2.16	0.46
3:C:1066:ALA:HB1	4:D:506:ARG:HA	1.96	0.46
4:D:102:THR:OG1	4:D:129:ILE:HD12	2.15	0.46
4:D:155:MET:CE	4:D:219:LEU:HD22	2.46	0.46
4:D:618:ALA:HB1	4:D:627:LEU:CD1	2.46	0.46
2:B:65:THR:HG22	2:B:66:VAL:N	2.31	0.46
3:C:96:LEU:HD22	3:C:98:PHE:HE1	1.79	0.46
3:C:781:VAL:HG21	3:C:838:VAL:HG21	1.98	0.46
4:D:226:PHE:CE1	4:D:248:TYR:HB3	2.50	0.46
4:D:693:ALA:O	4:D:697:ASN:HB2	2.16	0.46
4:D:699:LEU:CD1	4:D:711:THR:HG21	2.45	0.46
4:D:1041:PRO:HB3	4:D:1116:ALA:CB	2.46	0.46
6:F:234:LEU:HD23	6:F:270:VAL:HG21	1.97	0.46
8:P:11:DA:H2'	8:P:12:DA:H8	1.81	0.46
3:C:193:VAL:CG1	3:C:205:PHE:HB2	2.46	0.46
3:C:510:VAL:HG12	3:C:568:ASP:O	2.16	0.46
4:D:64:LYS:NZ	4:D:76:GLU:OE2	2.43	0.46
4:D:500:ARG:HB2	4:D:541:MET:HG2	1.98	0.46
4:D:875:ARG:HH2	4:D:1033:GLN:CD	2.18	0.46
4:D:1034:GLU:OE2	4:D:1041:PRO:HA	2.15	0.46
6:F:406:SER:HB3	6:F:409:GLU:HG3	1.98	0.46
3:C:809:GLU:O	3:C:813:ARG:HG2	2.15	0.46
4:D:60:CYS:SG	4:D:63:GLY:N	2.81	0.46
4:D:588:LEU:HD22	4:D:668:GLY:CA	2.44	0.46
4:D:590:THR:HG23	4:D:630:ARG:HE	1.81	0.46
4:D:863:ALA:O	4:D:866:THR:HG22	2.15	0.46
4:D:1174:THR:OG1	4:D:1175:GLU:CB	2.64	0.46
6:F:394:LEU:HB2	6:F:464:TYR:CE1	2.51	0.46
6:F:465:LEU:HD23	6:F:466:ASP:HB2	1.98	0.46
7:O:6:DA:C1'	7:O:7:DC:H5'	2.46	0.46
2:A:24:GLU:HB3	2:A:191:LYS:HB2	1.98	0.46
2:A:63:PHE:HE1	3:C:741:ILE:HD13	1.81	0.46
3:C:169:GLN:HB2	3:C:427:LEU:HD21	1.97	0.46
3:C:178:PHE:CD1	3:C:193:VAL:HB	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:659:GLN:OE1	3:C:659:GLN:N	2.48	0.46
3:C:984:LEU:CD1	3:C:989:GLY:HA2	2.46	0.46
4:D:140:ASP:OD2	4:D:143:MET:HB2	2.16	0.46
4:D:320:ILE:HG12	4:D:321:PRO:CD	2.46	0.46
4:D:633:ILE:O	4:D:665:THR:O	2.34	0.46
4:D:656:LYS:O	4:D:656:LYS:CE	2.64	0.46
4:D:1009:LEU:CD1	4:D:1146:GLN:HG3	2.44	0.46
2:A:42:LEU:HD23	2:A:211:ALA:HB2	1.98	0.45
2:A:56:ILE:HB	2:A:59:VAL:CG2	2.43	0.45
2:A:125:ILE:N	2:A:125:ILE:HD12	2.30	0.45
3:C:1118:GLU:OE1	4:D:412:ARG:HG3	2.17	0.45
4:D:518:GLU:O	14:D:2104:HOH:O	2.21	0.45
4:D:738:PRO:HA	4:D:791:PHE:HD2	1.81	0.45
4:D:755:ILE:HD12	4:D:776:ILE:CD1	2.46	0.45
4:D:823:VAL:HG12	4:D:824:THR:N	2.31	0.45
4:D:923:THR:OG1	4:D:962:ARG:HD2	2.16	0.45
6:F:201:LEU:HD11	6:F:219:MET:CB	2.42	0.45
7:O:2:DC:H2''	7:O:3:DT:O5'	2.16	0.45
7:O:28:DT:P	14:O:101:HOH:O	2.74	0.45
1:J:73:LYS:O	1:J:74:LYS:CG	2.64	0.45
2:B:66:VAL:HG12	2:B:69:VAL:HG22	1.98	0.45
2:B:76:ILE:HG23	2:B:125:ILE:HD12	1.97	0.45
3:C:766:ASN:HB3	6:F:465:LEU:HD21	1.98	0.45
4:D:765:ASN:ND2	4:D:767:THR:HG23	2.31	0.45
4:D:899:THR:O	4:D:957:THR:O	2.34	0.45
4:D:1036:PHE:HD2	4:D:1162:MET:HE1	1.81	0.45
4:D:1123:LEU:HB2	4:D:1131:VAL:HG21	1.97	0.45
6:F:454:HIS:CD2	6:F:456:SER:HG	2.34	0.45
7:O:6:DA:H1'	7:O:7:DC:C5'	2.46	0.45
2:A:11:GLU:OE2	2:B:225:LEU:HD22	2.16	0.45
2:B:28:PRO:HA	2:B:190:ASP:OD2	2.16	0.45
2:B:174:VAL:HA	2:B:195:ASP:O	2.16	0.45
3:C:62:ARG:HG3	3:C:66:ILE:HD11	1.98	0.45
4:D:271:ASP:HA	4:D:303:GLN:NE2	2.31	0.45
4:D:581:MET:HE2	4:D:716:LYS:HA	1.99	0.45
4:D:956:ILE:CD1	4:D:956:ILE:O	2.64	0.45
3:C:747:GLU:HG3	3:C:859:LEU:HD21	1.98	0.45
3:C:767:VAL:HB	3:C:771:VAL:CG2	2.46	0.45
3:C:1035:ARG:CZ	3:C:1047:PRO:HB3	2.45	0.45
3:C:1103:ILE:HD12	4:D:548:SER:CA	2.46	0.45
4:D:931:ALA:HA	4:D:932:ASN:HA	1.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:952:LEU:HD12	4:D:952:LEU:HA	1.85	0.45
6:F:176:VAL:CG1	6:F:177:ALA:N	2.79	0.45
6:F:408:ARG:HH21	11:F:506:EDO:H22	1.82	0.45
7:O:27:DA:H4'	7:O:28:DT:OP1	2.17	0.45
2:A:55:ARG:HH12	2:A:161:ARG:CZ	2.28	0.45
2:A:63:PHE:O	3:C:666:PHE:CD2	2.70	0.45
2:B:213:GLY:CA	2:B:216:VAL:HG12	2.45	0.45
3:C:130:PHE:CZ	3:C:403:ILE:HG13	2.52	0.45
3:C:523:THR:HG22	3:C:526:GLU:OE2	2.16	0.45
3:C:638:THR:HG23	3:C:688:GLU:HA	1.98	0.45
3:C:918:ASN:O	3:C:920:GLY:N	2.50	0.45
4:D:277:LEU:HD21	4:D:292:ALA:O	2.17	0.45
4:D:376:GLU:OE2	6:F:165:SER:OG	2.24	0.45
4:D:948:ILE:O	4:D:952:LEU:HB2	2.16	0.45
5:E:28:THR:HG23	5:E:28:THR:O	2.17	0.45
5:E:76:VAL:CG1	5:E:77:GLY:N	2.80	0.45
5:E:80:VAL:CG2	5:E:100:LEU:HD22	2.47	0.45
3:C:29:ARG:HD3	3:C:964:ALA:HB2	1.98	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
3:C:231:ALA:HB1	3:C:265:LEU:HD12	1.97	0.45
3:C:780:ILE:HD12	3:C:781:VAL:O	2.16	0.45
3:C:1048:LEU:HD23	3:C:1048:LEU:N	2.21	0.45
4:D:448:ALA:HB1	4:D:491:ILE:HD11	1.98	0.45
6:F:170:LEU:HA	6:F:173:ILE:HG12	1.98	0.45
8:P:17:DT:H5''	9:T:290:GLY:N	2.31	0.45
2:A:108:GLY:CA	2:A:121:PRO:HB3	2.47	0.45
2:B:153:LYS:N	2:B:154:ALA:CA	2.70	0.45
3:C:71:GLU:HA	3:C:71:GLU:OE2	2.17	0.45
3:C:77:LEU:HD23	3:C:77:LEU:HA	1.74	0.45
3:C:575:ARG:HE	3:C:967:VAL:CG2	2.25	0.45
3:C:850:ASP:HB3	3:C:851:GLU:H	1.55	0.45
4:D:287:GLN:HG3	4:D:288:LYS:HZ2	1.81	0.45
4:D:910:ILE:O	4:D:910:ILE:HG12	2.17	0.45
6:F:186:GLU:OE1	6:F:186:GLU:HA	2.17	0.45
