



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:27 PM UTC

PDB ID : 5TW1 / pdb_00005tw1
Title : Crystal structure of a Mycobacterium smegmatis transcription initiation complex with RbpA
Authors : Hubin, E.A.; Darst, S.A.; Campbell, E.A.
Deposited on : 2016-11-10
Resolution : 2.76 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

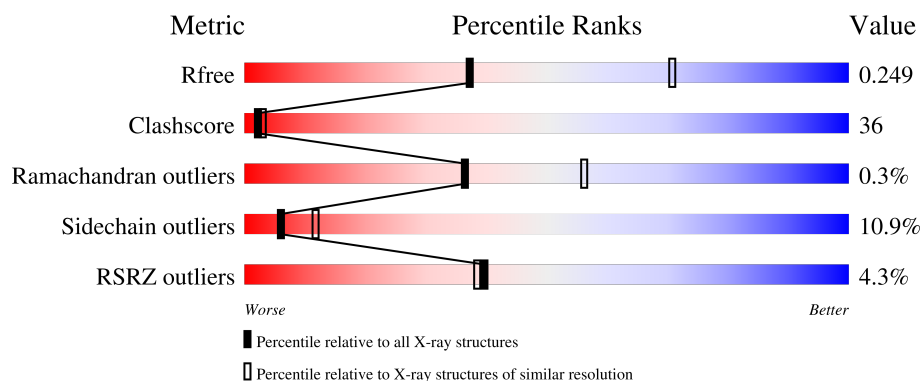
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

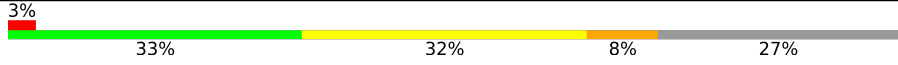
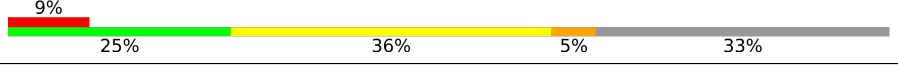
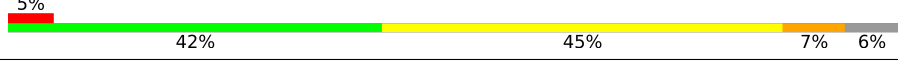
The reported resolution of this entry is 2.76 Å.

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}	180053	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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	
2	T	350	
3	C	1169	

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Mol	Chain	Length	Quality of chain
4	D	1317	
5	E	107	
6	F	466	
7	O	31	
8	P	26	
9	G	17	

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 26644 atoms, of which 36 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

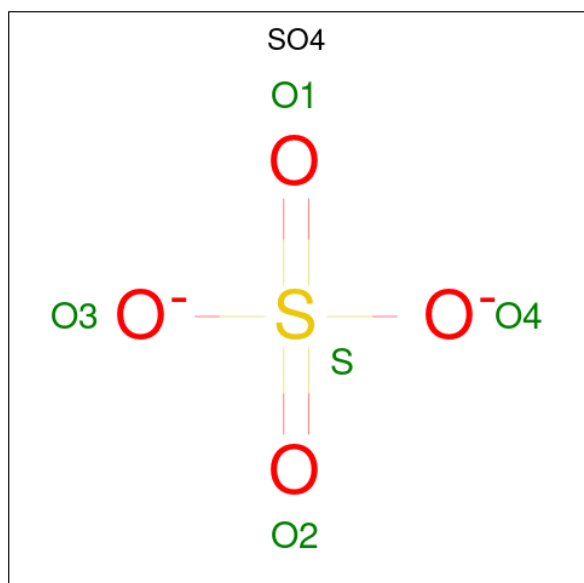
- Molecule 8 is a DNA chain called DNA (26-MER).

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

- Molecule 9 is a protein called Unknown peptide.

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

- Molecule 10 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



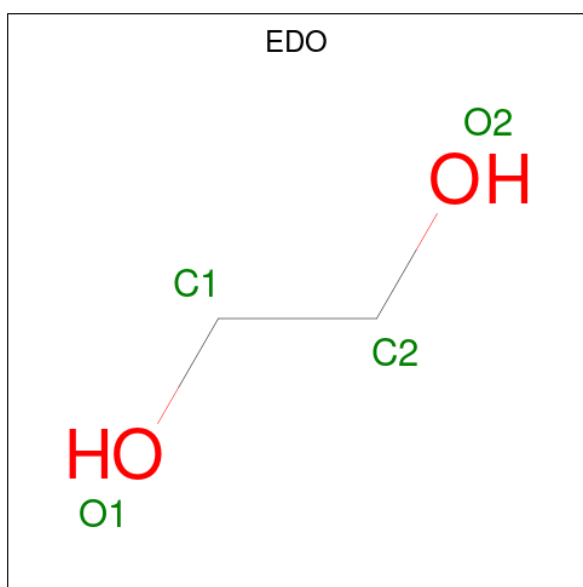
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	C	1	Total	O	S	0	0
			5	4	1		

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

- Molecule 11 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

- Molecule 12 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 13 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 14 is water.

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

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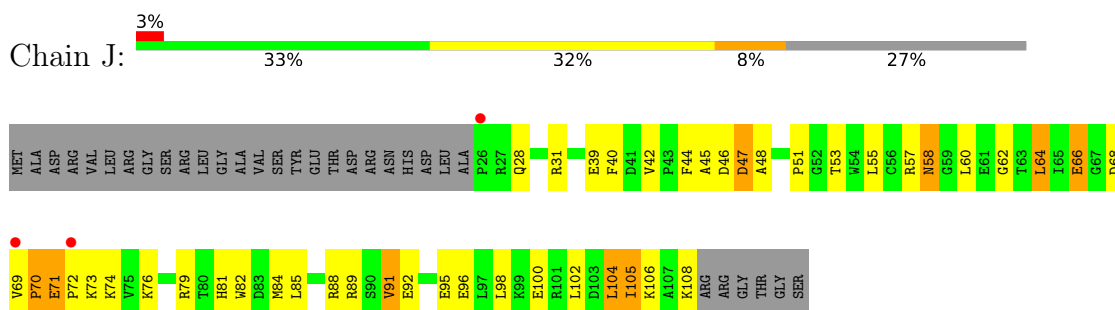
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	O	10	Total	O	0	0
			10	10		
14	P	3	Total	O	0	0
			3	3		

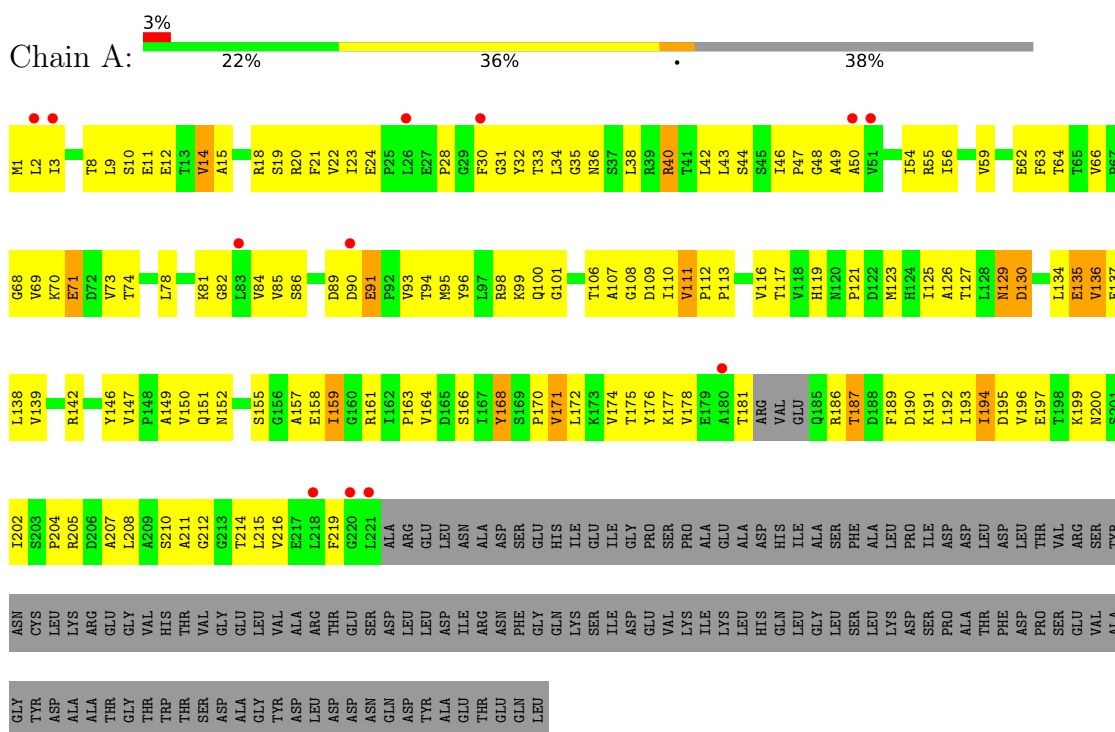
3 Residue-property plots

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

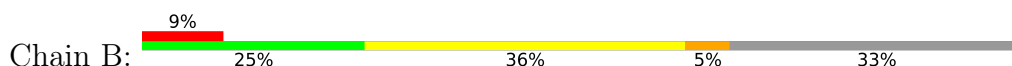
- Molecule 1: RNA polymerase-binding protein RbpA

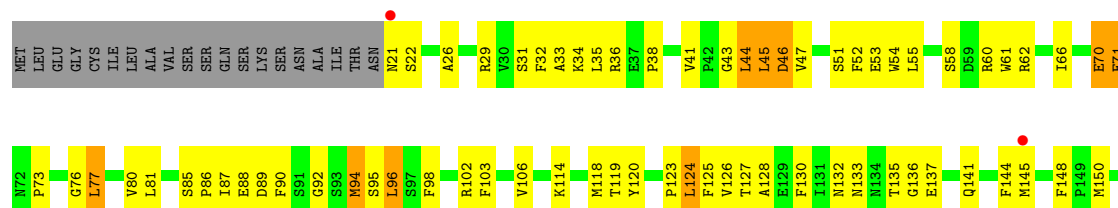


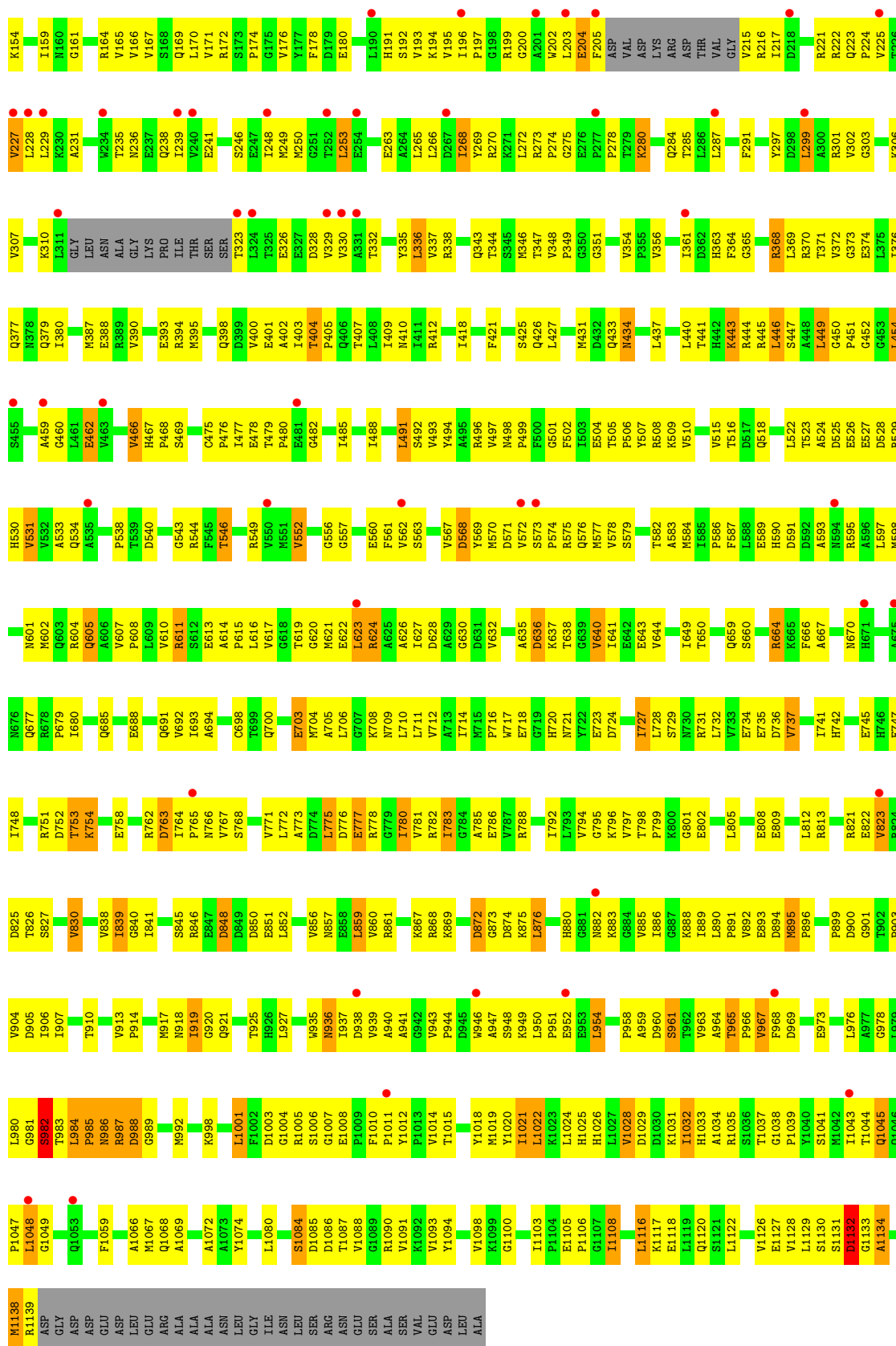
- Molecule 2: DNA-directed RNA polymerase subunit alpha



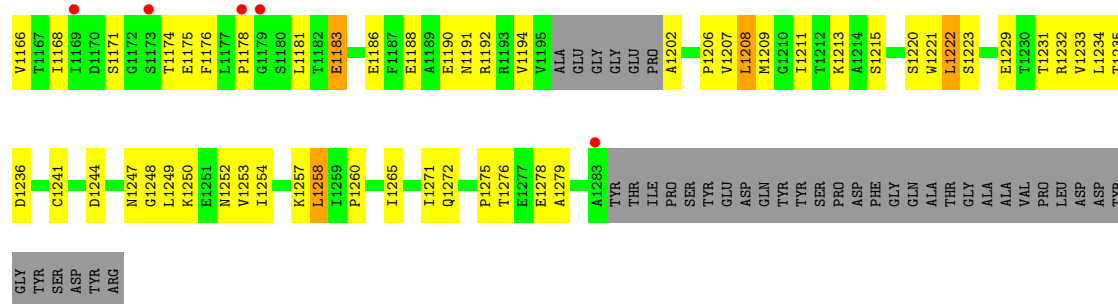
- Molecule 2: DNA-directed RNA polymerase subunit alpha



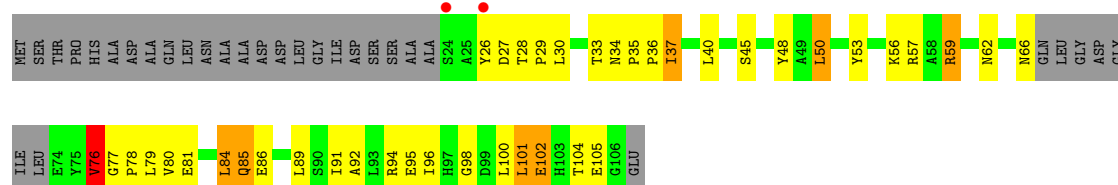




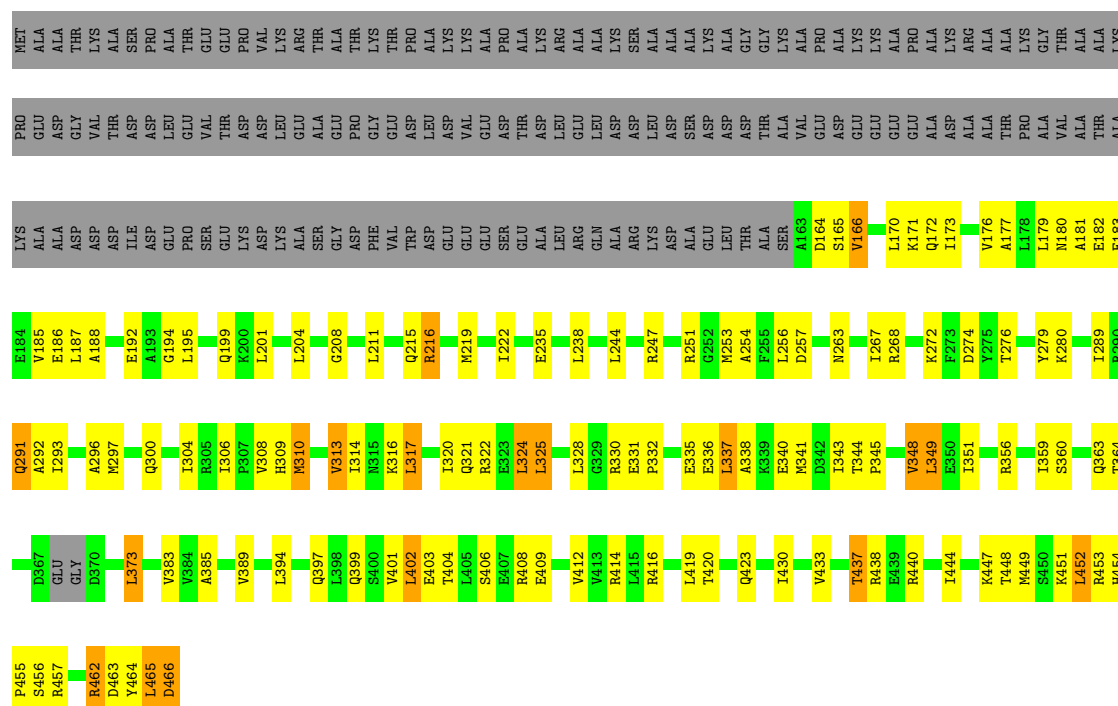




- Molecule 5: DNA-directed RNA polymerase subunit omega

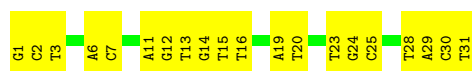


- Molecule 6: RNA polymerase sigma factor SigA

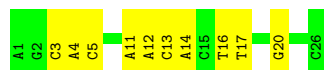


- Molecule 7: DNA (31-MER)





- Molecule 8: DNA (26-MER)



- Molecule 9: Unknown peptide



There are no outlier residues recorded for this chain.

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)	54.91 – 2.76 54.91 – 2.76	Depositor EDS
% Data completeness (in resolution range)	99.5 (54.91-2.76) 99.5 (54.91-2.76)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.16 (at 2.77Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155)	Depositor
R, R_{free}	0.239 , 0.280 (Not available) , 0.249	Depositor DCC
R_{free} test set	1989 reflections (1.37%)	wwPDB-VP
Wilson B-factor (Å ²)	78.4	Xtriage
Anisotropy	0.150	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 47.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.003 for l,k,h	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	26644	wwPDB-VP
Average B, all atoms (Å ²)	85.0	wwPDB-VP

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

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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, SO4, MG, 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	0.19	0/681	0.44	0/923
2	A	0.19	0/1641	0.43	0/2236
2	B	0.18	0/1693	0.47	0/2316
2	T	0.12	0/376	0.31	0/511
3	C	0.20	0/8394	0.46	2/11410 (0.0%)
4	D	0.22	0/9742	0.45	1/13189 (0.0%)
5	E	0.21	0/604	0.48	0/822
6	F	0.17	0/2426	0.37	0/3273
7	O	0.28	0/710	0.48	0/1095
8	P	0.29	0/589	0.49	0/906
All	All	0.21	0/26856	0.45	3/36681 (0.0%)

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

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

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	901	ALA	CB-CA-C	-9.54	104.44	115.79
3	C	949	LYS	N-CA-C	7.11	122.13	113.17
3	C	1132	ASP	N-CA-C	-6.81	99.42	108.34

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

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	55	0
2	A	1617	0	1636	182	0
2	B	1667	0	1636	194	0
2	T	374	0	344	29	0
3	C	8250	0	7989	712	0
4	D	9588	0	9552	651	0
5	E	592	0	583	53	0
6	F	2396	0	2422	146	0
7	O	634	0	350	33	0
8	P	526	0	296	16	0
9	G	85	0	19	0	0
10	C	15	0	0	2	0
10	D	20	0	0	2	0
10	F	25	0	0	1	0
11	C	8	12	12	1	0
11	D	12	18	18	3	0
11	F	4	6	6	1	0
12	D	2	0	0	0	0
13	D	1	0	0	0	0
14	A	2	0	0	0	0
14	B	2	0	0	0	0
14	C	30	0	0	16	0
14	D	57	0	0	17	0
14	E	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	F	16	0	0	3	0
14	J	2	0	0	0	0
14	O	10	0	0	3	0
14	P	3	0	0	1	0
All	All	26608	36	25512	1898	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 36.