1:J:51:PRO:O	1:J:64:LEU:HD12	2.16	0.45
3:C:346:MET:HB2	3:C:356:VAL:CG2	2.47	0.45
3:C:895:MET:HE2	3:C:895:MET:HB2	1.66	0.45
3:C:913:VAL:HB	3:C:914:PRO:HD3	1.97	0.45
3:C:1037:THR:HG22	3:C:1038:GLY:N	2.32	0.45
8:P:11:DA:H2''	8:P:12:DA:H5'	1.96	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:74:THR:OG1	4:D:608:GLU:OE1	2.35	0.45
2:B:99:LYS:HE2	2:B:99:LYS:HB3	1.65	0.45
3:C:394:ARG:HG3	3:C:398:GLN:CG	2.47	0.45
3:C:780:ILE:O	3:C:780:ILE:HG13	2.16	0.45
3:C:1043:ILE:HD12	3:C:1043:ILE:H	1.81	0.45
4:D:102:THR:HG23	4:D:258:ALA:CB	2.47	0.45
4:D:608:GLU:O	4:D:609:GLN:HB2	2.17	0.45
4:D:972:GLY:HA2	10:D:2005:SO4:O2	2.17	0.45
1:J:88:ARG:HG3	1:J:89:ARG:N	2.32	0.45
2:B:147:VAL:HG13	2:B:147:VAL:O	2.17	0.45
2:B:196:VAL:HG13	2:B:196:VAL:O	2.17	0.45
3:C:523:THR:HG23	3:C:526:GLU:HG2	1.99	0.45
3:C:614:ALA:HA	3:C:705:ALA:CB	2.47	0.45
4:D:1110:ASP:N	4:D:1110:ASP:OD1	2.50	0.45
2:B:28:PRO:HD3	2:B:189:PHE:CD1	2.52	0.44
3:C:193:VAL:HG22	3:C:194:LYS:N	2.32	0.44
3:C:632:VAL:HG13	3:C:694:ALA:O	2.17	0.44
3:C:1003:ASP:OD1	3:C:1005:ARG:HB3	2.17	0.44
4:D:720:PHE:O	4:D:724:THR:HG23	2.17	0.44
4:D:982:MET:HE3	4:D:1151:HIS:CG	2.52	0.44
1:J:57:ARG:HG3	4:D:25:TYR:HA	1.98	0.44
3:C:53:GLU:OE2	3:C:60:ARG:NH1	2.35	0.44
3:C:71:GLU:C	3:C:73:PRO:HD3	2.38	0.44
3:C:197:PRO:HB3	3:C:297:TYR:OH	2.16	0.44
4:D:243:GLU:HG2	4:D:247:ARG:HH21	1.81	0.44
8:P:3:DC:H2"	8:P:4:DA:H8	1.81	0.44
2:A:216:VAL:HG13	2:B:216:VAL:HG23	1.99	0.44
2:A:219:PHE:CE1	2:B:38:LEU:HD21	2.52	0.44
3:C:291:PHE:O	3:C:297:TYR:HB3	2.17	0.44
3:C:404:THR:HG23	3:C:407:THR:HG23	1.98	0.44
3:C:615:PRO:HB3	3:C:1020:TYR:CE2	2.51	0.44
3:C:723:GLU:HA	3:C:723:GLU:OE1	2.18	0.44
4:D:591:LEU:HD23	4:D:630:ARG:O	2.18	0.44
4:D:644:THR:HA	4:D:647:GLU:CD	2.36	0.44
5:E:53:TYR:CE1	5:E:101:LEU:HD12	2.53	0.44
6:F:394:LEU:HD13	6:F:464:TYR:CG	2.52	0.44
2:A:18:ARG:HA	2:A:204:PRO:CG	2.47	0.44
3:C:80:VAL:CG2	3:C:377:GLN:HG3	2.47	0.44
3:C:1015:THR:OG1	4:D:731:SER:OG	2.36	0.44
4:D:58:TRP:HH2	4:D:84:ARG:NH2	2.16	0.44
4:D:911:ARG:HG2	4:D:952:LEU:HD21	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:929:VAL:HG23	4:D:929:VAL:O	2.17	0.44
5:E:57:ARG:NH2	5:E:77:GLY:HA3	2.31	0.44
6:F:462:ARG:HA	6:F:462:ARG:HD3	1.79	0.44
1:J:58:ASN:HD21	1:J:60:LEU:CG	2.31	0.44
3:C:154:LYS:O	3:C:443:LYS:HE3	2.17	0.44
4:D:240:LEU:HD23	4:D:240:LEU:C	2.38	0.44
2:A:90:ASP:O	2:A:91:GLU:CG	2.66	0.44
2:A:174:VAL:O	3:C:901:GLY:HA3	2.18	0.44
2:A:187:THR:O	2:A:187:THR:HG23	2.17	0.44
2:B:150:VAL:HG13	2:B:150:VAL:O	2.17	0.44
4:D:130:TYR:O	4:D:372:ARG:HD3	2.17	0.44
4:D:814:ARG:O	4:D:817:ALA:O	2.36	0.44
4:D:884:ILE:HD11	4:D:886:ARG:CD	2.48	0.44
4:D:1165:ARG:HG2	4:D:1183:GLU:HA	1.99	0.44
4:D:1174:THR:CG2	4:D:1176:PHE:N	2.74	0.44
6:F:337:LEU:HD12	6:F:337:LEU:HA	1.78	0.44
1:J:28:GLN:N	1:J:44:PHE:O	2.50	0.44
1:J:69:VAL:N	1:J:70:PRO:HD3	2.33	0.44
2:A:48:GLY:O	2:A:142:ARG:HG2	2.16	0.44
2:A:78:LEU:CD1	3:C:611:ARG:HH11	2.31	0.44
3:C:41:VAL:HG22	3:C:494:TYR:HE1	1.83	0.44
3:C:291:PHE:HA	3:C:297:TYR:HB2	1.99	0.44
4:D:58:TRP:HA	4:D:82:VAL:HG23	2.00	0.44
4:D:129:ILE:HG12	4:D:130:TYR:CD2	2.53	0.44
4:D:439:HIS:O	4:D:513:GLU:N	2.48	0.44
4:D:525:HIS:O	4:D:528:VAL:HG22	2.18	0.44
4:D:600:GLN:CB	4:D:601:ALA:HA	2.48	0.44
4:D:633:ILE:HD13	4:D:635:VAL:HG13	1.99	0.44
4:D:739:PRO:HD3	4:D:791:PHE:CE2	2.53	0.44
9:T:280:GLU:HG3	9:T:294:ILE:HD13	2.00	0.44
1:J:104:LEU:HD23	1:J:104:LEU:O	2.18	0.44
2:A:10:SER:OG	2:A:22:VAL:HG13	2.18	0.44
2:A:96:TYR:O	2:A:111:VAL:HG13	2.17	0.44
2:A:193:ILE:HD12	2:A:193:ILE:C	2.38	0.44
3:C:62:ARG:HG3	3:C:66:ILE:CD1	2.47	0.44
3:C:619:THR:OG1	3:C:620:GLY:N	2.50	0.44
3:C:1066:ALA:CB	4:D:506:ARG:HA	2.48	0.44
4:D:12:ILE:HD11	4:D:1221:TRP:CE2	2.53	0.44
4:D:796:ASN:ND2	4:D:798:ILE:HB	2.28	0.44
5:E:29:PRO:CG	5:E:34:ASN:HB2	2.47	0.44
2:A:54:ILE:C	2:A:54:ILE:HD12	2.38	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:95:MET:CE	2:B:110:ILE:HD11	2.47	0.44
2:B:170:PRO:CB	2:B:202:ILE:HD11	2.43	0.44
2:B:191:LYS:HG2	2:B:193:ILE:HD11	1.99	0.44
4:D:735:VAL:CG1	4:D:816:LEU:HD22	2.48	0.44
4:D:735:VAL:CG1	4:D:840:ARG:HD2	2.42	0.44
6:F:320:ILE:HG22	6:F:337:LEU:HD12	2.00	0.44
2:B:79:ASN:O	2:B:123:MET:HE2	2.18	0.43
3:C:426:GLN:CD	3:C:450:GLY:HA2	2.37	0.43
3:C:498:ASN:HB2	3:C:502:PHE:O	2.18	0.43
4:D:397:ARG:HG3	4:D:397:ARG:O	2.18	0.43
4:D:1152:ASP:O	4:D:1156:GLU:HG3	2.18	0.43
9:T:269:VAL:O	9:T:269:VAL:HG23	2.17	0.43
2:B:17:ASN:OD1	2:B:17:ASN:N	2.36	0.43
2:B:111:VAL:O	2:B:111:VAL:HG13	2.17	0.43
3:C:166:VAL:CG1	3:C:372:VAL:HG23	2.48	0.43
3:C:228:LEU:HD23	3:C:228:LEU:HA	1.70	0.43
3:C:595:ARG:HA	3:C:595:ARG:HD2	1.90	0.43
3:C:706:LEU:N	14:C:1306:HOH:O	2.25	0.43
3:C:788:ARG:O	3:C:830:VAL:CG1	2.67	0.43