All (1898) 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)
6:F:253:MET:HE3	6:F:297:MET:HA	1.24	1.15
2:B:184:GLU:HA	2:B:187:THR:HG22	1.28	1.15
6:F:253:MET:HE2	6:F:300:GLN:HB2	1.26	1.15
3:C:940:ALA:HB1	3:C:941:ALA:HA	1.28	1.12
4:D:527:LEU:HD21	4:D:581:MET:HE1	1.31	1.12
3:C:228:LEU:HD21	3:C:268:ILE:HG12	1.29	1.11
3:C:982:SER:HB3	3:C:983:THR:HG23	1.35	1.08
4:D:622:MET:HE2	4:D:629:VAL:HG22	1.32	1.08
3:C:176:VAL:HG12	3:C:195:VAL:HG22	1.35	1.07
3:C:540:ASP:HB2	3:C:546:THR:HG23	1.32	1.07
4:D:106:TYR:HB3	4:D:312:MET:HE3	1.39	1.05
4:D:1275:PRO:HG3	5:E:76:VAL:HG11	1.34	1.04
4:D:641:ARG:HA	4:D:656:LYS:HE3	1.40	1.04
3:C:444:ARG:HH21	3:C:491:LEU:HD23	1.20	1.03
4:D:432:VAL:HG22	4:D:434:PRO:HD3	1.40	1.02
3:C:799:PRO:HA	3:C:823:VAL:HG12	1.36	1.02
3:C:602:MET:HE1	3:C:883:LYS:HB3	1.39	1.01
3:C:215:VAL:HG23	3:C:225:VAL:HA	1.41	0.99
4:D:622:MET:HE3	4:D:667:LEU:HD13	1.45	0.98
3:C:635:ALA:HB2	3:C:693:ILE:HD11	1.43	0.97
4:D:603:THR:HG22	4:D:604:LYS:HE2	1.47	0.96
6:F:308:VAL:HG21	7:O:23:DT:H71	1.45	0.96
2:A:1:MET:N	2:B:142:ARG:O	1.97	0.96
2:A:31:GLY:HA2	2:A:192:LEU:HD23	1.48	0.96
4:D:815:THR:HG22	4:D:820:LYS:HA	1.48	0.95
3:C:41:VAL:O	3:C:624:ARG:NH2	1.98	0.95
3:C:710:LEU:HD22	3:C:1021:ILE:HD11	1.46	0.95
3:C:478:GLU:OE2	3:C:604:ARG:NH2	1.98	0.95
4:D:1174:THR:HG23	4:D:1176:PHE:H	1.31	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:150:MET:HA	3:C:150:MET:HE2	1.49	0.93
4:D:573:PRO:HG2	4:D:576:MET:HE3	1.49	0.93
3:C:584:MET:O	14:C:1301:HOH:O	1.85	0.93
4:D:327:MET:HG3	4:D:337:THR:HB	1.49	0.93
3:C:338:ARG:HD2	3:C:346:MET:HG3	1.48	0.93
6:F:219:MET:HA	6:F:219:MET:HE2	1.51	0.92
3:C:1048:LEU:HD23	3:C:1048:LEU:H	1.34	0.92
3:C:217:ILE:HD11	3:C:272:LEU:HD11	1.52	0.92
2:A:89:ASP:CB	2:A:90:ASP:HA	1.99	0.92
3:C:783:ILE:HD12	3:C:783:ILE:H	1.33	0.92
3:C:191:HIS:HA	3:C:192:SER:HB3	1.49	0.91
2:B:63:PHE:CE2	4:D:603:THR:HG23	2.04	0.91
4:D:365:ILE:H	4:D:365:ILE:HD12	1.35	0.91
6:F:211:LEU:HB2	6:F:216:ARG:HD2	1.52	0.91
3:C:454:LEU:HD22	3:C:459:ALA:HB2	1.53	0.90
4:D:951:LEU:HB3	4:D:956:ILE:HD11	1.53	0.90
3:C:77:LEU:HD11	3:C:124:LEU:HD11	1.52	0.89
3:C:1132:ASP:HB3	3:C:1133:GLY:HA2	1.54	0.89
5:E:86:GLU:OE2	5:E:94:ARG:NH1	2.06	0.89
2:B:34:LEU:HD11	2:B:192:LEU:HD22	1.54	0.89
4:D:323:GLU:OE2	14:D:2102:HOH:O	1.91	0.89
4:D:599:TYR:HB2	4:D:610:GLY:HA3	1.52	0.89
4:D:740:GLN:HE21	4:D:740:GLN:H	1.19	0.89
2:B:152:ASN:C	2:B:154:ALA:HA	1.97	0.88
3:C:92:GLY:O	3:C:133:ASN:ND2	2.07	0.88
4:D:1074:GLU:O	14:D:2101:HOH:O	1.89	0.88
3:C:895:MET:SD	14:C:1326:HOH:O	2.30	0.88
3:C:508:ARG:HD3	3:C:515:VAL:HG11	1.56	0.87
3:C:938:ASP:O	3:C:944:PRO:HD3	1.74	0.87
3:C:159:ILE:HB	3:C:164:ARG:HD2	1.57	0.87
3:C:758:GLU:HG2	3:C:798:THR:HG22	1.54	0.87
3:C:935:TRP:HA	3:C:983:THR:HG23	1.54	0.87
2:A:98:ARG:HG2	2:A:135:GLU:HG2	1.56	0.87
4:D:655:TRP:HA	4:D:655:TRP:CE3	2.08	0.87
2:B:84:VAL:HB	2:B:199:LYS:HD3	1.56	0.86
4:D:155:MET:HE1	4:D:219:LEU:HD22	1.57	0.86
6:F:324:LEU:HD23	6:F:328:LEU:HD13	1.57	0.86
3:C:584:MET:HA	3:C:619:THR:HG21	1.56	0.86
4:D:269:ASP:HB3	4:D:272:ALA:HB3	1.57	0.86
2:B:153:LYS:N	2:B:154:ALA:HA	1.88	0.86
3:C:510:VAL:N	3:C:568:ASP:O	2.09	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:31:ARG:NH2	1:J:39:GLU:OE1	2.09	0.85
2:A:152:ASN:HB2	2:A:157:ALA:HB3	1.58	0.85
4:D:442:GLY:HA3	4:D:523:GLN:HB2	1.57	0.85
2:B:95:MET:HG2	2:B:113:PRO:HD2	1.59	0.85
6:F:280:LYS:HG2	7:O:30:DC:OP2	1.75	0.85
2:B:6:ARG:O	2:B:25:PRO:HD2	1.77	0.85
4:D:1088:ARG:HG2	4:D:1089:VAL:H	1.42	0.85
3:C:718:GLU:H	4:D:724:THR:HG21	1.42	0.85
4:D:612:TYR:HB2	4:D:635:VAL:HG12	1.57	0.84
4:D:1071:ASP:HB2	4:D:1073:GLY:N	1.93	0.84
2:B:32:TYR:HB3	3:C:1005:ARG:HG3	1.58	0.84
8:P:16:DT:OP2	14:P:101:HOH:O	1.95	0.84
2:A:48:GLY:HA2	2:A:49:ALA:HB3	1.58	0.84
4:D:930:ASP:O	4:D:933:GLY:HA3	1.77	0.84
3:C:574:PRO:O	3:C:575:ARG:HG2	1.78	0.84
4:D:1174:THR:HG21	4:D:1176:PHE:HB2	1.60	0.83
3:C:170:LEU:HA	3:C:369:LEU:H	1.44	0.83
3:C:379:GLN:HG2	3:C:421:PHE:HB2	1.61	0.83
2:B:21:PHE:HB2	2:B:194:ILE:HG22	1.61	0.83
4:D:901:ALA:H	4:D:912:ASP:HB2	1.44	0.83
2:B:151:GLN:HG2	2:B:154:ALA:HB1	1.61	0.82
2:T:289:PHE:HE2	2:T:294:ILE:HG13	1.44	0.82
2:B:100:GLN:HA	2:B:133:LYS:HA	1.61	0.82
2:A:157:ALA:HB1	2:A:161:ARG:HD2	1.60	0.82
3:C:649:ILE:HD11	3:C:679:PRO:HB3	1.61	0.82
2:A:56:ILE:HB	2:A:59:VAL:HG22	1.62	0.81
4:D:1248:GLY:O	4:D:1252:ASN:ND2	2.12	0.81
6:F:253:MET:CE	6:F:300:GLN:HB2	2.09	0.81
4:D:1174:THR:HG23	4:D:1176:PHE:N	1.96	0.81
4:D:642:PRO:HD3	4:D:656:LYS:HG2	1.62	0.81
3:C:940:ALA:HB1	3:C:941:ALA:CA	2.10	0.81
4:D:114:LEU:HG	4:D:312:MET:HE2	1.63	0.81
3:C:88:GLU:HG2	3:C:92:GLY:HA2	1.62	0.81
4:D:929:VAL:HG12	4:D:935:VAL:HG22	1.61	0.80
2:B:64:THR:O	2:B:65:THR:OG1	1.97	0.80
3:C:410:ASN:OD1	14:C:1302:HOH:O	1.98	0.80
4:D:1275:PRO:HB3	5:E:79:LEU:HD11	1.63	0.80
4:D:1165:ARG:HD2	4:D:1209:MET:HE1	1.63	0.80
5:E:84:LEU:H	5:E:84:LEU:HD12	1.45	0.80
1:J:102:LEU:O	1:J:105:ILE:HG22	1.81	0.80
5:E:85:GLN:HE21	5:E:85:GLN:H	1.30	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:573:PRO:HG2	4:D:576:MET:CE	2.12	0.80
3:C:891:PRO:HB2	3:C:893:GLU:HG2	1.64	0.80
2:B:18:ARG:HG3	2:B:197:GLU:HG3	1.64	0.79
4:D:1171:SER:CA	4:D:1174:THR:HG22	2.11	0.79
3:C:540:ASP:CB	3:C:546:THR:HG23	2.12	0.79
4:D:643:PRO:O	4:D:647:GLU:HB3	1.82	0.79
7:O:12:DG:N7	14:O:102:HOH:O	2.15	0.79
4:D:26:GLY:HA3	4:D:51:ILE:HG22	1.64	0.79
5:E:30:LEU:O	5:E:33:THR:HG22	1.83	0.79
4:D:818:GLY:O	4:D:838:SER:HB3	1.83	0.78
2:A:152:ASN:CB	2:A:157:ALA:HB3	2.13	0.78
6:F:454:HIS:ND1	6:F:455:PRO:HD2	1.98	0.78
2:B:95:MET:HE3	2:B:110:ILE:HD11	1.65	0.78
3:C:981:GLY:O	3:C:982:SER:OG	2.01	0.78
4:D:587:TYR:O	4:D:590:THR:HG22	1.84	0.78
4:D:599:TYR:CE1	4:D:601:ALA:HB2	2.19	0.78
4:D:735:VAL:HG12	4:D:840:ARG:HD2	1.64	0.78
6:F:308:VAL:HG22	14:F:601:HOH:O	1.82	0.78
3:C:51:SER:OG	3:C:373:GLY:N	2.14	0.78
4:D:859:LEU:O	4:D:862:THR:HG22	1.83	0.78
3:C:148:PHE:HE1	3:C:380:ILE:HD11	1.48	0.77
4:D:641:ARG:CA	4:D:656:LYS:HE3	2.13	0.77
4:D:951:LEU:C	4:D:956:ILE:HD11	2.09	0.77
5:E:45:SER:OG	5:E:105:GLU:OE2	2.01	0.77
2:T:279:THR:HG23	2:T:282:ASP:HB2	1.67	0.77
2:A:181:THR:N	2:A:189:PHE:O	2.18	0.77
3:C:763:ASP:HB3	3:C:821:ARG:HH22	1.50	0.77
4:D:642:PRO:HG3	4:D:661:TRP:CE2	2.19	0.77
4:D:1168:ILE:HD13	4:D:1176:PHE:HB3	1.64	0.77
7:O:11:DA:H2''	7:O:12:DG:H5''	1.65	0.77
3:C:412:ARG:HD2	6:F:322:ARG:HE	1.50	0.77
4:D:772:SER:O	4:D:776:ILE:HG13	1.85	0.77
4:D:937:ILE:HD12	4:D:951:LEU:HG	1.66	0.77
3:C:132:ASN:HB3	3:C:135:THR:HG22	1.65	0.76
3:C:494:TYR:HB3	3:C:506:PRO:HG3	1.67	0.76
3:C:637:LYS:HD2	3:C:659:GLN:HE22	1.50	0.76
3:C:231:ALA:HB1	3:C:265:LEU:CD1	2.14	0.76
3:C:1127:GLU:OE1	14:C:1304:HOH:O	2.02	0.76
4:D:417:LEU:HG	4:D:1254:ILE:HG23	1.66	0.76
2:A:40:ARG:HD3	2:B:33:THR:HG22	1.67	0.76
2:A:48:GLY:CA	2:A:49:ALA:HB3	2.16	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:509:LYS:O	3:C:516:THR:HG22	1.85	0.76
3:C:1003:ASP:OD1	3:C:1006:SER:N	2.17	0.76
2:B:170:PRO:HB2	2:B:202:ILE:HD11	1.67	0.76
2:B:184:GLU:CA	2:B:187:THR:HG22	2.13	0.76
2:A:86:SER:OG	2:A:119:HIS:NE2	2.15	0.76
3:C:368:ARG:NH1	14:C:1309:HOH:O	2.19	0.76
4:D:47:PHE:O	4:D:88:ARG:NH2	2.18	0.76
4:D:277:LEU:HD11	4:D:295:ARG:HG2	1.65	0.76
6:F:404:THR:O	6:F:457:ARG:NH2	2.19	0.76
4:D:143:MET:HE1	4:D:250:GLU:O	1.86	0.76
4:D:901:ALA:HB2	4:D:911:ARG:HA	1.68	0.76
3:C:984:LEU:HB2	3:C:985:PRO:HA	1.66	0.75
3:C:935:TRP:HA	3:C:983:THR:CG2	2.15	0.75
3:C:1059:PHE:HZ	3:C:1067:MET:HE3	1.52	0.75
2:A:28:PRO:HA	2:A:190:ASP:OD2	1.86	0.75
6:F:253:MET:HE2	6:F:300:GLN:CB	2.14	0.75
3:C:348:VAL:HB	3:C:351:GLY:HA3	1.69	0.75
3:C:711:LEU:HD23	3:C:904:VAL:HA	1.68	0.75
3:C:205:PHE:CE1	3:C:215:VAL:HG13	2.21	0.75
4:D:721:TYR:O	4:D:725:ARG:HG2	1.85	0.75
6:F:201:LEU:HD11	6:F:219:MET:HB3	1.68	0.75
2:B:22:VAL:HG12	2:B:193:ILE:HD12	1.69	0.75
3:C:940:ALA:CB	3:C:941:ALA:HA	2.12	0.75
4:D:951:LEU:HB3	4:D:956:ILE:CD1	2.15	0.75
4:D:655:TRP:HA	4:D:655:TRP:HE3	1.50	0.75
4:D:822:LEU:HD23	4:D:834:PRO:HA	1.67	0.75
2:B:32:TYR:HE1	2:B:178:VAL:HG21	1.51	0.75
3:C:720:HIS:CE1	3:C:888:LYS:HD3	2.22	0.75
2:A:66:VAL:O	2:A:69:VAL:HG22	1.86	0.74
1:J:68:ASP:HA	1:J:69:VAL:HB	1.68	0.74
4:D:237:ASP:HB3	4:D:240:LEU:HB3	1.69	0.74
3:C:1138:MET:O	3:C:1139:ARG:HG3	1.86	0.74
4:D:644:THR:HA	4:D:647:GLU:OE1	1.88	0.74
4:D:1009:LEU:HD12	4:D:1146:GLN:HG3	1.68	0.74
2:T:264:LEU:HB3	2:T:269:VAL:CG2	2.18	0.74
3:C:215:VAL:HG12	3:C:217:ILE:CG2	2.17	0.74
4:D:487:LEU:HG	4:D:491:ILE:HD12	1.70	0.74
3:C:249:MET:O	3:C:253:LEU:HD23	1.87	0.74
7:O:19:DA:H2''	7:O:20:DT:O5'	1.87	0.74
6:F:251:ARG:HB2	6:F:297:MET:HE1	1.70	0.74
4:D:111:PRO:O	4:D:113:ARG:NH1	2.20	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:773:ALA:O	3:C:782:ARG:NH2	2.21	0.74
7:O:14:DG:H2"	7:O:15:DT:OP2	1.86	0.74
3:C:982:SER:HB3	3:C:983:THR:CG2	2.16	0.73
3:C:1108:ILE:H	3:C:1108:ILE:HD12	1.52	0.73
4:D:647:GLU:HB2	4:D:655:TRP:CZ3	2.23	0.73
4:D:1069:PRO:HG2	4:D:1073:GLY:H	1.53	0.73
2:A:14:VAL:HG13	2:A:18:ARG:HG3	1.68	0.73
3:C:426:GLN:HE21	3:C:451:PRO:HD3	1.53	0.73
3:C:578:VAL:HG13	3:C:582:THR:HB	1.69	0.73
3:C:636:ASP:OD1	3:C:636:ASP:N	2.19	0.73
3:C:845:SER:N	3:C:850:ASP:OD2	2.19	0.73
2:A:14:VAL:HG12	2:A:19:SER:HA	1.69	0.73
4:D:26:GLY:HA3	4:D:51:ILE:CG2	2.18	0.73
4:D:278:ARG:O	4:D:281:ILE:HG13	1.88	0.73
3:C:720:HIS:O	4:D:432:VAL:HG11	1.89	0.73
3:C:742:HIS:CD2	3:C:868:ARG:HG3	2.23	0.73
7:O:15:DT:OP1	2:T:258:VAL:HG21	1.87	0.73
3:C:205:PHE:HE1	3:C:215:VAL:HG13	1.54	0.73
3:C:1018:TYR:O	14:C:1305:HOH:O	2.04	0.73
8:P:11:DA:H2"	8:P:12:DA:O5'	1.88	0.73
2:B:24:GLU:OE2	2:B:191:LYS:HD3	1.88	0.73
6:F:320:ILE:HG23	6:F:340:GLU:HG2	1.69	0.73
3:C:87:ILE:HD12	3:C:388:GLU:HG3	1.69	0.73
3:C:496:ARG:NH2	3:C:504:GLU:OE1	2.21	0.73
3:C:593:ALA:HB2	4:D:852:THR:HG22	1.71	0.73
4:D:962:ARG:NH1	4:D:977:CYS:SG	2.62	0.72
3:C:508:ARG:HD2	3:C:570:MET:HE2	1.71	0.72
3:C:204:GLU:OE1	3:C:216:ARG:NH1	2.21	0.72
3:C:191:HIS:HA	3:C:192:SER:CB	2.18	0.72
3:C:361:ILE:H	3:C:361:ILE:HD12	1.54	0.72
4:D:819:MET:HE2	4:D:821:GLY:HA2	1.70	0.72
3:C:754:LYS:HE2	3:C:754:LYS:H	1.55	0.72
4:D:88:ARG:NH1	14:D:2102:HOH:O	2.21	0.72
4:D:138:SER:HB3	4:D:253:THR:OG1	1.89	0.72
4:D:581:MET:HE3	4:D:716:LYS:HA	1.71	0.72
3:C:936:ASN:HD22	3:C:937:ILE:H	1.37	0.72
2:B:2:LEU:CB	2:B:231:HIS:HA	2.20	0.72
3:C:239:ILE:HG21	3:C:253:LEU:HD22	1.70	0.72
4:D:12:ILE:HD11	4:D:1221:TRP:CD2	2.25	0.72
4:D:668:GLY:HA2	4:D:671:MET:HE3	1.70	0.72