3:C:875:LYS:C	3:C:876:LEU:HD12	2.37	0.43
4:D:799:ILE:CG2	4:D:803:LYS:HE2	2.48	0.43
4:D:1123:LEU:HA	4:D:1131:VAL:HG22	2.01	0.43
6:F:244:LEU:HD12	6:F:289:ILE:HG21	2.00	0.43
8:P:4:DA:H2"	8:P:5:DC:H6	1.82	0.43
2:A:40:ARG:CZ	2:B:33:THR:HG22	2.48	0.43
2:B:104:VAL:O	2:B:104:VAL:HG13	2.18	0.43
2:B:151:GLN:HG2	2:B:151:GLN:O	2.17	0.43
3:C:947:ALA:O	3:C:951:PRO:HD2	2.19	0.43
3:C:1028:VAL:HG12	4:D:429:VAL:CG1	2.47	0.43
4:D:47:PHE:CD1	4:D:322:PRO:HB3	2.52	0.43
4:D:813:THR:O	4:D:813:THR:HG22	2.18	0.43
4:D:1181:LEU:HD22	4:D:1207:VAL:HG11	2.01	0.43
2:B:71:GLU:OE2	2:B:127:THR:HG23	2.18	0.43
4:D:23:TRP:HB3	4:D:92:MET:HE3	2.00	0.43
4:D:138:SER:HB3	4:D:253:THR:HG1	1.80	0.43
4:D:143:MET:HE2	4:D:251:TYR:CD1	2.54	0.43
4:D:901:ALA:HB2	4:D:912:ASP:H	1.82	0.43
6:F:345:PRO:HA	6:F:348:VAL:HG13	1.99	0.43
3:C:174:PRO:O	3:C:303:GLY:HA2	2.18	0.43
3:C:344:THR:O	3:C:344:THR:HG22	2.19	0.43
3:C:505:THR:HG22	3:C:506:PRO:HD2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:587:PHE:HB3	3:C:590:HIS:HD2	1.84	0.43
4:D:114:LEU:HG	4:D:312:MET:CE	2.47	0.43
6:F:321:GLN:NE2	6:F:331:GLU:OE2	2.52	0.43
6:F:349:LEU:HD12	6:F:349:LEU:HA	1.80	0.43
9:T:254:LEU:HB2	9:T:256:LEU:HG	2.01	0.43
1:J:69:VAL:N	1:J:70:PRO:CD	2.82	0.43
2:B:152:ASN:CA	2:B:154:ALA:HA	2.47	0.43
3:C:265:LEU:HD21	3:C:284:GLN:HA	2.00	0.43
3:C:390:VAL:HG11	3:C:394:ARG:HH21	1.84	0.43
3:C:667:ALA:HB3	3:C:675:ALA:HB3	2.01	0.43
3:C:973:GLU:CB	4:D:732:MET:HE1	2.49	0.43
3:C:1025:HIS:CD2	3:C:1025:HIS:O	2.72	0.43
4:D:163:GLU:HG2	4:D:166:ARG:HH21	1.83	0.43
6:F:171:LYS:HB3	6:F:171:LYS:HE2	1.78	0.43
6:F:465:LEU:O	6:F:466:ASP:HB2	2.17	0.43
1:J:106:LYS:HE2	1:J:106:LYS:HB3	1.77	0.43
2:B:74:THR:HG21	4:D:608:GLU:OE1	2.18	0.43
3:C:43:GLY:O	3:C:46:ASP:HB2	2.18	0.43
3:C:98:PHE:HE2	3:C:387:MET:HE1	1.84	0.43
3:C:577:MET:CE	4:D:849:PHE:HD1	2.30	0.43
3:C:1130:SER:HB3	3:C:1132:ASP:C	2.39	0.43
4:D:246:ASP:OD1	4:D:246:ASP:N	2.50	0.43
4:D:269:ASP:OD2	4:D:272:ALA:N	2.52	0.43
4:D:1119:PRO:O	4:D:1122:VAL:HG13	2.19	0.43
2:A:210:SER:CB	2:B:229:SER:CB	2.96	0.43
2:B:33:THR:OG1	2:B:34:LEU:N	2.51	0.43
3:C:361:ILE:H	3:C:361:ILE:CD1	2.28	0.43
3:C:447:SER:HB2	3:C:449:LEU:HD11	2.00	0.43
3:C:728:LEU:HD22	3:C:906:ILE:HG22	1.96	0.43
3:C:1100:GLY:CA	4:D:458:LYS:HE3	2.43	0.43
5:E:37:ILE:H	5:E:37:ILE:HG13	1.27	0.43
2:B:28:PRO:HA	2:B:29:GLY:HA2	1.80	0.43
2:B:64:THR:C	2:B:65:THR:HG1	2.04	0.43
3:C:51:SER:HB2	3:C:371:THR:OG1	2.19	0.43
3:C:365:GLY:HA3	3:C:525:ASP:OD1	2.19	0.43
3:C:369:LEU:HD12	3:C:369:LEU:HA	1.61	0.43
3:C:405:PRO:O	3:C:409:ILE:HG13	2.19	0.43
3:C:479:THR:OG1	3:C:480:PRO:CD	2.67	0.43
3:C:1001:LEU:HB2	3:C:1010:PHE:HD2	1.83	0.43
4:D:1140:GLN:NE2	4:D:1155:ILE:HD12	2.34	0.43
7:O:12:DG:C8	7:O:13:DT:H72	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:68:GLY:O	2:B:129:ASN:N	2.41	0.43
2:B:151:GLN:C	2:B:154:ALA:HB1	2.39	0.43
3:C:197:PRO:HB3	3:C:297:TYR:CZ	2.54	0.43
3:C:427:LEU:HD12	3:C:427:LEU:N	2.34	0.43
3:C:895:MET:HG3	3:C:896:PRO:CD	2.49	0.43
3:C:1049:GLY:HA3	4:D:421:ARG:CZ	2.49	0.43
4:D:131:PHE:HA	4:D:256:MET:HE2	2.01	0.43
4:D:656:LYS:O	4:D:656:LYS:HE2	2.19	0.43
5:E:53:TYR:HE1	5:E:101:LEU:HD12	1.84	0.43
2:A:40:ARG:CD	2:B:33:THR:HG22	2.41	0.42
3:C:113:CYS:HA	3:C:118:MET:HG3	2.01	0.42
3:C:128:ALA:CB	3:C:405:PRO:HB3	2.49	0.42
3:C:466:VAL:HG12	4:D:856:ARG:CZ	2.49	0.42
3:C:839:ILE:HD12	3:C:865:ALA:HB2	2.01	0.42
3:C:949:LYS:HG3	3:C:949:LYS:O	2.19	0.42
4:D:397:ARG:NH2	6:F:360:SER:OG	2.52	0.42
4:D:938:GLU:OE1	4:D:938:GLU:N	2.35	0.42
4:D:1056:LEU:HD23	4:D:1057:GLU:N	2.34	0.42
2:A:24:GLU:HB3	2:A:191:LYS:CG	2.49	0.42
2:A:147:VAL:CG1	2:A:166:SER:HB2	2.48	0.42
2:B:22:VAL:HG12	2:B:193:ILE:HG23	2.00	0.42
2:B:64:THR:HA	2:B:73:VAL:HG21	2.00	0.42
3:C:114:LYS:HG2	3:C:161:GLY:O	2.19	0.42
3:C:310:LYS:O	3:C:354:VAL:HG21	2.19	0.42
3:C:475:CYS:HB2	3:C:579:SER:HB3	2.00	0.42
3:C:1090:ARG:O	3:C:1093:VAL:HG12	2.19	0.42
4:D:599:TYR:CA	4:D:610:GLY:HA3	2.48	0.42
4:D:831:ILE:HA	4:D:831:ILE:HD12	1.72	0.42
6:F:263:ASN:O	6:F:267:ILE:HG13	2.19	0.42
6:F:440:ARG:O	6:F:444:ILE:HG13	2.19	0.42
1:J:58:ASN:HD21	1:J:60:LEU:HG	1.83	0.42
2:A:34:LEU:HD23	2:A:34:LEU:HA	1.77	0.42
2:A:84:VAL:HG13	2:A:84:VAL:O	2.19	0.42
3:C:31:SER:HA	3:C:964:ALA:O	2.19	0.42
3:C:562:VAL:HG12	3:C:563:SER:N	2.34	0.42
3:C:1001:LEU:N	3:C:1001:LEU:HD23	2.34	0.42
4:D:647:GLU:OE1	4:D:655:TRP:HH2	2.02	0.42
4:D:1034:GLU:O	14:D:2105:HOH:O	2.21	0.42
4:D:1163:LEU:HA	4:D:1163:LEU:HD23	1.79	0.42
5:E:81:GLU:O	5:E:94:ARG:NH2	2.48	0.42
6:F:452:LEU:HD12	6:F:452:LEU:HA	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:98:ARG:O	2:A:99:LYS:HD2	2.19	0.42
2:A:161:ARG:O	2:A:163:PRO:HD3	2.19	0.42
3:C:169:GLN:HB2	3:C:427:LEU:CD2	2.50	0.42
3:C:529:ARG:HB3	3:C:529:ARG:CZ	2.49	0.42
3:C:602:MET:HA	3:C:605:GLN:HB2	2.02	0.42
4:D:35:ASN:OD1	4:D:37:ARG:N	2.47	0.42
4:D:568:PRO:HB3	4:D:983:ALA:HB2	2.02	0.42
4:D:633:ILE:C	4:D:633:ILE:HD12	2.39	0.42
4:D:686:GLN:O	4:D:686:GLN:HG3	2.19	0.42
2:A:146:TYR:OH	3:C:869:LYS:NZ	2.53	0.42
3:C:454:LEU:HD12	3:C:454:LEU:O	2.19	0.42
3:C:1003:ASP:HB2	3:C:1010:PHE:CE1	2.54	0.42
3:C:1074:TYR:CZ	4:D:1258:LEU:HD21	2.55	0.42
4:D:51:ILE:H	4:D:51:ILE:HG12	1.67	0.42
4:D:83:THR:OG1	4:D:84:ARG:N	2.53	0.42
4:D:452:PHE:CE1	4:D:491:ILE:HG12	2.55	0.42
4:D:584:GLY:HA3	4:D:719:GLY:O	2.19	0.42
4:D:641:ARG:CZ	4:D:655:TRP:CZ2	3.02	0.42
4:D:687:MET:HE2	4:D:695:ILE:HD11	2.00	0.42
4:D:781:THR:CG2	4:D:814:ARG:HD2	2.49	0.42
4:D:900:LEU:HD11	4:D:948:ILE:HD12	2.02	0.42
4:D:1044:LYS:HE3	4:D:1118:ASP:HB2	2.01	0.42
4:D:1170:ASP:O	4:D:1202:ALA:HA	2.19	0.42
5:E:60:GLN:HG3	5:E:74:GLU:CB	2.49	0.42
6:F:325:LEU:HD23	6:F:330:ARG:O	2.18	0.42
2:A:175:THR:HG22	2:A:195:ASP:HB3	2.01	0.42
2:B:26:LEU:HD13	2:B:30:PHE:HB3	2.02	0.42
3:C:691:GLN:HG2	3:C:692:VAL:H	1.84	0.42
3:C:751:ARG:CD	3:C:856:VAL:HG22	2.50	0.42
4:D:117:LEU:O	4:D:117:LEU:HD22	2.19	0.42
4:D:334:ARG:HD3	6:F:356:ARG:NH2	2.35	0.42
4:D:735:VAL:HG11	4:D:816:LEU:CD2	2.50	0.42
4:D:934:ASN:OD1	4:D:934:ASN:N	2.53	0.42
4:D:1171:SER:HA	4:D:1174:THR:CG2	2.48	0.42
4:D:1208:LEU:HD23	4:D:1208:LEU:HA	1.85	0.42
3:C:985:PRO:HB3	3:C:989:GLY:HA2	2.01	0.42
4:D:653:ASN:HB2	4:D:654:GLY:HA2	1.99	0.42
2:B:50:ALA:HB2	2:B:167:ILE:O	2.19	0.42
2:B:182:ARG:C	2:B:184:GLU:H	2.21	0.42
3:C:203:LEU:HD22	3:C:217:ILE:HA	2.02	0.42
3:C:627:ILE:HD12	3:C:628:ASP:N	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:963:VAL:HG12	3:C:964:ALA:N	2.35	0.42
4:D:245:GLN:O	4:D:249:GLY:HA3	2.19	0.42
6:F:310:MET:O	6:F:314:ILE:HG13	2.20	0.42
2:A:40:ARG:NH2	2:B:32:TYR:HD2	2.18	0.42
3:C:616:LEU:HB2	3:C:709:ASN:CG	2.40	0.42
3:C:885:VAL:HG11	4:D:538:GLY:HA2	2.02	0.42
3:C:1122:LEU:HD12	3:C:1122:LEU:HA	1.83	0.42
4:D:250:GLU:HG3	4:D:251:TYR:CE2	2.55	0.42
4:D:640:LEU:O	4:D:656:LYS:HE3	2.19	0.42
4:D:991:GLY:HA2	4:D:1265:ILE:CD1	2.50	0.42
1:J:48:ALA:HB2	4:D:65:TYR:OH	2.19	0.42
2:A:93:VAL:CG2	2:A:113:PRO:HG3	2.49	0.42
2:B:226:ASN:O	2:B:227:ALA:HB3	2.19	0.42
3:C:89:ASP:OD1	3:C:89:ASP:N	2.51	0.42
3:C:178:PHE:CE1	3:C:193:VAL:HG21	2.55	0.42
3:C:263:GLU:HA	3:C:266:LEU:HD12	2.01	0.42
3:C:279:THR:H	3:C:282:SER:HG	1.66	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:870:ILE:HD12	3:C:870:ILE:HA	1.91	0.42
3:C:982:SER:CB	3:C:983:THR:HG23	2.29	0.42
4:D:556:ARG:O	4:D:560:LEU:HB2	2.19	0.42
4:D:579:LEU:HD23	4:D:807:THR:HB	2.02	0.42
4:D:742:GLN:O	4:D:746:GLU:HG2	2.19	0.42
4:D:951:LEU:HD22	4:D:956:ILE:HG12	2.01	0.42
6:F:320:ILE:O	6:F:324:LEU:HB2	2.19	0.42
2:A:95:MET:N	2:A:138:LEU:O	2.32	0.41
2:B:65:THR:N	2:B:73:VAL:HG23	2.35	0.41
2:B:147:VAL:CG1	2:B:166:SER:HB2	2.50	0.41
3:C:85:SER:HA	3:C:86:PRO:HA	1.68	0.41
3:C:400:VAL:C	3:C:402:ALA:H	2.22	0.41
3:C:939:VAL:HG22	3:C:940:ALA:CA	2.50	0.41
4:D:527:LEU:CD1	4:D:712:VAL:HG12	2.49	0.41
2:B:97:LEU:HD23	2:B:136:VAL:CG1	2.50	0.41
3:C:583:ALA:HB3	3:C:621:MET:HG3	2.01	0.41
4:D:110:VAL:O	4:D:110:VAL:HG13	2.20	0.41
4:D:740:GLN:H	4:D:740:GLN:NE2	2.04	0.41
4:D:1036:PHE:O	4:D:1211:ILE:HG23	2.20	0.41
4:D:1258:LEU:HD12	4:D:1258:LEU:HA	1.90	0.41
5:E:80:VAL:CG1	5:E:81:GLU:H	2.34	0.41
9:T:256:LEU:HB3	9:T:260:SER:HB2	2.00	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:71:GLU:HG2	1:J:72:PRO:HD2	2.02	0.41
2:A:2:LEU:HD12	2:B:143:GLY:CA	2.50	0.41
2:A:214:THR:HG23	2:B:231:HIS:CG	2.55	0.41
2:B:176:TYR:H	2:B:176:TYR:HD1	1.68	0.41
3:C:723:GLU:HB3	4:D:536:PHE:HD1	1.85	0.41
3:C:1014:VAL:HA	4:D:729:THR:HG21	2.02	0.41
4:D:82:VAL:HG13	4:D:82:VAL:O	2.21	0.41
4:D:433:GLY:HA3	4:D:436:LEU:HD12	2.01	0.41
6:F:246:LYS:HE2	6:F:246:LYS:HB3	1.96	0.41
2:B:8:THR:O	2:B:23:ILE:HA	2.21	0.41
2:B:47:PRO:HA	2:B:144:ARG:CG	2.45	0.41
3:C:493:VAL:HG23	3:C:578:VAL:O	2.20	0.41
3:C:851:GLU:O	3:C:852:LEU:CG	2.64	0.41
3:C:1031:LYS:NZ	10:C:1203:SO4:S	2.93	0.41
4:D:133:ALA:HB3	4:D:234:LEU:HD21	2.01	0.41
4:D:924:LEU:HD21	4:D:959:VAL:HG11	2.01	0.41
4:D:1249:LEU:HB3	4:D:1260:PRO:HD2	2.02	0.41
2:A:106:THR:HB	2:A:123:MET:O	2.20	0.41
2:B:161:ARG:HA	2:B:161:ARG:HD3	1.53	0.41
3:C:103:PHE:CE2	3:C:124:LEU:HG	2.56	0.41
3:C:186:THR:HG23	3:C:188:LYS:H	1.84	0.41
3:C:508:ARG:HD2	3:C:570:MET:HE2	2.01	0.41
3:C:508:ARG:CD	3:C:570:MET:HE2	2.51	0.41
3:C:610:VAL:HG23	3:C:611:ARG:N	2.36	0.41
4:D:92:MET:N	14:D:2109:HOH:O	2.32	0.41
4:D:699:LEU:HD11	4:D:711:THR:HG21	2.02	0.41
4:D:1191:ASN:OD1	4:D:1202:ALA:HB3	2.20	0.41
5:E:29:PRO:CB	5:E:33:THR:HG23	2.50	0.41
1:J:84:MET:CE	6:F:272:LYS:HB2	2.51	0.41
3:C:180:GLU:HB3	3:C:191:HIS:CD2	2.56	0.41
3:C:781:VAL:CG2	3:C:838:VAL:HG21	2.50	0.41