3:C:47:VAL:HG23	3:C:497:VAL:HG21	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:728:LEU:CD2	3:C:906:ILE:HG22	2.20	0.72
4:D:444:PRO:HG3	4:D:521:ALA:O	1.89	0.72
4:D:796:ASN:HD21	4:D:798:ILE:HB	1.54	0.72
6:F:397:GLN:O	6:F:401:VAL:HG23	1.89	0.72
8:P:11:DA:H2''	8:P:12:DA:C5'	2.20	0.71
3:C:637:LYS:HD2	3:C:659:GLN:NE2	2.03	0.71
4:D:590:THR:HG21	4:D:630:ARG:HH21	1.55	0.71
3:C:390:VAL:O	3:C:394:ARG:HB2	1.91	0.71
2:A:106:THR:HA	2:A:125:ILE:HD13	1.72	0.71
3:C:482:GLY:O	3:C:485:ILE:HG13	1.90	0.71
3:C:983:THR:OG1	14:C:1306:HOH:O	2.08	0.71
3:C:939:VAL:CG2	3:C:940:ALA:HA	2.21	0.71
3:C:982:SER:OG	14:C:1307:HOH:O	2.08	0.71
2:B:26:LEU:HD11	2:B:34:LEU:HD21	1.73	0.71
4:D:622:MET:O	14:D:2104:HOH:O	2.07	0.71
2:B:158:GLU:HB3	2:B:161:ARG:HB2	1.72	0.71
3:C:265:LEU:HD11	3:C:287:LEU:HD12	1.72	0.71
4:D:444:PRO:HD2	4:D:447:MET:HE2	1.71	0.71
4:D:488:GLU:HG3	4:D:516:LEU:HD12	1.72	0.71
7:O:28:DT:H2''	7:O:29:DA:H5'	1.72	0.71
3:C:246:SER:CB	3:C:337:VAL:HG11	2.21	0.71
3:C:1130:SER:HB3	3:C:1132:ASP:O	1.90	0.71
4:D:527:LEU:HD22	4:D:575:ALA:O	1.91	0.70
4:D:155:MET:CE	4:D:219:LEU:HB3	2.21	0.70
4:D:596:THR:HG22	4:D:626:ALA:O	1.91	0.70
3:C:239:ILE:CG2	3:C:253:LEU:HD22	2.21	0.70
3:C:328:ASP:O	3:C:332:THR:HG23	1.91	0.70
3:C:531:VAL:HG13	3:C:552:VAL:CG2	2.21	0.70
2:A:24:GLU:CD	2:A:191:LYS:HD3	2.16	0.70
3:C:650:THR:HG22	3:C:660:SER:OG	1.90	0.70
4:D:588:LEU:HD22	4:D:668:GLY:HA3	1.72	0.70
2:B:32:TYR:CB	3:C:1005:ARG:HG3	2.22	0.70
3:C:299:LEU:HB3	3:C:323:THR:HA	1.74	0.70
3:C:613:GLU:HB3	3:C:708:LYS:HD3	1.71	0.70
3:C:667:ALA:N	14:C:1303:HOH:O	2.01	0.70
3:C:1045:GLN:HG3	3:C:1090:ARG:HH21	1.55	0.70
2:A:38:LEU:HD13	2:A:208:LEU:HD11	1.74	0.70
2:B:79:ASN:O	2:B:123:MET:HE3	1.92	0.70
3:C:728:LEU:HB2	3:C:889:ILE:HG12	1.72	0.70
3:C:250:MET:HA	3:C:253:LEU:HD21	1.74	0.70
3:C:754:LYS:H	3:C:754:LYS:CE	2.05	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:32:TYR:CG	3:C:1005:ARG:HG3	2.26	0.70
6:F:253:MET:HE3	6:F:297:MET:CA	2.14	0.70
2:B:63:PHE:HE2	4:D:603:THR:HG23	1.52	0.70
2:B:181:THR:O	2:B:189:PHE:N	2.23	0.70
3:C:776:ASP:HB2	3:C:777:GLU:OE1	1.92	0.70
3:C:780:ILE:HD11	3:C:841:ILE:HD13	1.73	0.69
3:C:1068:GLN:NE2	4:D:1249:LEU:HD13	2.07	0.69
6:F:164:ASP:OD1	6:F:166:VAL:HG22	1.92	0.69
4:D:108:LYS:NZ	14:D:2109:HOH:O	2.21	0.69
5:E:35:PRO:HG2	5:E:40:LEU:HD11	1.74	0.69
2:B:30:PHE:HA	2:B:33:THR:HG23	1.73	0.69
3:C:981:GLY:O	14:C:1307:HOH:O	2.09	0.69
7:O:6:DA:H2''	7:O:7:DC:H5'	1.73	0.69
2:A:11:GLU:OE1	2:A:205:ARG:NE	2.24	0.69
3:C:727:ILE:HG22	3:C:888:LYS:HB3	1.72	0.69
3:C:910:THR:HG23	4:D:730:VAL:HG23	1.75	0.69
4:D:12:ILE:HD11	4:D:1221:TRP:CE3	2.28	0.69
2:A:82:GLY:HA3	2:A:123:MET:HE1	1.74	0.69
4:D:139:VAL:HG12	4:D:231:PRO:HD3	1.74	0.69
6:F:291:GLN:HG3	6:F:292:ALA:N	2.06	0.69
1:J:91:VAL:HG22	1:J:92:GLU:OE1	1.93	0.69
2:A:158:GLU:H	2:A:161:ARG:HH11	1.41	0.69
2:B:182:ARG:N	2:B:186:ARG:O	2.25	0.69
3:C:1100:GLY:HA3	4:D:458:LYS:HE3	1.75	0.69
1:J:84:MET:HE3	6:F:272:LYS:HE2	1.75	0.69
3:C:45:LEU:HD12	3:C:628:ASP:O	1.92	0.69
3:C:494:TYR:HD2	3:C:572:VAL:HG21	1.57	0.69
4:D:344:TYR:O	4:D:348:ILE:HG22	1.92	0.69
3:C:1026:HIS:HB3	3:C:1031:LYS:HE3	1.75	0.69
4:D:599:TYR:CB	4:D:610:GLY:HA3	2.23	0.69
4:D:795:ASP:O	14:D:2105:HOH:O	2.10	0.69
4:D:1166:VAL:HA	4:D:1207:VAL:HG23	1.75	0.69
3:C:444:ARG:NH2	3:C:492:SER:O	2.26	0.69
3:C:508:ARG:HD3	3:C:515:VAL:CG1	2.23	0.69
4:D:668:GLY:HA2	4:D:671:MET:CE	2.23	0.69
5:E:26:TYR:HE1	5:E:29:PRO:HD3	1.58	0.69
1:J:79:ARG:NH2	7:O:25:DC:OP1	2.27	0.68
4:D:708:VAL:O	4:D:712:VAL:HG23	1.93	0.68
4:D:1115:GLY:N	14:D:2110:HOH:O	2.22	0.68
4:D:1174:THR:HA	4:D:1175:GLU:CB	2.22	0.68
2:B:74:THR:HG21	4:D:611:VAL:HG11	1.73	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:718:GLU:H	4:D:724:THR:CG2	2.05	0.68
3:C:1045:GLN:HG2	3:C:1087:THR:HG22	1.75	0.68
4:D:780:ALA:O	4:D:784:VAL:HG22	1.93	0.68
8:P:13:DC:H2"	8:P:14:DA:C8	2.29	0.68
2:A:33:THR:HG21	2:B:37:SER:HA	1.76	0.68
2:A:95:MET:HE2	2:A:110:ILE:CG2	2.24	0.68
3:C:507:TYR:OH	3:C:527:GLU:OE2	2.11	0.68
3:C:1103:ILE:HD12	4:D:548:SER:HA	1.76	0.68
4:D:155:MET:HE1	4:D:219:LEU:CD2	2.24	0.68
4:D:238:GLU:HA	4:D:241:TYR:HB3	1.74	0.68
7:O:24:DG:OP2	14:O:101:HOH:O	2.11	0.68
4:D:578:ARG:HB2	11:D:2008:EDO:C2	2.24	0.68
6:F:330:ARG:NH2	6:F:336:GLU:OE2	2.25	0.68
2:T:256:LEU:HD22	2:T:297:VAL:HG22	1.76	0.68
1:J:89:ARG:NH2	6:F:276:THR:HG23	2.09	0.68
3:C:426:GLN:NE2	3:C:450:GLY:HA2	2.08	0.68
3:C:444:ARG:NH2	3:C:491:LEU:HD23	2.04	0.68
3:C:973:GLU:O	4:D:732:MET:HE1	1.94	0.68
4:D:603:THR:CG2	4:D:604:LYS:HE2	2.23	0.68
4:D:931:ALA:HB1	4:D:932:ASN:HD22	1.59	0.68
3:C:729:SER:OG	3:C:905:ASP:HA	1.94	0.67
4:D:1165:ARG:CD	4:D:1209:MET:HE1	2.25	0.67
4:D:73:ILE:O	4:D:82:VAL:HG12	1.94	0.67
3:C:191:HIS:HB2	3:C:336:LEU:HD21	1.76	0.67
2:B:47:PRO:HA	2:B:144:ARG:HG3	1.76	0.67
3:C:467:HIS:CG	3:C:468:PRO:HD2	2.29	0.67
2:B:216:VAL:HG13	2:B:217:GLU:H	1.59	0.67
4:D:143:MET:HE3	4:D:251:TYR:CD1	2.29	0.67
6:F:399:GLN:O	6:F:403:GLU:HG2	1.94	0.67
2:B:143:GLY:HA3	2:B:168:TYR:CD1	2.30	0.67
6:F:254:ALA:HA	10:F:502:SO4:O3	1.94	0.67
4:D:648:ALA:O	4:D:652:GLU:HB2	1.94	0.67
4:D:1087:LEU:HD23	4:D:1113:MET:HE2	1.77	0.67
4:D:1168:ILE:O	4:D:1178:PRO:HA	1.95	0.67
4:D:1232:ARG:NH1	4:D:1236:ASP:OD2	2.27	0.67
6:F:308:VAL:N	14:F:601:HOH:O	2.27	0.67
3:C:872:ASP:OD1	3:C:872:ASP:N	2.17	0.67
4:D:137:THR:HG22	4:D:253:THR:O	1.93	0.67
5:E:57:ARG:NE	5:E:95:GLU:OE1	2.23	0.67
2:A:40:ARG:NH1	2:B:33:THR:HG22	2.10	0.67
2:A:89:ASP:CB	2:A:90:ASP:CA	2.73	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:102:ARG:NH2	3:C:127:THR:OG1	2.27	0.67
4:D:108:LYS:O	4:D:108:LYS:HG3	1.94	0.67
1:J:42:VAL:HG13	4:D:74:ILE:HD12	1.75	0.66
3:C:44:LEU:HD13	3:C:440:LEU:HD21	1.75	0.66
2:B:3:ILE:HA	2:B:232:ILE:CB	2.25	0.66
4:D:627:LEU:HD13	4:D:667:LEU:HD12	1.77	0.66
2:A:94:THR:HG22	2:A:139:VAL:HG22	1.76	0.66
3:C:772:LEU:HA	3:C:775:LEU:HD22	1.78	0.66
4:D:889:ASP:OD2	4:D:891:GLU:N	2.28	0.66
2:A:177:LYS:HE2	2:A:193:ILE:CD1	2.25	0.66
3:C:44:LEU:CD1	3:C:440:LEU:HD21	2.25	0.66
3:C:454:LEU:HD22	3:C:459:ALA:CB	2.24	0.66
3:C:799:PRO:CA	3:C:823:VAL:HG12	2.21	0.66
3:C:1059:PHE:CZ	3:C:1067:MET:HE3	2.30	0.66
4:D:230:ALA:N	4:D:233:GLN:OE1	2.25	0.66
6:F:338:ALA:HB1	6:F:343:ILE:O	1.95	0.66
3:C:148:PHE:CE1	3:C:380:ILE:HD11	2.31	0.66
3:C:176:VAL:HG12	3:C:195:VAL:CG2	2.21	0.66
3:C:613:GLU:O	3:C:705:ALA:HB1	1.96	0.66
4:D:980:ARG:HD3	4:D:985:GLY:O	1.96	0.66
2:A:42:LEU:O	2:A:171:VAL:HG11	1.96	0.66
2:A:66:VAL:HB	2:A:69:VAL:HG21	1.76	0.66
4:D:237:ASP:OD1	4:D:239:VAL:HG13	1.96	0.66
4:D:576:MET:HE2	4:D:693:ALA:HA	1.78	0.66
4:D:642:PRO:CD	4:D:656:LYS:HG2	2.26	0.66
2:A:95:MET:HE2	2:A:110:ILE:HG22	1.77	0.66
3:C:77:LEU:CD1	3:C:124:LEU:HD11	2.25	0.66
2:A:177:LYS:HE2	2:A:193:ILE:HD11	1.77	0.66
3:C:203:LEU:HD13	3:C:217:ILE:HG22	1.78	0.66
3:C:250:MET:HA	3:C:253:LEU:CD2	2.26	0.66
3:C:533:ALA:HB2	3:C:567:VAL:HG11	1.78	0.66
3:C:732:LEU:HA	3:C:737:VAL:CG1	2.26	0.66
3:C:851:GLU:O	3:C:852:LEU:HG	1.96	0.66
4:D:878:ASP:OD2	4:D:1250:LYS:NZ	2.29	0.66
4:D:320:ILE:HG12	4:D:321:PRO:HD2	1.78	0.66
4:D:647:GLU:HG2	4:D:648:ALA:N	2.11	0.66
4:D:881:GLN:HE22	4:D:1250:LYS:HE2	1.61	0.66
3:C:685:GLN:OE1	14:C:1308:HOH:O	2.15	0.65
3:C:1045:GLN:HG3	3:C:1090:ARG:NH2	2.10	0.65
3:C:1086:ASP:O	3:C:1090:ARG:HG2	1.96	0.65
4:D:137:THR:HG22	4:D:253:THR:C	2.21	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:665:THR:HG22	4:D:684:ASN:ND2	2.12	0.65
4:D:1089:VAL:HG13	4:D:1098:GLY:C	2.21	0.65
5:E:40:LEU:HB3	5:E:50:LEU:HD11	1.79	0.65
3:C:721:ASN:HD22	3:C:727:ILE:HD11	1.62	0.65
4:D:193:VAL:O	4:D:197:VAL:HG23	1.96	0.65
4:D:1174:THR:CG2	4:D:1176:PHE:HB2	2.26	0.65
4:D:59:GLU:OE2	4:D:66:LYS:NZ	2.29	0.65
4:D:826:PRO:HD3	4:D:853:HIS:ND1	2.12	0.65
4:D:262:LYS:HG3	4:D:310:MET:HE1	1.77	0.65
4:D:599:TYR:CZ	4:D:601:ALA:HB2	2.31	0.65
4:D:1100:LEU:HD23	4:D:1101:SER:N	2.11	0.65
2:B:105:VAL:HB	2:B:125:ILE:HG23	1.79	0.65
3:C:685:GLN:HB3	14:C:1308:HOH:O	1.96	0.65
3:C:712:VAL:HB	3:C:906:ILE:HD11	1.78	0.65
2:A:33:THR:CG2	2:B:37:SER:HA	2.27	0.65
2:B:79:ASN:OD1	4:D:636:ARG:NH2	2.26	0.65
3:C:236:ASN:OD1	3:C:253:LEU:HD13	1.96	0.65
3:C:796:LYS:HB3	3:C:826:THR:O	1.96	0.65
4:D:218:ARG:O	4:D:222:ILE:HG13	1.95	0.65
5:E:29:PRO:HG2	5:E:34:ASN:HB2	1.78	0.65
3:C:575:ARG:HE	3:C:967:VAL:HG22	1.61	0.65
3:C:710:LEU:HD13	3:C:1021:ILE:HG12	1.78	0.65
4:D:438:LEU:HA	4:D:525:HIS:CD2	2.31	0.65
2:A:99:LYS:HE3	2:A:109:ASP:CG	2.22	0.65
3:C:1028:VAL:O	3:C:1032:ILE:HG22	1.97	0.65
2:B:32:TYR:CE1	2:B:178:VAL:HG21	2.31	0.65
3:C:531:VAL:HG13	3:C:552:VAL:HG23	1.79	0.65
3:C:771:VAL:HG23	3:C:772:LEU:CD1	2.27	0.65
1:J:64:LEU:HD22	1:J:66:GLU:H	1.61	0.64
2:A:157:ALA:CB	2:A:161:ARG:HD2	2.27	0.64
2:B:83:LEU:N	2:B:123:MET:HE1	2.11	0.64
3:C:1098:VAL:HG11	4:D:469:ILE:HD12	1.78	0.64
4:D:106:TYR:HB3	4:D:312:MET:CE	2.20	0.64
6:F:181:ALA:O	6:F:185:VAL:HG23	1.97	0.64
3:C:338:ARG:HD3	3:C:343:GLN:NE2	2.11	0.64
4:D:6:PHE:CD1	4:D:1257:LYS:HE3	2.33	0.64
4:D:642:PRO:HG3	4:D:661:TRP:CD2	2.31	0.64
4:D:706:ILE:HD12	5:E:36:PRO:HB3	1.78	0.64
4:D:177:LEU:HD23	4:D:177:LEU:O	1.98	0.64
4:D:726:SER:OG	4:D:728:VAL:HG23	1.96	0.64
2:A:14:VAL:CG1	2:A:18:ARG:HG3	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:846:ARG:N	3:C:857:ASN:O	2.28	0.64
3:C:135:THR:HG23	3:C:137:GLU:H	1.63	0.64
6:F:462:ARG:NH1	6:F:465:LEU:HD12	2.13	0.64
2:B:85:VAL:HG23	2:B:117:THR:C	2.23	0.64
4:D:661:TRP:HZ3	4:D:663:ALA:HB2	1.63	0.64
4:D:400:LYS:HE3	4:D:404:ASP:HB3	1.80	0.64
4:D:846:LEU:O	4:D:850:ILE:HG12	1.98	0.64
6:F:289:ILE:O	6:F:293:ILE:HG13	1.98	0.64
4:D:924:LEU:HD21	4:D:943:LEU:HD11	1.79	0.64
2:B:144:ARG:NH1	2:B:144:ARG:HB2	2.13	0.64
4:D:144:ARG:NH2	4:D:229:LEU:O	2.32	0.63
4:D:190:LYS:HE3	4:D:193:VAL:HG23	1.80	0.63
4:D:638:THR:HA	4:D:659:ASP:O	1.98	0.63
4:D:1119:PRO:HA	4:D:1122:VAL:CG1	2.27	0.63
2:A:8:THR:OG1	2:A:24:GLU:O	2.13	0.63
4:D:139:VAL:CG1	4:D:231:PRO:HD3	2.28	0.63
4:D:1168:ILE:HD13	4:D:1176:PHE:CB	2.28	0.63
2:A:177:LYS:HG2	2:A:193:ILE:HD11	1.81	0.63
3:C:235:THR:N	3:C:238:GLN:OE1	2.31	0.63
6:F:451:LYS:O	6:F:454:HIS:HB3	1.99	0.63
2:A:48:GLY:HA2	2:A:49:ALA:CB	2.28	0.63
3:C:876:LEU:HD11	3:C:886:ILE:CD1	2.29	0.63
3:C:937:ILE:CB	3:C:939:VAL:HG12	2.27	0.63
4:D:31:PRO:HB2	4:D:345:ARG:HG2	1.80	0.63
4:D:755:ILE:HD12	4:D:776:ILE:HD11	1.79	0.63
2:A:36:ASN:HB2	2:A:176:TYR:OH	1.99	0.63
2:B:95:MET:HG2	2:B:113:PRO:CD	2.28	0.63
3:C:52:PHE:HZ	3:C:150:MET:HE2	1.63	0.63
3:C:508:ARG:CD	3:C:570:MET:HE2	2.28	0.63