3:C:870:ILE:HG13	3:C:886:ILE:CD1	2.50	0.41
3:C:946:TRP:CE2	3:C:978:GLY:HA3	2.56	0.41
4:D:113:ARG:HB2	4:D:312:MET:CE	2.46	0.41
4:D:740:GLN:O	4:D:744:ILE:HG13	2.19	0.41
4:D:788:LEU:C	4:D:788:LEU:HD23	2.41	0.41
4:D:884:ILE:HD11	4:D:886:ARG:HD3	2.03	0.41
9:T:297:VAL:O	9:T:301:LEU:HG	2.20	0.41
2:A:12:GLU:HB2	2:A:20:ARG:O	2.20	0.41
2:A:42:LEU:O	2:A:46:ILE:HG12	2.21	0.41
3:C:400:VAL:O	3:C:401:GLU:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:506:PRO:O	3:C:572:VAL:HG13	2.20	0.41
3:C:727:ILE:O	3:C:728:LEU:HD23	2.21	0.41
3:C:967:VAL:HG23	3:C:968:PHE:N	2.33	0.41
4:D:755:ILE:HD13	4:D:772:SER:OG	2.20	0.41
4:D:791:PHE:O	4:D:791:PHE:HD1	2.04	0.41
4:D:877:VAL:O	4:D:881:GLN:HB3	2.21	0.41
4:D:1122:VAL:HG23	4:D:1126:GLN:HE21	1.84	0.41
4:D:1168:ILE:HD13	4:D:1176:PHE:CG	2.55	0.41
4:D:1181:LEU:CD1	4:D:1213:LYS:HE2	2.51	0.41
1:J:85:LEU:O	1:J:85:LEU:HD12	2.20	0.41
2:B:158:GLU:CB	2:B:161:ARG:HB2	2.46	0.41
3:C:189:THR:O	3:C:190:LEU:HG	2.20	0.41
3:C:783:ILE:H	3:C:783:ILE:CD1	2.07	0.41
2:A:46:ILE:HA	2:A:47:PRO:HD3	1.91	0.41
2:B:30:PHE:CA	2:B:33:THR:HG23	2.47	0.41
2:B:151:GLN:CG	2:B:151:GLN:O	2.68	0.41
2:B:191:LYS:HE2	2:B:191:LYS:HB3	1.90	0.41
3:C:165:VAL:HG23	3:C:431:MET:HB2	2.02	0.41
3:C:434:ASN:HA	3:C:673:THR:OG1	2.21	0.41
3:C:494:TYR:HD2	3:C:572:VAL:CG2	2.28	0.41
3:C:538:PRO:O	3:C:546:THR:OG1	2.38	0.41
3:C:644:VAL:O	3:C:644:VAL:HG23	2.21	0.41
3:C:708:LYS:HG3	3:C:737:VAL:HG23	2.03	0.41
3:C:1011:PRO:HB2	3:C:1012:TYR:CD2	2.56	0.41
4:D:155:MET:HE1	4:D:219:LEU:HB3	2.03	0.41
4:D:229:LEU:HA	4:D:233:GLN:OE1	2.21	0.41
4:D:365:ILE:HD11	6:F:235:GLU:OE2	2.21	0.41
4:D:680:TYR:HA	4:D:681:PRO:HD3	1.94	0.41
4:D:797:PRO:O	4:D:801:ILE:HG13	2.21	0.41
4:D:815:THR:CG2	4:D:820:LYS:HA	2.35	0.41
4:D:1004:GLU:HB3	4:D:1005:PRO:HD3	2.03	0.41
4:D:1069:PRO:HB2	4:D:1071:ASP:OD1	2.21	0.41
5:E:78:PRO:O	5:E:80:VAL:O	2.39	0.41
5:E:80:VAL:CG1	5:E:81:GLU:N	2.83	0.41
6:F:306:ILE:HG22	6:F:310:MET:HB3	2.03	0.41
7:O:31:DT:H5'	7:O:31:DT:C6	2.56	0.41
9:T:279:THR:CG2	9:T:282:ASP:HB2	2.44	0.41
9:T:283:LEU:HD23	9:T:283:LEU:HA	1.87	0.41
2:B:134:LEU:HD23	2:B:135:GLU:N	2.36	0.41
3:C:31:SER:O	3:C:954:LEU:HD11	2.21	0.41
3:C:574:PRO:HB2	3:C:968:PHE:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:758:GLU:CG	3:C:798:THR:HG22	2.38	0.41
3:C:1041:SER:HB3	3:C:1044:THR:O	2.21	0.41
4:D:31:PRO:HB3	4:D:348:ILE:HG23	2.03	0.41
4:D:412:ARG:HA	4:D:416:ASN:HD22	1.86	0.41
4:D:831:ILE:O	4:D:831:ILE:HG22	2.19	0.41
6:F:324:LEU:CD2	6:F:328:LEU:HD22	2.51	0.41
6:F:359:ILE:HG22	6:F:360:SER:N	2.35	0.41
7:O:6:DA:H2 [?]	7:O:7:DC:OP2	2.20	0.41
2:B:105:VAL:HB	2:B:125:ILE:CG2	2.47	0.40
3:C:33:ALA:HB2	3:C:966:PRO:CG	2.50	0.40
3:C:270:ARG:O	3:C:274:PRO:HG3	2.21	0.40
4:D:243:GLU:HA	4:D:246:ASP:OD1	2.21	0.40
4:D:281:ILE:HD12	4:D:282:ARG:N	2.36	0.40
4:D:1181:LEU:CD2	4:D:1207:VAL:HG11	2.51	0.40
6:F:332:PRO:HA	6:F:336:GLU:OE1	2.21	0.40
1:J:58:ASN:HD21	1:J:60:LEU:CD1	2.33	0.40
2:A:95:MET:HE2	2:A:110:ILE:HG22	2.03	0.40
2:A:218:LEU:HD12	2:A:218:LEU:HA	1.84	0.40
2:B:183:VAL:O	2:B:183:VAL:CG1	2.70	0.40
3:C:44:LEU:HD11	3:C:628:ASP:HB2	2.03	0.40
3:C:169:GLN:O	3:C:369:LEU:HA	2.20	0.40
3:C:273:ARG:N	3:C:274:PRO:HD3	2.35	0.40
3:C:778:ARG:H	3:C:778:ARG:HG3	1.63	0.40
4:D:592:VAL:HG23	4:D:630:ARG:HB3	2.03	0.40
4:D:600:GLN:CB	4:D:601:ALA:CA	2.98	0.40
4:D:873:THR:O	4:D:877:VAL:HG23	2.22	0.40
4:D:1129:ARG:O	4:D:1133:ILE:HG12	2.20	0.40
4:D:1171:SER:CB	4:D:1172:GLY:CA	2.99	0.40
9:T:279:THR:O	9:T:282:ASP:N	2.50	0.40
2:A:36:ASN:HB2	3:C:1007:GLY:HA3	2.03	0.40
2:B:89:ASP:O	2:B:90:ASP:HB2	2.21	0.40
2:B:230:GLU:OE1	2:B:230:GLU:HA	2.21	0.40
3:C:196:ILE:HD12	3:C:196:ILE:HA	1.94	0.40
3:C:412:ARG:NH1	6:F:322:ARG:HH11	2.19	0.40
3:C:571:ASP:HB3	3:C:576:GLN:HE21	1.86	0.40
4:D:656:LYS:HA	4:D:659:ASP:HB2	2.03	0.40
4:D:859:LEU:HD12	4:D:862:THR:HG21	2.03	0.40
6:F:437:THR:OG1	7:O:3:DT:OP2	2.39	0.40
6:F:439:GLU:OE1	8:P:22:DC:H5	2.04	0.40
2:B:51:VAL:CG1	2:B:164:VAL:HG21	2.50	0.40
3:C:228:LEU:O	3:C:231:ALA:N	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:444:ARG:O	3:C:446:LEU:HD23	2.22	0.40
3:C:523:THR:OG1	3:C:524:ALA:N	2.54	0.40
4:D:34:ILE:O	6:F:304:ILE:HG23	2.21	0.40
4:D:153:ALA:O	4:D:157:VAL:HG23	2.21	0.40
4:D:277:LEU:O	4:D:277:LEU:HD23	2.21	0.40
4:D:644:THR:O	4:D:647:GLU:HG2	2.21	0.40
4:D:666:THR:HG23	4:D:669:ARG:HD2	2.04	0.40
4:D:1004:GLU:N	4:D:1005:PRO:HD2	2.35	0.40
4:D:1165:ARG:HD2	4:D:1209:MET:CE	2.50	0.40
2:B:198:THR:HG22	2:B:199:LYS:N	2.37	0.40
3:C:698:CYS:O	3:C:705:ALA:O	2.38	0.40
3:C:754:LYS:H	3:C:754:LYS:NZ	2.20	0.40
4:D:640:LEU:O	4:D:656:LYS:CE	2.70	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:777:GLU:OE2	4:D:209:ARG:NH1[2_356]	2.19	0.01

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%)	201 (94%)	13 (6%)	0	100	100
2	B	231/350 (66%)	216 (94%)	13 (6%)	2 (1%)	17	31
3	C	1093/1169 (94%)	1039 (95%)	50 (5%)	4 (0%)	34	53
4	D	1238/1317 (94%)	1190 (96%)	45 (4%)	3 (0%)	47	69
5	E	72/107 (67%)	65 (90%)	5 (7%)	2 (3%)	5	7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	F	313/466 (67%)	307 (98%)	6 (2%)	0	100	100
9	T	51/100 (51%)	51 (100%)	0	0	100	100
All	All	3293/3973 (83%)	3144 (96%)	138 (4%)	11 (0%)	41	60

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	E	76	VAL
3	C	982	SER
3	C	544	ARG
3	C	1134	ALA
4	D	902	GLU
4	D	1194	VAL
2	B	184	GLU
5	E	78	PRO
2	B	183	VAL
3	C	967	VAL
4	D	935	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%)	10	19
2	A	178/297 (60%)	161 (90%)	17 (10%)	8	14
2	B	171/297 (58%)	152 (89%)	19 (11%)	6	10
3	C	857/984 (87%)	780 (91%)	77 (9%)	9	16
4	D	994/1095 (91%)	904 (91%)	90 (9%)	9	16
5	E	62/86 (72%)	50 (81%)	12 (19%)	1	2
6	F	252/379 (66%)	232 (92%)	20 (8%)	12	22
9	T	36/86 (42%)	29 (81%)	7 (19%)	1	2
All	All	2621/3322 (79%)	2373 (90%)	248 (10%)	8	15