2:B:43:LEU:HD12	2:B:171:VAL:HG23	1.81	0.63
3:C:250:MET:O	3:C:253:LEU:HG	1.99	0.63
4:D:21:ARG:NE	4:D:96:GLU:OE2	2.27	0.63
3:C:176:VAL:HG22	3:C:307:VAL:HG12	1.81	0.63
3:C:1072:ALA:HB1	4:D:554:GLU:OE2	1.99	0.63
4:D:1275:PRO:HG3	5:E:76:VAL:CG1	2.20	0.63
6:F:204:LEU:O	6:F:208:GLY:N	2.32	0.63
3:C:792:ILE:HD12	3:C:792:ILE:H	1.64	0.63
3:C:510:VAL:HG12	3:C:568:ASP:C	2.24	0.62
3:C:727:ILE:HG13	3:C:907:ILE:HB	1.80	0.62
3:C:1048:LEU:HD23	3:C:1048:LEU:N	2.12	0.62
4:D:956:ILE:HD12	4:D:956:ILE:O	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:1188:GLU:O	4:D:1192:ARG:HG3	1.99	0.62
6:F:444:ILE:O	6:F:448:THR:HG23	1.99	0.62
2:B:30:PHE:HA	2:B:33:THR:CG2	2.29	0.62
2:B:85:VAL:HG23	2:B:117:THR:O	1.98	0.62
4:D:102:THR:HG23	4:D:258:ALA:HB2	1.81	0.62
4:D:238:GLU:OE2	4:D:242:ARG:NH2	2.31	0.62
4:D:275:GLU:HA	4:D:278:ARG:HB2	1.81	0.62
2:B:50:ALA:HB3	2:B:168:TYR:HD2	1.63	0.62
2:B:198:THR:HG21	2:B:202:ILE:HD12	1.81	0.62
3:C:302:VAL:HG11	3:C:368:ARG:HD3	1.81	0.62
4:D:578:ARG:HB2	11:D:2008:EDO:H21	1.81	0.62
4:D:1114:GLU:HG3	14:D:2110:HOH:O	2.00	0.62
3:C:876:LEU:HD13	3:C:886:ILE:HG13	1.81	0.62
4:D:614:SER:HB2	4:D:615:PRO:HD2	1.80	0.62
7:O:19:DA:H4'	7:O:20:DT:OP1	1.98	0.62
4:D:527:LEU:CD2	4:D:581:MET:HE1	2.20	0.62
1:J:45:ALA:HB2	4:D:73:ILE:HD12	1.80	0.62
3:C:299:LEU:HD12	3:C:299:LEU:O	2.00	0.62
4:D:1171:SER:HA	4:D:1174:THR:HG22	1.79	0.62
8:P:11:DA:H4'	8:P:12:DA:OP1	1.99	0.62
3:C:766:ASN:O	3:C:767:VAL:HG13	2.00	0.62
3:C:876:LEU:CD1	3:C:886:ILE:HG13	2.29	0.62
4:D:363:PRO:HB2	4:D:365:ILE:CD1	2.30	0.62
4:D:602:ALA:HB3	4:D:607:PRO:O	2.00	0.62
4:D:1249:LEU:HD12	4:D:1250:LYS:N	2.15	0.62
1:J:47:ASP:OD1	1:J:47:ASP:N	2.19	0.61
3:C:765:PRO:HD2	3:C:825:ASP:HB2	1.81	0.61
4:D:190:LYS:NZ	4:D:192:ASP:HB3	2.15	0.61
2:A:158:GLU:H	2:A:161:ARG:NH1	1.97	0.61
2:B:120:ASN:ND2	2:B:123:MET:SD	2.72	0.61
3:C:215:VAL:HG12	3:C:217:ILE:HG23	1.82	0.61
2:T:279:THR:HG23	2:T:282:ASP:CB	2.29	0.61
6:F:180:ASN:OD1	6:F:183:GLU:HG3	2.00	0.61
3:C:348:VAL:HB	3:C:351:GLY:CA	2.30	0.61
3:C:477:ILE:CD1	4:D:852:THR:HG21	2.30	0.61
3:C:876:LEU:HD11	3:C:886:ILE:HD11	1.82	0.61
1:J:44:PHE:HE2	4:D:76:GLU:HA	1.66	0.61
1:J:98:LEU:O	1:J:102:LEU:HD13	1.99	0.61
4:D:622:MET:CE	4:D:629:VAL:HG22	2.21	0.61
4:D:647:GLU:HB2	4:D:655:TRP:CH2	2.36	0.61
4:D:676:LEU:HD12	4:D:676:LEU:N	2.16	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:785:GLY:O	4:D:789:GLU:HG3	1.99	0.61
3:C:231:ALA:HB1	3:C:265:LEU:HD13	1.80	0.61
3:C:299:LEU:HD12	3:C:299:LEU:C	2.26	0.61
2:A:138:LEU:HD12	2:A:138:LEU:N	2.15	0.61
2:B:74:THR:CG2	4:D:611:VAL:HG11	2.30	0.61
3:C:32:PHE:O	3:C:34:LYS:HD2	2.01	0.61
4:D:957:THR:O	4:D:958:THR:HG23	2.01	0.61
2:A:3:ILE:O	2:A:3:ILE:HG13	1.99	0.61
3:C:302:VAL:O	3:C:306:LYS:HG2	2.01	0.61
3:C:572:VAL:HG22	3:C:576:GLN:CD	2.26	0.61
3:C:805:LEU:HD12	3:C:809:GLU:CD	2.25	0.61
4:D:88:ARG:HD2	14:D:2102:HOH:O	2.00	0.61
5:E:80:VAL:HG12	5:E:81:GLU:N	2.15	0.61
5:E:80:VAL:HG12	5:E:81:GLU:H	1.65	0.61
6:F:324:LEU:HD22	6:F:332:PRO:HB3	1.82	0.61
2:A:40:ARG:NH2	3:C:894:ASP:OD2	2.34	0.61
3:C:132:ASN:CB	3:C:135:THR:HG22	2.29	0.61
3:C:148:PHE:HD2	3:C:150:MET:HE3	1.66	0.61
3:C:732:LEU:HD22	3:C:737:VAL:HG11	1.83	0.61
3:C:795:GLY:HA2	3:C:827:SER:OG	2.01	0.61
1:J:95:GLU:OE1	1:J:95:GLU:HA	2.01	0.61
2:A:113:PRO:HD2	2:A:116:VAL:HG21	1.83	0.61
2:A:210:SER:HB3	2:B:229:SER:HB2	1.83	0.60
2:B:39:ARG:NH2	4:D:623:ASP:OD2	2.34	0.60
3:C:421:PHE:O	3:C:425:SER:HB3	2.01	0.60
4:D:275:GLU:O	4:D:278:ARG:N	2.34	0.60
6:F:293:ILE:O	6:F:297:MET:HG3	2.01	0.60
8:P:17:DT:O5'	2:T:290:GLY:HA3	2.00	0.60
2:A:24:GLU:OE1	2:A:191:LYS:HD3	2.01	0.60
2:B:213:GLY:HA2	2:B:216:VAL:HG12	1.83	0.60
2:B:76:ILE:HA	2:B:79:ASN:HB2	1.83	0.60
3:C:216:ARG:HG2	3:C:221:ARG:HA	1.82	0.60
3:C:745:GLU:OE2	3:C:861:ARG:HD2	2.02	0.60
4:D:594:GLY:HA2	4:D:598:GLU:OE1	2.01	0.60
6:F:176:VAL:HG12	6:F:177:ALA:N	2.16	0.60
1:J:74:LYS:HG3	1:J:74:LYS:O	2.01	0.60
4:D:612:TYR:HB2	4:D:635:VAL:CG1	2.31	0.60
6:F:272:LYS:HE3	7:O:25:DC:OP1	2.01	0.60
3:C:38:PRO:HB3	3:C:508:ARG:HH21	1.66	0.60
3:C:363:HIS:NE2	3:C:528:ASP:OD2	2.34	0.60
3:C:584:MET:HA	3:C:619:THR:CG2	2.28	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:96:GLU:O	1:J:100:GLU:HG3	2.02	0.60
2:A:82:GLY:CA	2:A:123:MET:HE1	2.31	0.60
2:B:21:PHE:HB2	2:B:194:ILE:CG2	2.30	0.60
3:C:480:PRO:O	3:C:485:ILE:HG12	2.02	0.60
4:D:1071:ASP:HB2	4:D:1072:GLY:C	2.27	0.60
2:B:200:ASN:H	2:B:200:ASN:ND2	2.00	0.60
3:C:714:ILE:O	3:C:714:ILE:HG22	2.00	0.60
4:D:920:PHE:CE2	4:D:948:ILE:HG13	2.35	0.60
3:C:712:VAL:HA	3:C:906:ILE:HG13	1.84	0.60
3:C:1034:ALA:HB2	4:D:447:MET:HG3	1.84	0.60
3:C:394:ARG:HG3	3:C:398:GLN:HG3	1.84	0.59
3:C:998:LYS:NZ	4:D:734:ASP:OD2	2.30	0.59
1:J:82:TRP:CE2	6:F:199:GLN:HG2	2.37	0.59
3:C:982:SER:CB	3:C:983:THR:HG23	2.23	0.59
4:D:622:MET:HE2	4:D:629:VAL:CG2	2.21	0.59
4:D:846:LEU:H	4:D:846:LEU:HD12	1.66	0.59
4:D:1171:SER:CB	4:D:1174:THR:HG22	2.31	0.59
6:F:462:ARG:HH12	6:F:465:LEU:HD12	1.66	0.59
2:B:101:GLY:N	2:B:132:GLY:O	2.35	0.59
3:C:710:LEU:CD2	3:C:1021:ILE:HD11	2.28	0.59
4:D:435:GLN:OE1	4:D:435:GLN:N	2.30	0.59
4:D:1036:PHE:HA	4:D:1162:MET:HE1	1.84	0.59
2:B:52:THR:OG1	2:B:141:GLU:HG2	2.02	0.59
3:C:523:THR:HG22	3:C:526:GLU:CD	2.27	0.59
2:B:22:VAL:CG1	2:B:193:ILE:HD12	2.32	0.59
2:B:212:GLY:O	2:B:216:VAL:HG12	2.02	0.59
3:C:338:ARG:HB3	3:C:343:GLN:HE21	1.68	0.59
3:C:556:GLY:N	3:C:557:GLY:HA2	2.17	0.59
4:D:453:LYS:HB3	4:D:454:PRO:HD3	1.85	0.59
4:D:1062:PHE:CD2	4:D:1080:LYS:HD2	2.38	0.59
6:F:321:GLN:O	6:F:325:LEU:HB2	2.02	0.59
2:A:14:VAL:HG13	2:A:15:ALA:H	1.66	0.59
3:C:202:TRP:C	3:C:203:LEU:HD23	2.27	0.59
3:C:530:HIS:HB3	3:C:568:ASP:CG	2.27	0.59
3:C:751:ARG:HG2	3:C:856:VAL:HG22	1.84	0.59
4:D:6:PHE:HD1	4:D:1257:LYS:HE3	1.67	0.59
4:D:1079:ASP:N	4:D:1079:ASP:OD1	2.34	0.59
5:E:85:GLN:H	5:E:85:GLN:NE2	1.97	0.59
2:A:106:THR:CA	2:A:125:ILE:HD13	2.32	0.59
4:D:1171:SER:C	4:D:1174:THR:HG22	2.27	0.59
7:O:6:DA:C2'	7:O:7:DC:H5'	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:751:ARG:NH1	4:D:332:GLY:O	2.36	0.59
3:C:1028:VAL:HG12	4:D:429:VAL:HG12	1.85	0.59
3:C:1116:LEU:O	3:C:1120:GLN:HG3	2.03	0.59
4:D:334:ARG:HD3	6:F:356:ARG:HH21	1.68	0.59
4:D:585:LEU:HD12	4:D:692:GLN:NE2	2.17	0.59
4:D:850:ILE:O	4:D:853:HIS:HB2	2.02	0.59
6:F:176:VAL:HG12	6:F:177:ALA:H	1.67	0.59
3:C:736:ASP:OD1	3:C:869:LYS:HE2	2.03	0.59
4:D:1054:VAL:HG12	4:D:1104:ASP:O	2.03	0.59
3:C:203:LEU:HD22	3:C:217:ILE:HG22	1.85	0.58
4:D:58:TRP:CD2	4:D:68:VAL:HG22	2.38	0.58
4:D:1121:GLU:OE2	4:D:1124:ARG:NH2	2.29	0.58
2:A:40:ARG:HD3	2:B:33:THR:CG2	2.33	0.58
2:B:198:THR:CG2	2:B:202:ILE:HD12	2.32	0.58
3:C:434:ASN:O	3:C:608:PRO:HD3	2.03	0.58
3:C:768:SER:O	3:C:771:VAL:HG22	2.04	0.58
4:D:745:LEU:O	4:D:749:GLU:HG2	2.02	0.58
2:A:89:ASP:CB	2:A:142:ARG:HD2	2.33	0.58
2:A:199:LYS:O	2:A:200:ASN:HB2	2.03	0.58
3:C:937:ILE:HA	3:C:938:ASP:CB	2.33	0.58
2:A:30:PHE:CE1	2:B:40:ARG:HG3	2.38	0.58
2:B:167:ILE:HD11	4:D:617:GLU:HG3	1.84	0.58
3:C:335:TYR:CE1	3:C:356:VAL:HG13	2.38	0.58
3:C:338:ARG:CD	3:C:346:MET:HG3	2.29	0.58
4:D:436:LEU:O	4:D:716:LYS:NZ	2.35	0.58
4:D:743:GLU:O	4:D:747:ARG:HG3	2.04	0.58
6:F:345:PRO:HA	6:F:348:VAL:CG1	2.33	0.58
2:B:151:GLN:CG	2:B:154:ALA:HB1	2.34	0.58
3:C:910:THR:CG2	4:D:730:VAL:HG23	2.34	0.58
3:C:986:ASN:OD1	3:C:986:ASN:N	2.31	0.58
4:D:76:GLU:CD	4:D:76:GLU:H	2.11	0.58
4:D:673:ASN:HA	4:D:676:LEU:HD13	1.84	0.58
3:C:224:PRO:HB2	3:C:227:VAL:HG13	1.86	0.58
3:C:498:ASN:OD1	3:C:499:PRO:HD2	2.03	0.58
3:C:783:ILE:HG13	3:C:841:ILE:HD12	1.85	0.58
3:C:229:LEU:O	3:C:229:LEU:HD12	2.04	0.58
4:D:17:ALA:O	4:D:21:ARG:HG3	2.03	0.58
2:B:183:VAL:O	2:B:183:VAL:HG12	2.03	0.58
3:C:32:PHE:HE1	3:C:963:VAL:CG1	2.16	0.58
3:C:166:VAL:HG11	3:C:372:VAL:HG23	1.86	0.58
3:C:712:VAL:HG11	3:C:925:THR:HG23	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:412:ARG:HD2	6:F:322:ARG:NE	2.18	0.58
3:C:578:VAL:HG12	3:C:579:SER:O	2.03	0.58
3:C:590:HIS:O	3:C:919:ILE:HD11	2.04	0.58
4:D:930:ASP:HB3	4:D:954:ALA:HB1	1.85	0.58
3:C:509:LYS:HA	3:C:569:TYR:HA	1.85	0.58
4:D:723:ALA:O	4:D:726:SER:HB3	2.03	0.58
4:D:1231:THR:O	4:D:1235:THR:HG23	2.03	0.58
5:E:84:LEU:HB2	5:E:85:GLN:HE21	1.69	0.58
6:F:402:LEU:HD23	6:F:414:ARG:HE	1.68	0.58
2:A:100:GLN:OE1	2:A:101:GLY:N	2.31	0.57
2:B:34:LEU:HD12	2:B:35:GLY:N	2.19	0.57
4:D:269:ASP:HB3	4:D:272:ALA:CB	2.32	0.57
4:D:641:ARG:NE	4:D:655:TRP:HZ2	2.02	0.57
4:D:988:VAL:HG23	4:D:992:GLU:HG3	1.85	0.57
4:D:1041:PRO:HB3	4:D:1116:ALA:HB3	1.85	0.57
7:O:6:DA:H1'	7:O:7:DC:H5'	1.86	0.57
3:C:649:ILE:HG21	3:C:693:ILE:HG21	1.86	0.57
3:C:1026:HIS:HB3	3:C:1031:LYS:CE	2.32	0.57
4:D:460:LEU:HD11	4:D:472:ALA:HB1	1.86	0.57
2:T:256:LEU:CD2	2:T:297:VAL:HG22	2.34	0.57
2:A:192:LEU:C	2:A:192:LEU:HD12	2.30	0.57
3:C:534:GLN:NE2	4:D:846:LEU:HD11	2.19	0.57
4:D:248:TYR:HA	4:D:251:TYR:CD2	2.39	0.57
2:B:162:ILE:HG23	4:D:607:PRO:HG2	1.85	0.57
3:C:742:HIS:HD2	3:C:868:ARG:HG3	1.66	0.57
2:A:50:ALA:HB3	2:A:168:TYR:CD1	2.39	0.57
2:A:93:VAL:HG22	2:A:113:PRO:HG3	1.87	0.57
3:C:132:ASN:CG	3:C:135:THR:HG22	2.30	0.57
3:C:221:ARG:HG3	3:C:222:ARG:HG3	1.87	0.57
3:C:506:PRO:HB2	3:C:572:VAL:HG11	1.86	0.57
3:C:748:ILE:O	3:C:859:LEU:HD23	2.04	0.57
4:D:273:GLU:O	4:D:277:LEU:HB2	2.05	0.57
6:F:345:PRO:O	6:F:348:VAL:HG13	2.04	0.57
1:J:68:ASP:HA	1:J:69:VAL:CB	2.34	0.57
2:A:9:LEU:HD13	2:A:23:ILE:CG1	2.34	0.57
3:C:203:LEU:HD22	3:C:217:ILE:CB	2.35	0.57
3:C:368:ARG:HB3	3:C:501:GLY:O	2.05	0.57
3:C:522:LEU:HB3	3:C:526:GLU:HG3	1.86	0.57
2:B:97:LEU:HB3	2:B:136:VAL:CG1	2.35	0.57
3:C:540:ASP:O	3:C:543:GLY:N	2.32	0.57
3:C:710:LEU:HD13	3:C:1021:ILE:CG1	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:984:LEU:HD13	3:C:989:GLY:O	2.04	0.57
4:D:143:MET:CE	4:D:251:TYR:HA	2.34	0.57
4:D:602:ALA:HB3	4:D:607:PRO:C	2.29	0.57
2:A:85:VAL:HG22	2:A:86:SER:H	1.70	0.57
2:A:112:PRO:HB2	2:A:116:VAL:HG23	1.86	0.57
2:B:144:ARG:HB2	2:B:144:ARG:HH11	1.70	0.57
3:C:38:PRO:HB3	3:C:508:ARG:NH2	2.20	0.57
3:C:505:THR:CG2	3:C:506:PRO:HD2	2.35	0.57
3:C:575:ARG:NH2	3:C:966:PRO:HB2	2.19	0.57
10:C:1203:SO4:O1	4:D:540:GLN:NE2	2.37	0.57
4:D:155:MET:HE1	4:D:219:LEU:HB3	1.85	0.57
4:D:368:ASN:ND2	14:D:2116:HOH:O	2.37	0.57
2:A:9:LEU:HD23	2:B:221:LEU:O	2.05	0.57
3:C:476:PRO:O	4:D:856:ARG:NH2	2.35	0.57
3:C:763:ASP:CB	3:C:821:ARG:HH22	2.16	0.57
3:C:602:MET:HE1	3:C:883:LYS:CB	2.27	0.57
3:C:984:LEU:HB2	3:C:985:PRO:CA	2.33	0.57
4:D:641:ARG:CZ	4:D:655:TRP:HZ2	2.17	0.57
4:D:781:THR:HG22	4:D:814:ARG:HD2	1.87	0.57
4:D:885:VAL:O	4:D:990:ILE:O	2.23	0.57
4:D:1009:LEU:HB3	4:D:1029:LEU:HD13	1.87	0.57
8:P:3:DC:H2"	8:P:4:DA:C8	2.40	0.57
2:A:197:GLU:OE1	3:C:987:ARG:NH1	2.36	0.56
2:B:41:THR:O	2:B:45:SER:HB3	2.05	0.56
2:B:210:SER:O	2:B:214:THR:HG23	2.05	0.56
3:C:510:VAL:HG11	3:C:567:VAL:HB	1.86	0.56
4:D:924:LEU:HD22	4:D:959:VAL:CG1	2.35	0.56
4:D:982:MET:HE2	4:D:1153:LYS:HE3	1.86	0.56
1:J:89:ARG:HH22	6:F:274:ASP:CG	2.11	0.56
3:C:717:TRP:HH2	3:C:1005:ARG:NH2	2.03	0.56
3:C:1045:GLN:HG2	3:C:1087:THR:CG2	2.34	0.56
4:D:661:TRP:CZ3	4:D:663:ALA:HB2	2.38	0.56
6:F:317:LEU:HD21	6:F:337:LEU:HG	1.87	0.56
2:A:85:VAL:HG22	2:A:86:SER:N	2.19	0.56
2:A:99:LYS:HE3	2:A:109:ASP:OD1	2.05	0.56
2:B:180:ALA:HA	2:B:189:PHE:O	2.05	0.56
2:B:213:GLY:HA2	2:B:216:VAL:CG1	2.36	0.56
3:C:45:LEU:HD21	3:C:443:LYS:HD2	1.86	0.56
3:C:873:GLY:HA3	3:C:1028:VAL:HG11	1.87	0.56
3:C:966:PRO:HG2	3:C:969:ASP:O	2.05	0.56
4:D:735:VAL:HG22	4:D:798:ILE:HD11	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:89:ARG:NH2	6:F:274:ASP:OD1	2.26	0.56
2:B:76:ILE:HG23	2:B:125:ILE:CD1	2.35	0.56
2:B:143:GLY:HA3	2:B:168:TYR:CE1	2.41	0.56
4:D:1168:ILE:CD1	4:D:1176:PHE:HB3	2.35	0.56
3:C:21:ASN:O	3:C:22:SER:OG	2.21	0.56
3:C:649:ILE:HD13	3:C:693:ILE:HG22	1.87	0.56
3:C:891:PRO:HB2	3:C:893:GLU:CG	2.34	0.56
3:C:1029:ASP:OD1	4:D:520:LYS:HD2	2.06	0.56
4:D:1132:GLN:HE21	4:D:1163:LEU:HD12	1.71	0.56
2:A:211:ALA:O	2:A:215:LEU:N	2.36	0.56
3:C:721:ASN:HD22	3:C:727:ILE:CD1	2.18	0.56
4:D:240:LEU:HD23	4:D:244:LEU:HG	1.86	0.56
4:D:706:ILE:HD11	5:E:36:PRO:HA	1.87	0.56
4:D:1088:ARG:HG2	4:D:1089:VAL:N	2.18	0.56
5:E:26:TYR:CE1	5:E:29:PRO:HD3	2.40	0.56
6:F:219:MET:HE2	6:F:219:MET:CA	2.32	0.56
2:B:105:VAL:HG23	2:B:128:LEU:CD1	2.35	0.56
3:C:171:VAL:N	3:C:368:ARG:O	2.38	0.56
4:D:203:ARG:NE	4:D:203:ARG:HA	2.20	0.56
4:D:1275:PRO:CG	5:E:76:VAL:HG11	2.23	0.56
3:C:771:VAL:HG23	3:C:772:LEU:HD12	1.86	0.56
4:D:653:ASN:HB2	4:D:654:GLY:CA	2.35	0.56
4:D:753:ASP:O	4:D:757:ARG:N	2.38	0.56
4:D:901:ALA:HB1	4:D:910:ILE:O	2.06	0.56
6:F:449:MET:O	6:F:453:ARG:HG3	2.06	0.56
6:F:465:LEU:HD23	6:F:466:ASP:N	2.21	0.56
2:T:251:ILE:O	2:T:254:LEU:HG	2.06	0.56
3:C:921:GLN:HB2	3:C:1019:MET:HE3	1.87	0.56
3:C:937:ILE:CA	3:C:938:ASP:CB	2.84	0.56
4:D:170:LEU:HD13	4:D:209:ARG:NH2	2.21	0.56
4:D:262:LYS:CG	4:D:310:MET:HE1	2.36	0.56
6:F:438:ARG:NH1	8:P:20:DG:N7	2.53	0.56
2:A:8:THR:O	2:A:23:ILE:HA	2.06	0.55
2:B:50:ALA:HB3	2:B:168:TYR:CD2	2.41	0.55
3:C:369:LEU:HB3	3:C:501:GLY:O	2.06	0.55
3:C:549:ARG:HB2	3:C:561:PHE:CE2	2.41	0.55
3:C:680:ILE:HD11	3:C:692:VAL:O	2.05	0.55
4:D:270:ILE:O	4:D:274:ALA:N	2.38	0.55
4:D:924:LEU:CD2	4:D:959:VAL:HG11	2.36	0.55
5:E:76:VAL:HG13	5:E:77:GLY:N	2.20	0.55
3:C:549:ARG:HA	3:C:563:SER:HA	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:338:ALA:HB2	6:F:348:VAL:HG11	1.87	0.55
2:A:31:GLY:HA2	2:A:192:LEU:CD2	2.29	0.55
3:C:578:VAL:HG13	3:C:582:THR:CB	2.36	0.55
4:D:1128:PRO:HG3	4:D:1206:PRO:CB	2.37	0.55
6:F:308:VAL:HG21	7:O:23:DT:C7	2.27	0.55
7:O:11:DA:C2'	7:O:12:DG:H5"	2.36	0.55
6:F:462:ARG:NH1	6:F:465:LEU:HB2	2.21	0.55
2:T:251:ILE:HG21	2:T:270:HIS:O	2.06	0.55
2:A:170:PRO:HB3	2:A:202:ILE:HG12	1.86	0.55
2:A:192:LEU:HD12	2:A:192:LEU:O	2.06	0.55
2:B:177:LYS:HG3	2:B:193:ILE:HB	1.89	0.55
3:C:446:LEU:N	3:C:446:LEU:HD23	2.21	0.55
3:C:839:ILE:HG22	3:C:840:GLY:N	2.21	0.55
3:C:936:ASN:HD22	3:C:937:ILE:N	2.04	0.55
3:C:1003:ASP:HB2	3:C:1010:PHE:CZ	2.42	0.55
4:D:183:GLU:O	4:D:187:GLU:HG2	2.07	0.55
1:J:88:ARG:HG3	1:J:89:ARG:H	1.72	0.55
2:B:84:VAL:HB	2:B:199:LYS:CD	2.33	0.55
3:C:338:ARG:HB3	3:C:343:GLN:NE2	2.21	0.55
4:D:962:ARG:HB3	4:D:977:CYS:HA	1.89	0.55
5:E:29:PRO:HB2	5:E:33:THR:HG23	1.87	0.55
2:B:97:LEU:HB3	2:B:136:VAL:HG13	1.89	0.55
3:C:132:ASN:HB3	3:C:135:THR:CG2	2.35	0.55
3:C:275:GLY:O	6:F:171:LYS:HD2	2.06	0.55
3:C:1126:VAL:HG12	4:D:12:ILE:HG23	1.89	0.55
4:D:631:ALA:O	4:D:666:THR:HA	2.06	0.55
4:D:844:THR:H	4:D:847:GLU:HB2	1.71	0.55
6:F:254:ALA:HB3	6:F:257:ASP:OD2	2.07	0.55
6:F:364:THR:O	6:F:364:THR:HG23	2.07	0.55
2:A:2:LEU:HD12	2:B:143:GLY:HA2	1.88	0.55
3:C:228:LEU:HD21	3:C:268:ILE:CG1	2.19	0.55
3:C:721:ASN:ND2	3:C:727:ILE:HD11	2.22	0.55
4:D:129:ILE:HD11	4:D:130:TYR:CZ	2.41	0.55
4:D:872:LEU:HG	4:D:876:LEU:HD22	1.88	0.55
4:D:937:ILE:CD1	4:D:951:LEU:HG	2.34	0.55
4:D:1056:LEU:HD21	4:D:1063:PHE:HD1	1.72	0.55
2:A:90:ASP:O	2:A:91:GLU:HG2	2.07	0.55
2:A:152:ASN:HA	2:A:155:SER:OG	2.06	0.55
3:C:348:VAL:HG13	3:C:349:PRO:HD2	1.89	0.55
3:C:1014:VAL:HG13	4:D:729:THR:HG21	1.89	0.55
5:E:92:ALA:O	5:E:96:ILE:HG13	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:92:GLU:OE1	1:J:92:GLU:N	2.39	0.55
2:B:66:VAL:O	2:B:69:VAL:HG22	2.06	0.55
3:C:176:VAL:HG13	3:C:307:VAL:HG11	1.87	0.55
4:D:363:PRO:HG2	4:D:366:ILE:HD12	1.88	0.55
4:D:1276:THR:HG22	5:E:102:GLU:CG	2.36	0.55
6:F:324:LEU:HD23	6:F:328:LEU:CD1	2.33	0.55
3:C:269:TYR:CE2	3:C:278:PRO:HB3	2.41	0.54
3:C:727:ILE:CG1	3:C:907:ILE:HB	2.37	0.54
4:D:12:ILE:HG12	4:D:1221:TRP:CZ2	2.43	0.54
4:D:460:LEU:HD11	4:D:472:ALA:CB	2.37	0.54
2:B:44:SER:HA	2:B:145:GLY:HA2	1.88	0.54
3:C:202:TRP:H	3:C:202:TRP:CD1	2.25	0.54
3:C:346:MET:HB2	3:C:356:VAL:HG21	1.89	0.54
4:D:579:LEU:HG	11:D:2008:EDO:H22	1.89	0.54
3:C:614:ALA:HB1	3:C:615:PRO:HD2	1.88	0.54
3:C:1045:GLN:CG	3:C:1090:ARG:HH21	2.19	0.54
2:A:106:THR:C	2:A:125:ILE:HD13	2.33	0.54
2:A:210:SER:HB3	2:B:229:SER:CB	2.37	0.54
2:B:162:ILE:CG2	4:D:607:PRO:HG2	2.38	0.54
3:C:935:TRP:HB2	3:C:982:SER:CB	2.38	0.54
4:D:706:ILE:O	4:D:710:GLN:HG3	2.07	0.54
4:D:1037:GLU:HG2	4:D:1039:ARG:NH1	2.22	0.54
3:C:493:VAL:HG12	3:C:494:TYR:CD1	2.42	0.54
4:D:848:TYR:O	4:D:852:THR:HG23	2.07	0.54
2:B:24:GLU:HG3	2:B:191:LYS:HG3	1.88	0.54
3:C:885:VAL:CG1	4:D:538:GLY:HA2	2.38	0.54
3:C:1039:PRO:HB2	3:C:1048:LEU:HD21	1.89	0.54
4:D:932:ASN:N	4:D:933:GLY:HA2	2.22	0.54
4:D:1087:LEU:CD2	4:D:1113:MET:HE2	2.38	0.54
5:E:81:GLU:OE1	5:E:81:GLU:HA	2.08	0.54
2:A:66:VAL:HB	2:A:69:VAL:CG2	2.38	0.54
3:C:141:GLN:OE1	3:C:404:THR:OG1	2.26	0.54
3:C:917:MET:HE2	4:D:839:PHE:CD2	2.43	0.54
6:F:219:MET:HA	6:F:219:MET:CE	2.31	0.54
2:A:43:LEU:HD11	2:A:174:VAL:HB	1.90	0.54
4:D:706:ILE:CD1	5:E:36:PRO:HB3	2.37	0.54
6:F:385:ALA:O	6:F:389:VAL:HG23	2.08	0.54
2:A:21:PHE:HB2	2:A:194:ILE:HG12	1.89	0.54
2:A:40:ARG:HD3	2:B:33:THR:CB	2.38	0.54
3:C:380:ILE:HG12	3:C:418:ILE:HD11	1.89	0.54
4:D:468:ASN:ND2	6:F:463:ASP:OD2	2.35	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:687:MET:HE2	4:D:695:ILE:CD1	2.38	0.54
4:D:901:ALA:N	4:D:912:ASP:HB2	2.20	0.54
2:A:111:VAL:O	2:A:111:VAL:HG22	2.08	0.53
2:A:210:SER:CB	2:B:229:SER:HB2	2.38	0.53
3:C:892:VAL:CG2	3:C:903:PRO:HG2	2.38	0.53
3:C:939:VAL:HG23	3:C:940:ALA:HA	1.88	0.53
4:D:39:LEU:HD13	4:D:335:PHE:HZ	1.72	0.53
2:B:205:ARG:CZ	2:B:205:ARG:HB2	2.37	0.53
3:C:41:VAL:HG13	3:C:493:VAL:HG12	1.91	0.53
3:C:148:PHE:HD2	3:C:150:MET:CE	2.21	0.53
3:C:268:ILE:O	3:C:272:LEU:HD13	2.08	0.53
3:C:431:MET:O	3:C:670:ASN:ND2	2.41	0.53
3:C:876:LEU:N	3:C:876:LEU:HD12	2.24	0.53
3:C:988:ASP:OD1	3:C:988:ASP:N	2.40	0.53
3:C:1085:ASP:OD2	4:D:420:LYS:NZ	2.40	0.53
4:D:915:VAL:HG23	4:D:920:PHE:CE2	2.43	0.53
6:F:215:GLN:O	6:F:219:MET:HG2	2.08	0.53
7:O:15:DT:H2"	7:O:16:DT:OP2	2.08	0.53
2:A:9:LEU:HD23	2:B:221:LEU:C	2.33	0.53
3:C:102:ARG:O	3:C:124:LEU:HD23	2.07	0.53
3:C:777:GLU:CD	3:C:777:GLU:H	2.15	0.53
3:C:1117:LYS:HD2	3:C:1120:GLN:NE2	2.23	0.53
4:D:982:MET:CE	4:D:1153:LYS:HE3	2.38	0.53
2:A:48:GLY:CA	2:A:49:ALA:CB	2.85	0.53
2:A:197:GLU:OE1	3:C:987:ARG:NH2	2.42	0.53
3:C:338:ARG:HD3	3:C:343:GLN:HE22	1.73	0.53
3:C:712:VAL:CG1	3:C:925:THR:HG23	2.38	0.53
3:C:948:SER:C	3:C:950:LEU:CB	2.82	0.53
4:D:826:PRO:HG3	4:D:853:HIS:CE1	2.43	0.53
4:D:1229:GLU:O	4:D:1233:VAL:HG23	2.07	0.53
3:C:368:ARG:HA	3:C:369:LEU:CB	2.39	0.53
3:C:822:GLU:HG2	3:C:823:VAL:HG22	1.91	0.53
4:D:131:PHE:HA	4:D:256:MET:HE2	1.91	0.53
4:D:285:LYS:HA	4:D:289:LYS:HD2	1.90	0.53
4:D:622:MET:HE3	4:D:667:LEU:CD1	2.30	0.53
4:D:1045:ALA:O	14:D:2106:HOH:O	2.19	0.53
1:J:102:LEU:HA	1:J:105:ILE:HG22	1.90	0.53
2:B:103:GLY:O	2:B:128:LEU:HB2	2.08	0.53
4:D:744:ILE:O	4:D:748:HIS:HD2	1.92	0.53
4:D:1034:GLU:OE2	4:D:1042:ARG:HG2	2.09	0.53
4:D:872:LEU:HG	4:D:876:LEU:CD2	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:82:GLY:HA3	2:A:123:MET:CE	2.39	0.53
3:C:704:MET:CE	3:C:706:LEU:HD21	2.39	0.53
3:C:729:SER:OG	3:C:904:VAL:O	2.27	0.53
3:C:808:GLU:O	3:C:812:LEU:HD13	2.09	0.53
3:C:973:GLU:OE1	4:D:840:ARG:NH2	2.42	0.53
4:D:443:LEU:HD22	4:D:514:PRO:HB3	1.91	0.53
3:C:76:GLY:O	3:C:80:VAL:HG23	2.09	0.53
3:C:169:GLN:OE1	3:C:370:ARG:NH2	2.42	0.53
4:D:373:MET:SD	6:F:256:LEU:HB3	2.49	0.53
1:J:40:PHE:CZ	1:J:58:ASN:HB2	2.44	0.53
2:B:216:VAL:HG13	2:B:217:GLU:N	2.23	0.53
3:C:921:GLN:HB2	3:C:1019:MET:CE	2.38	0.53
2:B:97:LEU:HD21	2:B:105:VAL:HG11	1.90	0.52
3:C:280:LYS:O	3:C:284:GLN:HG2	2.10	0.52
3:C:967:VAL:HG23	3:C:968:PHE:H	1.73	0.52
4:D:1069:PRO:O	4:D:1072:GLY:HA2	2.09	0.52
2:B:60:LEU:HD22	2:B:60:LEU:N	2.24	0.52
3:C:329:VAL:O	3:C:332:THR:OG1	2.26	0.52
4:D:602:ALA:HB1	4:D:606:ALA:HB3	1.89	0.52
4:D:653:ASN:CB	4:D:654:GLY:CA	2.87	0.52
4:D:767:THR:O	4:D:771:GLU:HB2	2.09	0.52
4:D:951:LEU:CB	4:D:956:ILE:HD11	2.33	0.52
1:J:82:TRP:CZ2	6:F:199:GLN:HG2	2.44	0.52
3:C:29:ARG:CD	3:C:964:ALA:HB2	2.39	0.52
3:C:62:ARG:O	3:C:66:ILE:HG13	2.09	0.52
3:C:426:GLN:CD	3:C:450:GLY:HA2	2.34	0.52
3:C:1084:SER:HB2	4:D:421:ARG:O	2.10	0.52
4:D:781:THR:O	4:D:784:VAL:HG23	2.09	0.52
4:D:815:THR:HG22	4:D:820:LYS:CA	2.33	0.52
4:D:936:ILE:CG2	4:D:951:LEU:HD23	2.38	0.52
5:E:98:GLY:O	5:E:100:LEU:HD12	2.09	0.52
6:F:335:GLU:OE1	6:F:335:GLU:N	2.41	0.52
8:P:17:DT:P	2:T:290:GLY:HA3	2.49	0.52
2:T:260:SER:O	2:T:264:LEU:HG	2.08	0.52
2:A:33:THR:HG22	2:B:37:SER:OG	2.10	0.52
3:C:90:PHE:HA	14:C:1323:HOH:O	2.09	0.52
3:C:202:TRP:O	3:C:203:LEU:HD23	2.08	0.52
3:C:335:TYR:O	3:C:335:TYR:HD1	1.91	0.52
3:C:393:GLU:OE2	6:F:247:ARG:HD3	2.09	0.52
3:C:895:MET:HG3	3:C:896:PRO:HD2	1.91	0.52
3:C:939:VAL:HG22	3:C:940:ALA:HA	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:585:LEU:HD12	4:D:692:GLN:HE21	1.73	0.52
2:T:251:ILE:HD12	2:T:254:LEU:HD11	1.91	0.52
2:A:56:ILE:HB	2:A:59:VAL:CG2	2.37	0.52
3:C:494:TYR:HB3	3:C:506:PRO:CG	2.37	0.52
3:C:568:ASP:OD1	3:C:568:ASP:N	2.43	0.52
3:C:958:PRO:O	3:C:961:SER:OG	2.28	0.52
2:A:68:GLY:HA3	2:A:129:ASN:HD21	1.74	0.52
3:C:33:ALA:HB2	3:C:966:PRO:HG3	1.90	0.52