All (248) 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	A	188	ASP
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

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Mol	Chain	Res	Type
3	C	44	LEU
3	C	45	LEU
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	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	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	623	LEU
3	C	624	ARG
3	C	636	ASP

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Mol	Chain	Res	Type
3	C	640	VAL
3	C	703	GLU
3	C	727	ILE
3	C	737	VAL
3	C	753	THR
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	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
4	D	88	ARG

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Mol	Chain	Res	Type
4	D	101	VAL
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	504	LEU
4	D	507	LEU
4	D	513	GLU
4	D	518	GLU
4	D	558	LEU
4	D	566	LEU
4	D	567	SER
4	D	574	LEU
4	D	576	MET
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	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	939	ARG
4	D	945	ASP
4	D	961	VAL
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
5	E	37	ILE

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Mol	Chain	Res	Type
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	348	VAL
6	F	349	LEU
6	F	373	LEU
6	F	383	VAL
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
9	T	252	ASP
9	T	254	LEU
9	T	255	ASP
9	T	260	SER
9	T	279	THR
9	T	284	LEU
9	T	288	ASN

Sometimes 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	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	911	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 [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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	D	2007	-	4,4,4	0.14	0	6,6,6	0.06	0
11	EDO	F	506	-	3,3,3	0.47	0	2,2,2	0.26	0
10	SO4	D	2005	-	4,4,4	0.14	0	6,6,6	0.04	0
10	SO4	D	2006	-	4,4,4	0.14	0	6,6,6	0.05	0
10	SO4	F	503	-	4,4,4	0.14	0	6,6,6	0.06	0
10	SO4	F	502	-	4,4,4	0.13	0	6,6,6	0.07	0
10	SO4	F	504	-	4,4,4	0.14	0	6,6,6	0.06	0
11	EDO	C	1205	-	3,3,3	0.46	0	2,2,2	0.29	0
11	EDO	D	2009	-	3,3,3	0.45	0	2,2,2	0.30	0
10	SO4	C	1203	-	4,4,4	0.14	0	6,6,6	0.05	0
10	SO4	F	501	6	4,4,4	0.13	0	6,6,6	0.07	0
10	SO4	C	1201	-	4,4,4	0.14	0	6,6,6	0.05	0
10	SO4	D	2004	-	4,4,4	0.14	0	6,6,6	0.07	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	SO4	F	505	-	4,4,4	0.14	0	6,6,6	0.05	0
10	SO4	C	1202	-	4,4,4	0.14	0	6,6,6	0.07	0
11	EDO	D	2010	-	3,3,3	0.47	0	2,2,2	0.18	0
11	EDO	C	1204	-	3,3,3	0.45	0	2,2,2	0.34	0
11	EDO	D	2008	-	3,3,3	0.46	0	2,2,2	0.28	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
11	EDO	F	506	-	-	1/1/1/1	-
11	EDO	D	2009	-	-	0/1/1/1	-
11	EDO	C	1205	-	-	1/1/1/1	-
11	EDO	D	2010	-	-	0/1/1/1	-
11	EDO	C	1204	-	-	1/1/1/1	-
11	EDO	D	2008	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	C	1204	EDO	O1-C1-C2-O2
11	D	2008	EDO	O1-C1-C2-O2
11	C	1205	EDO	O1-C1-C2-O2
11	F	506	EDO	O1-C1-C2-O2

There are no ring outliers.

6 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	F	506	EDO	1	0
10	D	2005	SO4	2	0
10	F	502	SO4	1	0
11	C	1205	EDO	1	0
10	C	1203	SO4	2	0
11	D	2008	EDO	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	J	83/114 (72%)	0.45	10 (12%) 4 4	65, 98, 141, 159	0
2	A	218/350 (62%)	0.20	6 (2%) 53 62	60, 88, 120, 139	0
2	B	233/350 (66%)	0.90	37 (15%) 1 2	82, 112, 136, 148	0
3	C	1099/1169 (94%)	0.62	100 (9%) 9 10	43, 86, 149, 168	0
4	D	1248/1317 (94%)	0.35	40 (3%) 47 56	39, 74, 127, 157	0
5	E	76/107 (71%)	0.39	2 (2%) 56 65	52, 79, 113, 118	0
6	F	319/466 (68%)	0.12	6 (1%) 66 75	40, 74, 136, 159	0
7	O	31/31 (100%)	-0.68	0 100 100	52, 65, 85, 90	0
8	P	26/26 (100%)	-0.78	0 100 100	60, 70, 84, 94	0
9	T	53/100 (53%)	3.61	44 (83%) 0 0	115, 149, 167, 170	0
All	All	3386/4030 (84%)	0.48	245 (7%) 15 18	39, 83, 143, 170	0

All (245) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	228	LEU	8.8
9	T	275	LEU	7.7
9	T	261	TYR	7.1
9	T	256	LEU	6.9
9	T	269	VAL	6.8
3	C	215	VAL	6.4
3	C	330	VAL	6.0
9	T	297	VAL	5.9
2	B	183	VAL	5.9
3	C	354	VAL	5.8
3	C	287	LEU	5.8
3	C	239	ILE	5.6
9	T	298	LYS	5.5

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Mol	Chain	Res	Type	RSRZ
2	B	157	ALA	5.4
9	T	289	PHE	5.3
9	T	293	SER	5.3
3	C	189	THR	5.2
2	A	218	LEU	5.2
9	T	283	LEU	5.2
9	T	291	GLN	5.1
9	T	264	LEU	5.1
9	T	281	SER	5.1
3	C	459	ALA	5.0
9	T	253	ASP	4.9
9	T	254	LEU	4.9
3	C	243	PHE	4.9
9	T	299	ILE	4.9
2	B	140	VAL	4.7
3	C	349	PRO	4.7
9	T	279	THR	4.6
3	C	254	GLU	4.6
3	C	227	VAL	4.6
3	C	252	THR	4.5
9	T	273	GLY	4.5
3	C	182	ILE	4.5
9	T	268	GLY	4.3
3	C	225	VAL	4.3
9	T	259	ARG	4.2
3	C	242	ARG	4.2
3	C	203	LEU	4.2
3	C	352	VAL	4.0
3	C	226	THR	4.0
9	T	278	ARG	4.0
2	B	21	PHE	4.0
3	C	337	VAL	4.0
6	F	145	ALA	4.0
3	C	550	VAL	3.9
4	D	1009	LEU	3.9
3	C	335	TYR	3.9
2	B	66	VAL	3.8
3	C	351	GLY	3.8
3	C	235	THR	3.8
3	C	185	SER	3.8
3	C	66	ILE	3.8
3	C	244	GLY	3.7

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Mol	Chain	Res	Type	RSRZ
3	C	333	ILE	3.7
3	C	186	THR	3.7
3	C	131	ILE	3.7
3	C	181	THR	3.7
9	T	263	CYS	3.6
3	C	350	GLY	3.6
9	T	296	GLU	3.6
9	T	294	ILE	3.6
9	T	267	GLU	3.5
2	B	128	LEU	3.5
3	C	229	LEU	3.5
4	D	193	VAL	3.5
3	C	205	PHE	3.5
1	J	105	ILE	3.5
3	C	240	VAL	3.5
4	D	66	LYS	3.4
3	C	191	HIS	3.4
3	C	455	SER	3.4
3	C	943	VAL	3.4
9	T	301	LEU	3.4
2	B	110	ILE	3.4
3	C	190	LEU	3.4
9	T	255	ASP	3.4
2	B	134	LEU	3.4
9	T	272	VAL	3.4
3	C	561	PHE	3.3
3	C	234	TRP	3.3
2	B	107	ALA	3.3
4	D	655	TRP	3.3
3	C	765	PRO	3.3
4	D	1178	PRO	3.3
2	A	26	LEU	3.3
3	C	336	LEU	3.3
3	C	938	ASP	3.3
9	T	265	LYS	3.3
3	C	968	PHE	3.2
2	B	138	LEU	3.2
4	D	762	GLY	3.2
3	C	353	GLU	3.2
9	T	276	VAL	3.2
9	T	270	HIS	3.2
3	C	248	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
9	T	286	ILE	3.2
4	D	849	PHE	3.2
4	D	769	ARG	3.1
3	C	348	VAL	3.1
4	D	197	VAL	3.1
9	T	280	GLU	3.1
9	T	277	ALA	3.1
1	J	74	LYS	3.1
3	C	271	LYS	3.1
2	A	2	LEU	3.1
3	C	286	LEU	3.1
3	C	70	GLU	3.1
3	C	250	MET	3.1
2	B	164	VAL	3.1
9	T	274	GLU	3.0
3	C	355	PRO	3.0
2	B	56	ILE	3.0
3	C	1133	GLY	3.0
2	B	154	ALA	3.0
3	C	302	VAL	3.0
3	C	346	MET	2.9
4	D	761	ARG	2.9
6	F	213	VAL	2.9
9	T	251	ILE	2.9
2	B	1	MET	2.9
3	C	358	VAL	2.9
4	D	1173	SER	2.9
3	C	192	SER	2.9
1	J	68	ASP	2.8
2	B	3	ILE	2.8
3	C	98	PHE	2.8
1	J	69	VAL	2.8
2	B	59	VAL	2.8
3	C	259	SER	2.8
9	T	266	ARG	2.8
4	D	190	LYS	2.8
4	D	1191	ASN	2.8
1	J	73	LYS	2.8
9	T	295	ASP	2.8
1	J	97	LEU	2.8
9	T	257	THR	2.7
1	J	103	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
3	C	456	ARG	2.7
2	B	32	TYR	2.7
4	D	920	PHE	2.7
9	T	252	ASP	2.7
3	C	949	LYS	2.7
4	D	1067	ILE	2.7
4	D	192	ASP	2.6
3	C	71	GLU	2.6
2	B	15	ALA	2.6
4	D	901	ALA	2.6
2	B	104	VAL	2.6
3	C	260	GLY	2.6
3	C	180	GLU	2.5
3	C	196	ILE	2.5
3	C	184	LYS	2.5
3	C	687	VAL	2.5
3	C	253	LEU	2.5
1	J	31	ARG	2.5
3	C	268	ILE	2.5
6	F	460	VAL	2.5
4	D	186	ALA	2.5
9	T	300	LYS	2.5
3	C	202	TRP	2.4
3	C	237	GLU	2.4
4	D	188	GLY	2.4
6	F	215	GLN	2.4
2	B	65	THR	2.4
4	D	611	VAL	2.4
3	C	201	ALA	2.4
3	C	96	LEU	2.4
3	C	339	LEU	2.4
2	B	64	THR	2.4
2	B	130	ASP	2.4
4	D	932	ASN	2.4
3	C	488	ILE	2.4
3	C	519	ILE	2.4
3	C	522	LEU	2.3
3	C	233	GLY	2.3
3	C	245	PHE	2.3
2	B	184	GLU	2.3
9	T	302	HIS	2.3
2	B	58	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
6	F	143	ALA	2.3
2	B	108	GLY	2.3
2	A	181	THR	2.3
3	C	542	ASN	2.3
4	D	1190	GLU	2.3
4	D	640	LEU	2.3
4	D	822	LEU	2.3
2	B	127	THR	2.3
4	D	469	ILE	2.3
4	D	936	ILE	2.3
9	T	292	LYS	2.3
2	B	172	LEU	2.3
4	D	1063	PHE	2.3
3	C	249	MET	2.2
2	A	194	ILE	2.2
3	C	560	GLU	2.2
3	C	32	PHE	2.2
4	D	467	GLN	2.2
3	C	87	ILE	2.2
4	D	1112	LEU	2.2
3	C	279	THR	2.2
4	D	779	ASP	2.2
2	B	118	VAL	2.2
3	C	552	VAL	2.2
3	C	572	VAL	2.2
2	B	152	ASN	2.2
9	T	284	LEU	2.2
4	D	1179	GLY	2.2
9	T	282	ASP	2.2
3	C	812	LEU	2.2
4	D	832	PRO	2.1
2	B	69	VAL	2.1
1	J	76	LYS	2.1
4	D	191	SER	2.1
5	E	79	LEU	2.1
3	C	270	ARG	2.1
2	B	194	ILE	2.1
4	D	1172	GLY	2.1
3	C	69	GLY	2.1
4	D	195	ARG	2.1
3	C	177	TYR	2.1
3	C	487	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
3	C	727	ILE	2.1
3	C	341	GLU	2.1
2	B	208	LEU	2.1
3	C	559	VAL	2.1
2	B	70	LYS	2.1
2	B	95	MET	2.1
3	C	1043	ILE	2.1
5	E	75	TYR	2.1
1	J	67	GLY	2.1
3	C	564	ALA	2.0
4	D	913	ALA	2.0
3	C	503	ILE	2.0
4	D	607	PRO	2.0
2	B	85	VAL	2.0
3	C	62	ARG	2.0
2	B	54	ILE	2.0
4	D	332	GLY	2.0
4	D	304	GLN	2.0
6	F	151	SER	2.0
2	B	63	PHE	2.0
2	A	38	LEU	2.0
4	D	768	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [\(i\)](#)

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

6.3 Carbohydrates [\(i\)](#)

There are no monosaccharides in this entry.

6.4 Ligands [\(i\)](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
12	ZN	D	2002	1/1	0.58	0.39	222,222,222,222	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
10	SO4	C	1203	5/5	0.74	0.26	106,115,140,197	0
11	EDO	D	2008	4/4	0.81	0.20	73,90,108,108	0
10	SO4	F	505	5/5	0.84	0.43	79,86,117,167	0
10	SO4	C	1202	5/5	0.85	0.19	108,111,116,178	0
11	EDO	F	506	4/4	0.87	0.21	74,88,95,95	0
11	EDO	D	2010	4/4	0.87	0.36	63,76,77,90	0
11	EDO	D	2009	4/4	0.88	0.14	74,89,104,104	0
10	SO4	D	2006	5/5	0.89	0.20	85,104,119,125	0
10	SO4	F	504	5/5	0.89	0.23	115,115,118,128	0
11	EDO	C	1204	4/4	0.90	0.23	52,66,79,80	0
10	SO4	C	1201	5/5	0.91	0.16	113,115,126,138	0
10	SO4	D	2007	5/5	0.91	0.14	95,100,113,141	0
11	EDO	C	1205	4/4	0.92	0.20	74,94,102,113	0
10	SO4	D	2005	5/5	0.94	0.16	86,87,98,125	0
10	SO4	D	2004	5/5	0.95	0.16	70,77,85,88	0
10	SO4	F	502	5/5	0.95	0.12	88,88,104,107	0
10	SO4	F	503	5/5	0.95	0.08	86,95,99,116	0
13	MG	D	2003	1/1	0.95	0.35	79,79,79,79	0
10	SO4	F	501	5/5	0.96	0.06	100,100,118,124	0
12	ZN	D	2001	1/1	0.98	0.26	78,78,78,78	0

6.5 Other polymers [i](#)

There are no such residues in this entry.