3:C:538:PRO:HB2	3:C:546:THR:OG1	2.10	0.52
3:C:549:ARG:HD3	3:C:561:PHE:CE2	2.44	0.52
3:C:874:ASP:OD1	3:C:1028:VAL:HG22	2.10	0.52
6:F:173:ILE:HG22	6:F:238:LEU:CD1	2.40	0.52
2:A:177:LYS:HG2	2:A:193:ILE:CD1	2.40	0.52
3:C:44:LEU:HG	3:C:628:ASP:OD2	2.09	0.52
3:C:573:SER:HB2	3:C:574:PRO:HD2	1.92	0.52
3:C:635:ALA:CB	3:C:693:ILE:HD11	2.30	0.52
4:D:898:VAL:HG11	4:D:919:ALA:HB2	1.91	0.52
2:A:18:ARG:HA	2:A:204:PRO:HG3	1.92	0.52
2:A:181:THR:H	2:A:189:PHE:C	2.15	0.52
3:C:984:LEU:HD13	3:C:989:GLY:CA	2.40	0.52
6:F:394:LEU:HB2	6:F:464:TYR:CD1	2.45	0.52
2:A:50:ALA:HB3	2:A:168:TYR:CE1	2.45	0.52
2:B:22:VAL:HA	2:B:192:LEU:O	2.10	0.52
3:C:299:LEU:HD23	3:C:323:THR:N	2.24	0.52
3:C:193:VAL:HG12	3:C:205:PHE:HB2	1.92	0.52
3:C:479:THR:OG1	3:C:480:PRO:HD2	2.10	0.52
4:D:27:GLU:HB2	4:D:94:HIS:CE1	2.45	0.52
4:D:248:TYR:HA	4:D:251:TYR:HD2	1.75	0.52
4:D:354:LEU:O	4:D:358:ILE:HG12	2.10	0.52
2:B:64:THR:C	2:B:65:THR:HG1	2.02	0.51
3:C:910:THR:O	3:C:914:PRO:HD3	2.10	0.51
3:C:1133:GLY:O	3:C:1134:ALA:HB3	2.09	0.51
4:D:432:VAL:CG2	4:D:434:PRO:HD3	2.28	0.51
4:D:607:PRO:O	4:D:609:GLN:HG2	2.10	0.51
6:F:309:HIS:O	6:F:313:VAL:HG12	2.09	0.51
3:C:641:ILE:HG21	3:C:644:VAL:HG13	1.91	0.51
4:D:330:LEU:HD22	4:D:330:LEU:H	1.74	0.51
4:D:653:ASN:CB	4:D:654:GLY:HA3	2.39	0.51
4:D:716:LYS:HE3	4:D:717:ASP:OD1	2.10	0.51
4:D:1123:LEU:HA	4:D:1131:VAL:CG2	2.40	0.51
4:D:1132:GLN:CG	4:D:1163:LEU:HD12	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:150:MET:HA	3:C:150:MET:CE	2.33	0.51
3:C:624:ARG:NH1	3:C:628:ASP:OD2	2.43	0.51
3:C:852:LEU:CD2	3:C:856:VAL:HG12	2.40	0.51
3:C:1069:ALA:HB3	4:D:506:ARG:HB3	1.93	0.51
3:C:1132:ASP:HB3	3:C:1133:GLY:CA	2.35	0.51
4:D:1164:ARG:NH1	10:D:2005:SO4:O1	2.43	0.51
5:E:62:ASN:O	5:E:66:ASN:ND2	2.44	0.51
2:A:147:VAL:HG12	2:A:168:TYR:HE2	1.74	0.51
2:B:74:THR:OG1	4:D:608:GLU:OE1	2.29	0.51
2:B:102:PRO:HB3	2:B:130:ASP:HA	1.93	0.51
3:C:87:ILE:CD1	3:C:388:GLU:HG3	2.40	0.51
3:C:404:THR:HG23	3:C:407:THR:H	1.75	0.51
4:D:240:LEU:HD23	4:D:240:LEU:C	2.35	0.51
4:D:1009:LEU:HD23	4:D:1029:LEU:HD12	1.91	0.51
1:J:64:LEU:HD22	1:J:66:GLU:HB2	1.93	0.51
3:C:272:LEU:C	3:C:274:PRO:HD3	2.35	0.51
3:C:764:ILE:HB	3:C:767:VAL:HG21	1.91	0.51
3:C:959:ALA:O	3:C:960:ASP:HB2	2.09	0.51
4:D:1174:THR:CA	4:D:1175:GLU:CB	2.87	0.51
2:B:79:ASN:O	2:B:123:MET:CE	2.58	0.51
3:C:1074:TYR:CE1	4:D:1258:LEU:HD21	2.46	0.51
4:D:190:LYS:HZ2	4:D:192:ASP:HB3	1.74	0.51
2:A:36:ASN:CB	3:C:1007:GLY:HA3	2.41	0.51
3:C:123:PRO:HB3	3:C:144:PHE:HE1	1.75	0.51
3:C:346:MET:HE2	3:C:348:VAL:HA	1.92	0.51
4:D:736:LEU:N	4:D:792:TYR:OH	2.33	0.51
8:P:11:DA:H2''	8:P:12:DA:H5'	1.90	0.51
3:C:94:MET:CE	3:C:395:MET:HB3	2.40	0.51
3:C:584:MET:CA	3:C:619:THR:HG21	2.36	0.51
4:D:70:PHE:O	4:D:82:VAL:HG11	2.10	0.51
4:D:588:LEU:HD22	4:D:668:GLY:CA	2.38	0.51
4:D:932:ASN:N	4:D:933:GLY:CA	2.74	0.51
2:A:159:ILE:HD11	3:C:785:ALA:HA	1.92	0.51
2:A:172:LEU:HD13	2:A:197:GLU:OE2	2.11	0.51
3:C:35:LEU:N	3:C:35:LEU:HD12	2.26	0.50
3:C:171:VAL:HG12	3:C:172:ARG:N	2.26	0.50
3:C:578:VAL:HG13	3:C:582:THR:CG2	2.41	0.50
4:D:656:LYS:HD3	4:D:656:LYS:H	1.75	0.50
6:F:164:ASP:OD1	6:F:166:VAL:N	2.42	0.50
6:F:304:ILE:HB	14:F:606:HOH:O	2.10	0.50
2:A:177:LYS:HE2	2:A:193:ILE:HG12	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:193:ILE:HD12	2:A:193:ILE:O	2.11	0.50
2:A:210:SER:CB	2:B:229:SER:CB	2.90	0.50
2:B:170:PRO:O	2:B:199:LYS:HB2	2.12	0.50
3:C:516:THR:HG21	3:C:518:GLN:HB2	1.92	0.50
2:B:198:THR:HG22	2:B:199:LYS:O	2.10	0.50
3:C:577:MET:HE3	4:D:849:PHE:HD1	1.75	0.50
3:C:852:LEU:HD22	3:C:856:VAL:HG12	1.92	0.50
4:D:411:GLY:O	4:D:415:GLN:HB3	2.12	0.50
4:D:981:SER:HB3	4:D:984:THR:OG1	2.10	0.50
6:F:465:LEU:HD23	6:F:465:LEU:C	2.37	0.50
2:A:70:LYS:HB3	2:A:71:GLU:OE1	2.12	0.50
3:C:106:VAL:HG11	3:C:120:TYR:CE1	2.46	0.50
3:C:180:GLU:HG3	3:C:180:GLU:O	2.10	0.50
3:C:572:VAL:H	3:C:576:GLN:NE2	2.10	0.50
3:C:894:ASP:HA	3:C:1004:GLY:HA3	1.93	0.50
4:D:880:SER:O	4:D:995:GLY:HA3	2.11	0.50
2:A:54:ILE:C	2:A:54:ILE:HD12	2.36	0.50
3:C:41:VAL:HG13	3:C:493:VAL:CG1	2.41	0.50
3:C:797:VAL:CG1	3:C:823:VAL:HB	2.41	0.50
4:D:103:HIS:CE1	4:D:105:TRP:HB2	2.46	0.50
4:D:137:THR:HG23	4:D:253:THR:OG1	2.12	0.50
4:D:363:PRO:HB2	4:D:365:ILE:HD13	1.93	0.50
4:D:875:ARG:HH22	4:D:1033:GLN:CD	2.19	0.50
6:F:166:VAL:O	6:F:170:LEU:HG	2.10	0.50
2:A:113:PRO:HD2	2:A:116:VAL:CG2	2.41	0.50
2:B:172:LEU:O	4:D:616:ALA:HB1	2.10	0.50
4:D:54:PRO:HG3	4:D:81:GLU:O	2.12	0.50
6:F:176:VAL:CG1	6:F:177:ALA:H	2.25	0.50
6:F:462:ARG:HH11	6:F:465:LEU:HB2	1.75	0.50
3:C:762:ARG:HG3	3:C:762:ARG:O	2.10	0.50
3:C:797:VAL:HG12	3:C:823:VAL:HB	1.94	0.50
14:C:1321:HOH:O	4:D:733:ALA:HB2	2.12	0.50
2:T:289:PHE:HE2	2:T:294:ILE:CG1	2.20	0.50
2:B:93:VAL:HG11	2:B:116:VAL:HG11	1.92	0.50
2:B:147:VAL:HG13	2:B:166:SER:HB2	1.93	0.50
3:C:946:TRP:CZ2	3:C:978:GLY:HA3	2.46	0.50
3:C:1043:ILE:HD12	3:C:1043:ILE:N	2.25	0.50
4:D:581:MET:HE3	4:D:716:LYS:CA	2.41	0.50
4:D:644:THR:HA	4:D:647:GLU:CD	2.35	0.50
4:D:937:ILE:HD12	4:D:951:LEU:CG	2.38	0.50
4:D:1056:LEU:HD21	4:D:1063:PHE:CD1	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:1062:PHE:CE2	4:D:1080:LYS:HD2	2.47	0.50
3:C:199:ARG:HG2	3:C:200:GLY:N	2.27	0.50
4:D:1054:VAL:HG11	4:D:1100:LEU:HD21	1.94	0.50
6:F:416:ARG:HA	6:F:430:ILE:HD11	1.94	0.50
1:J:76:LYS:HG3	1:J:76:LYS:O	2.11	0.49
2:A:1:MET:O	2:A:1:MET:HG2	2.11	0.49
2:B:139:VAL:HG21	2:B:161:ARG:HH21	1.76	0.49
3:C:36:ARG:O	3:C:38:PRO:HD3	2.11	0.49
3:C:51:SER:OG	3:C:371:THR:HG23	2.12	0.49
3:C:404:THR:CG2	3:C:407:THR:HG23	2.42	0.49
3:C:710:LEU:O	3:C:1018:TYR:HA	2.12	0.49
3:C:754:LYS:HE2	3:C:754:LYS:N	2.24	0.49
4:D:236:VAL:O	4:D:236:VAL:HG12	2.12	0.49
4:D:704:PRO:HD2	4:D:707:VAL:HG21	1.94	0.49
4:D:890:CYS:SG	4:D:892:THR:HG22	2.52	0.49
2:A:130:ASP:N	2:A:130:ASP:OD1	2.44	0.49
2:B:105:VAL:HG12	2:B:125:ILE:HG21	1.93	0.49
3:C:96:LEU:HD22	3:C:98:PHE:CE1	2.47	0.49
3:C:196:ILE:HG23	3:C:196:ILE:O	2.12	0.49
3:C:268:ILE:HG23	3:C:272:LEU:HD22	1.95	0.49
3:C:467:HIS:ND1	3:C:468:PRO:HD2	2.27	0.49
3:C:475:CYS:CB	3:C:579:SER:HB3	2.42	0.49
3:C:572:VAL:O	3:C:573:SER:HB3	2.12	0.49
4:D:331:ASP:N	4:D:331:ASP:OD1	2.45	0.49
6:F:194:GLY:HA2	6:F:222:ILE:HG22	1.94	0.49
6:F:454:HIS:CD2	6:F:456:SER:HG	2.30	0.49
2:A:24:GLU:HB3	2:A:191:LYS:HB2	1.95	0.49
3:C:126:VAL:HB	3:C:145:MET:HE2	1.94	0.49
3:C:370:ARG:HH22	3:C:452:GLY:HA3	1.77	0.49
4:D:285:LYS:HG3	4:D:289:LYS:HD2	1.94	0.49
4:D:430:ILE:HD13	4:D:541:MET:HG3	1.93	0.49
4:D:432:VAL:HG22	4:D:434:PRO:CD	2.28	0.49
5:E:56:LYS:HA	5:E:59:ARG:HG3	1.93	0.49
2:T:289:PHE:CE2	2:T:294:ILE:HG13	2.34	0.49
2:B:99:LYS:O	2:B:133:LYS:HG3	2.12	0.49
3:C:753:THR:HG21	3:C:799:PRO:HD2	1.95	0.49
3:C:965:THR:O	3:C:965:THR:OG1	2.25	0.49
3:C:1117:LYS:HE2	4:D:90:GLU:O	2.13	0.49
4:D:362:ALA:HB3	4:D:367:VAL:HG23	1.93	0.49
4:D:992:GLU:OE1	5:E:48:TYR:OH	2.31	0.49
4:D:1275:PRO:CB	5:E:79:LEU:HD11	2.38	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:211:ALA:O	2:A:215:LEU:HB2	2.12	0.49
2:B:183:VAL:O	2:B:184:GLU:CB	2.61	0.49
3:C:203:LEU:C	3:C:204:GLU:HG3	2.37	0.49
4:D:599:TYR:HA	4:D:610:GLY:HA3	1.94	0.49
4:D:936:ILE:HG23	4:D:951:LEU:HD23	1.95	0.49
2:A:32:TYR:CE1	2:A:178:VAL:HG22	2.47	0.49
2:A:95:MET:HE2	2:A:110:ILE:HG21	1.95	0.49
2:A:108:GLY:HA2	2:A:121:PRO:HB3	1.94	0.49
2:B:26:LEU:CD1	2:B:34:LEU:HD21	2.42	0.49
3:C:523:THR:CG2	3:C:526:GLU:HG2	2.43	0.49
3:C:680:ILE:HG12	3:C:693:ILE:O	2.13	0.49
3:C:727:ILE:HG13	3:C:907:ILE:HD12	1.94	0.49
4:D:113:ARG:HB2	4:D:312:MET:CE	2.43	0.49
4:D:119:ASP:C	4:D:120:LEU:HD12	2.37	0.49
4:D:1153:LYS:O	4:D:1157:VAL:HG23	2.13	0.49
4:D:1276:THR:HG22	5:E:102:GLU:HG3	1.95	0.49
6:F:253:MET:CE	6:F:297:MET:HA	2.18	0.49
3:C:626:ALA:HB2	3:C:704:MET:HG2	1.95	0.49
4:D:603:THR:HG22	4:D:604:LYS:CE	2.30	0.49
4:D:755:ILE:HD12	4:D:776:ILE:CD1	2.43	0.49
4:D:901:ALA:HB2	4:D:911:ARG:CA	2.39	0.49
4:D:915:VAL:O	4:D:920:PHE:HD2	1.96	0.49
4:D:988:VAL:CG2	4:D:992:GLU:HG3	2.42	0.49
4:D:1271:ILE:HG12	5:E:105:GLU:HA	1.94	0.49
2:A:71:GLU:OE2	2:A:126:ALA:HA	2.11	0.49
2:B:85:VAL:HB	2:B:118:VAL:HA	1.94	0.49
3:C:176:VAL:O	3:C:176:VAL:HG23	2.11	0.49
4:D:177:LEU:HD12	4:D:201:GLY:HA3	1.95	0.49
4:D:1222:LEU:HD23	4:D:1244:ASP:OD2	2.12	0.49
2:T:283:LEU:O	2:T:286:ILE:HG22	2.13	0.49
2:A:129:ASN:H	2:A:129:ASN:HD22	1.60	0.49
3:C:26:ALA:HB1	3:C:623:LEU:HD21	1.94	0.49
3:C:508:ARG:HD2	3:C:570:MET:CE	2.41	0.49
4:D:618:ALA:HB1	4:D:627:LEU:CD1	2.43	0.49
5:E:95:GLU:HB3	5:E:101:LEU:CD2	2.43	0.49
2:A:31:GLY:O	2:A:35:GLY:N	2.34	0.49
2:A:49:ALA:HB1	2:A:85:VAL:O	2.12	0.49
2:B:105:VAL:HG23	2:B:128:LEU:HD13	1.95	0.49
3:C:45:LEU:HD21	3:C:443:LYS:CD	2.43	0.49
3:C:284:GLN:HG3	3:C:285:THR:N	2.28	0.49
3:C:326:GLU:O	3:C:330:VAL:HG23	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:510:VAL:HG11	3:C:567:VAL:CG1	2.43	0.49
4:D:140:ASP:OD2	4:D:143:MET:HB2	2.13	0.49
4:D:243:GLU:O	4:D:247:ARG:HG3	2.13	0.49
4:D:915:VAL:HG23	4:D:920:PHE:HE2	1.78	0.49
6:F:313:VAL:CG2	6:F:351:ILE:HD13	2.43	0.49
2:B:171:VAL:HG23	2:B:171:VAL:O	2.12	0.48
2:B:172:LEU:HD12	4:D:620:MET:SD	2.53	0.48
3:C:71:GLU:C	3:C:73:PRO:HD3	2.38	0.48
3:C:410:ASN:ND2	3:C:412:ARG:HG3	2.28	0.48
4:D:1117:ALA:O	4:D:1119:PRO:HD3	2.13	0.48
6:F:317:LEU:CD2	6:F:337:LEU:HG	2.43	0.48
1:J:84:MET:CE	6:F:272:LYS:HB2	2.43	0.48
2:A:9:LEU:HD13	2:A:23:ILE:HG13	1.96	0.48
3:C:781:VAL:HG21	3:C:838:VAL:HG21	1.95	0.48
4:D:105:TRP:CE2	4:D:1231:THR:HG23	2.48	0.48
4:D:1069:PRO:HG2	4:D:1073:GLY:N	2.24	0.48
7:O:29:DA:N7	14:O:103:HOH:O	2.35	0.48
1:J:81:HIS:CG	6:F:195:LEU:HD21	2.48	0.48
2:A:11:GLU:CD	2:A:205:ARG:HG2	2.38	0.48
2:A:186:ARG:O	2:A:187:THR:HG22	2.13	0.48
3:C:505:THR:HG22	3:C:506:PRO:HD2	1.95	0.48
3:C:919:ILE:HD12	3:C:920:GLY:N	2.28	0.48
4:D:1034:GLU:OE2	4:D:1042:ARG:N	2.46	0.48
7:O:15:DT:H1'	7:O:16:DT:H5''	1.95	0.48
2:A:177:LYS:HE2	2:A:193:ILE:CG1	2.44	0.48
3:C:174:PRO:HD2	3:C:302:VAL:HB	1.94	0.48
3:C:616:LEU:HB2	3:C:709:ASN:CG	2.38	0.48
3:C:771:VAL:HG23	3:C:772:LEU:HD13	1.93	0.48
4:D:608:GLU:O	4:D:609:GLN:HB2	2.13	0.48
4:D:653:ASN:N	4:D:654:GLY:HA3	2.28	0.48
4:D:735:VAL:HG22	4:D:798:ILE:CD1	2.43	0.48
1:J:58:ASN:HD21	1:J:60:LEU:HD12	1.78	0.48
2:B:76:ILE:HG23	2:B:125:ILE:HD11	1.94	0.48
3:C:32:PHE:HE1	3:C:963:VAL:HG13	1.79	0.48
3:C:708:LYS:HG3	3:C:737:VAL:HG23	1.95	0.48
3:C:723:GLU:O	3:C:724:ASP:HB2	2.14	0.48
3:C:845:SER:O	3:C:850:ASP:HB2	2.13	0.48
4:D:363:PRO:HB2	4:D:365:ILE:HD12	1.95	0.48
4:D:1071:ASP:N	4:D:1072:GLY:HA2	2.28	0.48
2:A:18:ARG:HB2	2:A:196:VAL:O	2.13	0.48
2:A:18:ARG:NH1	2:A:195:ASP:OD2	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:29:ARG:HG2	3:C:964:ALA:HB2	1.96	0.48
3:C:55:LEU:HD22	3:C:376:ILE:HB	1.95	0.48
3:C:174:PRO:HB2	3:C:303:GLY:CA	2.43	0.48
4:D:665:THR:HG21	4:D:682:PHE:CE2	2.49	0.48
4:D:1005:PRO:HG3	4:D:1150:ILE:HD11	1.95	0.48
6:F:272:LYS:HE3	7:O:25:DC:P	2.53	0.48
7:O:6:DA:C1'	7:O:7:DC:H5'	2.44	0.48
2:B:95:MET:HE3	2:B:110:ILE:CD1	2.39	0.48
3:C:1098:VAL:HG11	4:D:469:ILE:CD1	2.42	0.48
4:D:336:ALA:HA	6:F:359:ILE:O	2.14	0.48
4:D:935:VAL:O	4:D:935:VAL:HG12	2.13	0.48
4:D:1088:ARG:HD2	4:D:1111:GLN:HB3	1.95	0.48
4:D:1276:THR:HG22	5:E:102:GLU:HG2	1.95	0.48
1:J:51:PRO:O	1:J:64:LEU:HD12	2.13	0.48
2:B:65:THR:HG22	2:B:66:VAL:N	2.29	0.48
4:D:153:ALA:O	4:D:157:VAL:HG23	2.13	0.48
2:B:22:VAL:HG12	2:B:193:ILE:CD1	2.40	0.48
3:C:202:TRP:H	3:C:202:TRP:HD1	1.59	0.48
3:C:231:ALA:HB1	3:C:265:LEU:HD12	1.94	0.48
3:C:1080:LEU:HD12	4:D:1253:VAL:HG13	1.96	0.48
4:D:58:TRP:CE3	4:D:68:VAL:HG22	2.49	0.48
4:D:365:ILE:HD13	6:F:235:GLU:HG2	1.96	0.48
4:D:924:LEU:CD2	4:D:943:LEU:HD11	2.43	0.48
6:F:244:LEU:HD12	6:F:289:ILE:CG2	2.44	0.48
6:F:360:SER:HB3	6:F:363:GLN:HG3	1.95	0.48
7:O:28:DT:H2''	7:O:29:DA:C5'	2.40	0.48
1:J:53:THR:HA	1:J:62:GLY:O	2.13	0.48
2:A:152:ASN:HB3	2:A:157:ALA:HB3	1.93	0.48
3:C:1084:SER:OG	3:C:1085:ASP:N	2.45	0.48
2:A:112:PRO:HB2	2:A:116:VAL:CG2	2.43	0.47
2:B:64:THR:HA	2:B:73:VAL:HG21	1.95	0.47
3:C:203:LEU:HD13	3:C:217:ILE:CG2	2.42	0.47
3:C:203:LEU:HD22	3:C:217:ILE:CG2	2.44	0.47
3:C:215:VAL:O	3:C:223:GLN:HB2	2.14	0.47
3:C:265:LEU:CD1	3:C:287:LEU:HD12	2.44	0.47
3:C:477:ILE:HD11	4:D:852:THR:HG21	1.95	0.47
3:C:1048:LEU:H	3:C:1048:LEU:CD2	2.17	0.47
4:D:226:PHE:CE1	4:D:248:TYR:HB3	2.48	0.47
4:D:1165:ARG:NE	4:D:1209:MET:HE1	2.29	0.47
4:D:1171:SER:O	4:D:1202:ALA:HB2	2.14	0.47
2:A:55:ARG:HH12	2:A:161:ARG:CZ	2.26	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:52:THR:O	2:B:164:VAL:HG22	2.13	0.47
2:B:198:THR:HG21	2:B:202:ILE:O	2.14	0.47
3:C:178:PHE:CD1	3:C:193:VAL:HB	2.49	0.47
3:C:372:VAL:O	3:C:376:ILE:HG12	2.14	0.47
3:C:589:GLU:OE1	3:C:589:GLU:N	2.37	0.47
3:C:731:ARG:NH1	3:C:735:GLU:OE1	2.47	0.47
3:C:752:ASP:OD1	3:C:857:ASN:ND2	2.45	0.47
6:F:310:MET:O	6:F:313:VAL:HG13	2.14	0.47
2:A:40:ARG:HH21	2:B:32:TYR:HD2	1.62	0.47
2:A:197:GLU:CD	3:C:987:ARG:HH22	2.20	0.47
3:C:523:THR:HG23	3:C:526:GLU:HG2	1.96	0.47
3:C:649:ILE:HG21	3:C:693:ILE:CG2	2.44	0.47
5:E:81:GLU:O	5:E:94:ARG:NH2	2.47	0.47
7:O:6:DA:H1'	7:O:7:DC:C5'	2.44	0.47
2:A:42:LEU:HD23	2:A:211:ALA:HB2	1.96	0.47
2:A:147:VAL:HG13	2:A:147:VAL:O	2.14	0.47
3:C:716:PRO:O	4:D:724:THR:HB	2.14	0.47
3:C:788:ARG:O	3:C:830:VAL:HG11	2.14	0.47
4:D:246:ASP:OD1	4:D:246:ASP:N	2.46	0.47
4:D:1119:PRO:HA	4:D:1122:VAL:HG12	1.95	0.47
8:P:11:DA:H2'	8:P:12:DA:C8	2.48	0.47
2:A:9:LEU:HB2	2:A:23:ILE:HG12	1.96	0.47
2:A:31:GLY:CA	2:A:192:LEU:HD23	2.32	0.47
2:B:18:ARG:HG3	2:B:197:GLU:CG	2.41	0.47
2:B:213:GLY:CA	2:B:216:VAL:HG12	2.43	0.47
3:C:87:ILE:O	3:C:95:SER:HA	2.13	0.47
3:C:203:LEU:HD22	3:C:217:ILE:HA	1.96	0.47
3:C:602:MET:HE2	3:C:1024:LEU:HD21	1.95	0.47
4:D:602:ALA:CB	4:D:607:PRO:O	2.62	0.47
6:F:279:TYR:CE1	7:O:28:DT:H5''	2.49	0.47
2:A:78:LEU:HD12	3:C:611:ARG:HH11	1.79	0.47
2:B:63:PHE:N	2:B:63:PHE:CD1	2.81	0.47
3:C:560:GLU:HG3	3:C:562:VAL:HG23	1.97	0.47
4:D:66:LYS:HG2	4:D:66:LYS:O	2.13	0.47
4:D:869:SER:HB2	4:D:1029:LEU:HD21	1.97	0.47
4:D:948:ILE:O	4:D:952:LEU:HB2	2.14	0.47
5:E:57:ARG:O	5:E:57:ARG:HD3	2.14	0.47
2:A:78:LEU:O	2:A:81:LYS:HB2	2.15	0.47
3:C:124:LEU:HD23	3:C:125:PHE:H	1.80	0.47
3:C:128:ALA:CB	3:C:405:PRO:HB3	2.45	0.47
3:C:130:PHE:CZ	3:C:403:ILE:HG13	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:269:TYR:CD2	3:C:278:PRO:HB3	2.50	0.47
3:C:498:ASN:HB2	3:C:502:PHE:O	2.15	0.47
3:C:549:ARG:HB2	3:C:561:PHE:CZ	2.50	0.47
3:C:586:PRO:O	3:C:880:HIS:HE1	1.98	0.47
3:C:614:ALA:HA	3:C:705:ALA:HB2	1.97	0.47
3:C:882:ASN:ND2	3:C:1019:MET:HE1	2.29	0.47
4:D:320:ILE:HG12	4:D:321:PRO:CD	2.45	0.47
4:D:846:LEU:HD12	4:D:846:LEU:N	2.29	0.47
7:O:2:DC:H2''	7:O:3:DT:O5'	2.15	0.47
2:B:214:THR:O	2:B:218:LEU:HB2	2.13	0.47
3:C:794:VAL:HG11	3:C:860:VAL:HG11	1.96	0.47
3:C:896:PRO:HB2	3:C:1001:LEU:HD13	1.97	0.47
1:J:88:ARG:HG3	1:J:89:ARG:N	2.30	0.47
2:A:107:ALA:HB3	2:A:121:PRO:HA	1.96	0.47
2:A:161:ARG:O	2:A:163:PRO:HD3	2.15	0.47
2:A:219:PHE:CE1	2:B:38:LEU:HD21	2.50	0.47
3:C:516:THR:CG2	3:C:518:GLN:HB2	2.45	0.47
3:C:728:LEU:HD23	3:C:906:ILE:HG22	1.97	0.47
8:P:17:DT:H5''	2:T:290:GLY:N	2.30	0.47
2:T:264:LEU:HB3	2:T:269:VAL:HG21	1.93	0.47
2:B:69:VAL:HG23	2:B:71:GLU:O	2.14	0.47
2:B:153:LYS:N	2:B:154:ALA:CA	2.72	0.47
3:C:368:ARG:HA	3:C:369:LEU:HB3	1.97	0.47
3:C:460:GLY:HA3	3:C:462:GLU:OE1	2.15	0.47
3:C:587:PHE:HB3	3:C:590:HIS:HD2	1.80	0.47
3:C:664:ARG:HB2	3:C:677:GLN:OE1	2.15	0.47
3:C:792:ILE:HD12	3:C:792:ILE:N	2.28	0.47
3:C:1093:VAL:HG13	3:C:1094:TYR:N	2.30	0.47
4:D:287:GLN:HG3	4:D:288:LYS:HZ2	1.80	0.47
4:D:590:THR:CG2	4:D:630:ARG:HE	2.28	0.47
3:C:475:CYS:HA	3:C:577:MET:O	2.15	0.46
3:C:1103:ILE:HD12	4:D:548:SER:CA	2.45	0.46
3:C:1103:ILE:CD1	4:D:547:LEU:HB3	2.44	0.46
4:D:129:ILE:HD11	4:D:130:TYR:CE2	2.49	0.46
4:D:656:LYS:O	4:D:656:LYS:CE	2.63	0.46
4:D:788:LEU:C	4:D:788:LEU:HD23	2.40	0.46
4:D:1056:LEU:HD23	4:D:1057:GLU:H	1.79	0.46
6:F:320:ILE:HG22	6:F:337:LEU:HD12	1.97	0.46
1:J:40:PHE:HZ	1:J:58:ASN:HB2	1.80	0.46
2:B:66:VAL:HG12	2:B:69:VAL:HG22	1.97	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)
3:C:1031:LYS:NZ	10:C:1203:SO4:S	2.88	0.46
4:D:889:ASP:OD2	4:D:962:ARG:NH2	2.48	0.46
6:F:414:ARG:HG2	6:F:419:LEU:HD12	1.98	0.46
2:T:257:THR:OG1	2:T:260:SER:OG	2.33	0.46
2:A:56:ILE:HG12	2:A:136:VAL:HB	1.98	0.46
3:C:29:ARG:HD3	3:C:964:ALA:HB2	1.97	0.46
3:C:475:CYS:HB2	3:C:579:SER:HB3	1.96	0.46
3:C:477:ILE:O	3:C:477:ILE:HG22	2.16	0.46
3:C:643:GLU:OE2	14:C:1310:HOH:O	2.21	0.46
3:C:875:LYS:C	3:C:876:LEU:HD12	2.39	0.46
3:C:1003:ASP:HB2	3:C:1010:PHE:CE1	2.50	0.46
3:C:1130:SER:HB3	3:C:1132:ASP:C	2.41	0.46
4:D:738:PRO:HA	4:D:791:PHE:HD2	1.80	0.46
2:A:108:GLY:CA	2:A:121:PRO:HB3	2.46	0.46
2:B:94:THR:HA	2:B:138:LEU:O	2.16	0.46
3:C:52:PHE:CZ	3:C:150:MET:HE2	2.49	0.46
3:C:913:VAL:HB	3:C:914:PRO:HD3	1.96	0.46
5:E:80:VAL:CG1	5:E:94:ARG:HH21	2.29	0.46
6:F:316:LYS:HD3	6:F:341:MET:HE3	1.96	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:A:175:THR:OG1	3:C:899:PRO:O	2.27	0.46
4:D:58:TRP:HH2	4:D:84:ARG:NH2	2.14	0.46
4:D:285:LYS:HA	4:D:289:LYS:HB2	1.96	0.46
4:D:397:ARG:HG3	4:D:397:ARG:O	2.15	0.46
4:D:720:PHE:O	4:D:724:THR:HG23	2.15	0.46
2:T:286:ILE:HG22	2:T:289:PHE:CB	2.45	0.46
3:C:71:GLU:OE2	3:C:71:GLU:HA	2.16	0.46
3:C:400:VAL:C	3:C:402:ALA:H	2.23	0.46
4:D:400:LYS:CE	4:D:404:ASP:HB3	2.44	0.46
4:D:517:VAL:HG12	4:D:518:GLU:O	2.15	0.46
4:D:765:ASN:ND2	4:D:767:THR:HG23	2.30	0.46
4:D:1152:ASP:O	4:D:1156:GLU:HG3	2.16	0.46
6:F:170:LEU:HA	6:F:173:ILE:HG12	1.97	0.46
8:P:4:DA:H2"	8:P:5:DC:C6	2.51	0.46
2:B:152:ASN:O	2:B:153:LYS:CB	2.64	0.46
2:B:196:VAL:HG13	2:B:196:VAL:O	2.16	0.46
2:B:230:GLU:OE1	2:B:230:GLU:HA	2.16	0.46
3:C:80:VAL:CG2	3:C:377:GLN:HG3	2.45	0.46
3:C:615:PRO:HB3	3:C:1020:TYR:CE2	2.50	0.46
3:C:780:ILE:HD12	3:C:781:VAL:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:850:ASP:HB3	3:C:851:GLU:H	1.55	0.46
3:C:1066:ALA:HB1	4:D:506:ARG:HA	1.96	0.46
4:D:129:ILE:HG12	4:D:130:TYR:CD2	2.51	0.46
4:D:676:LEU:HD12	4:D:676:LEU:H	1.79	0.46
4:D:991:GLY:HA2	4:D:1265:ILE:HD12	1.98	0.46
4:D:1034:GLU:O	14:D:2107:HOH:O	2.20	0.46
1:J:73:LYS:O	1:J:74:LYS:HG3	2.16	0.46
2:A:63:PHE:O	3:C:666:PHE:CD2	2.69	0.46
2:B:28:PRO:HA	2:B:190:ASP:OD2	2.16	0.46
2:B:63:PHE:N	2:B:63:PHE:HD1	2.13	0.46
2:B:80:LEU:HG	2:B:125:ILE:HD13	1.97	0.46
2:B:182:ARG:C	2:B:184:GLU:H	2.22	0.46
3:C:38:PRO:CB	3:C:508:ARG:HH21	2.28	0.46
3:C:427:LEU:HD12	3:C:427:LEU:N	2.31	0.46
3:C:767:VAL:HB	3:C:771:VAL:HG21	1.97	0.46
3:C:984:LEU:CD1	3:C:989:GLY:HA2	2.46	0.46
3:C:1032:ILE:HG21	4:D:520:LYS:HD3	1.98	0.46
3:C:1033:HIS:HB3	11:C:1205:EDO:O1	2.15	0.46
3:C:1084:SER:OG	4:D:420:LYS:HD3	2.16	0.46
4:D:125:LEU:O	4:D:129:ILE:HG23	2.16	0.46
4:D:823:VAL:HG12	4:D:824:THR:N	2.30	0.46
4:D:924:LEU:HD22	4:D:959:VAL:HG11	1.95	0.46
5:E:80:VAL:HG12	5:E:94:ARG:HH21	1.81	0.46
6:F:201:LEU:HD11	6:F:219:MET:CB	2.40	0.46
6:F:251:ARG:CB	6:F:297:MET:HE1	2.44	0.46
3:C:193:VAL:HG22	3:C:194:LYS:N	2.31	0.46
3:C:766:ASN:HB3	6:F:465:LEU:HD21	1.98	0.46
3:C:848:ASP:OD1	3:C:848:ASP:N	2.49	0.46
4:D:735:VAL:CG1	4:D:840:ARG:HD2	2.40	0.46
4:D:1123:LEU:HB2	4:D:1131:VAL:HG21	1.97	0.46
5:E:37:ILE:H	5:E:37:ILE:HG13	1.26	0.46
1:J:73:LYS:O	1:J:74:LYS:CG	2.63	0.46
2:B:9:LEU:HD21	2:B:208:LEU:HD21	1.98	0.46
2:B:26:LEU:HD13	2:B:30:PHE:HB3	1.98	0.46
2:B:202:ILE:HD13	2:B:207:ALA:HB2	1.97	0.46
3:C:447:SER:HB2	3:C:449:LEU:HD11	1.98	0.46
4:D:231:PRO:O	4:D:232:LYS:HB2	2.15	0.46
4:D:931:ALA:HA	4:D:932:ASN:HA	1.63	0.46
6:F:176:VAL:CG1	6:F:177:ALA:N	2.78	0.46
6:F:440:ARG:O	6:F:444:ILE:HG13	2.16	0.46
2:B:105:VAL:HG23	2:B:128:LEU:HD11	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:150:VAL:HG13	2:B:150:VAL:O	2.16	0.45
3:C:96:LEU:HD22	3:C:98:PHE:HE1	1.79	0.45
3:C:577:MET:CE	4:D:849:PHE:HD1	2.29	0.45
3:C:601:ASN:O	3:C:604:ARG:HG2	2.16	0.45
3:C:632:VAL:CG1	3:C:692:VAL:HG13	2.46	0.45
3:C:727:ILE:HA	3:C:888:LYS:O	2.16	0.45
4:D:67:ARG:HH12	6:F:423:GLN:HA	1.81	0.45
4:D:629:VAL:CG1	4:D:671:MET:HE1	2.46	0.45
2:A:137:GLU:C	2:A:138:LEU:HD12	2.41	0.45
2:B:43:LEU:HD12	2:B:43:LEU:HA	1.78	0.45
4:D:85:ALA:O	4:D:88:ARG:HB2	2.17	0.45
4:D:163:GLU:HG2	4:D:166:ARG:HH21	1.81	0.45
4:D:647:GLU:HB2	4:D:655:TRP:HZ3	1.76	0.45
4:D:1086:ARG:O	4:D:1087:LEU:HD23	2.17	0.45
2:A:48:GLY:O	2:A:142:ARG:HG2	2.15	0.45
2:A:125:ILE:N	2:A:125:ILE:HD12	2.31	0.45
2:B:28:PRO:HD3	2:B:189:PHE:CD1	2.51	0.45
3:C:361:ILE:HD12	3:C:361:ILE:N	2.25	0.45
3:C:405:PRO:O	3:C:409:ILE:HG13	2.16	0.45
3:C:638:THR:HG23	3:C:688:GLU:HA	1.97	0.45
3:C:797:VAL:HG11	3:C:823:VAL:CG2	2.46	0.45
3:C:888:LYS:HG2	3:C:890:LEU:HD13	1.99	0.45
3:C:935:TRP:HB2	3:C:982:SER:HB2	1.98	0.45
4:D:666:THR:HG23	4:D:669:ARG:HD2	1.98	0.45
4:D:1009:LEU:CD1	4:D:1146:GLN:HG3	2.44	0.45
5:E:29:PRO:CG	5:E:34:ASN:HB2	2.46	0.45
5:E:57:ARG:NH2	5:E:77:GLY:HA3	2.30	0.45
2:B:151:GLN:C	2:B:154:ALA:HB1	2.42	0.45
2:B:174:VAL:HA	2:B:195:ASP:O	2.16	0.45
3:C:767:VAL:HB	3:C:771:VAL:CG2	2.46	0.45
3:C:859:LEU:HD22	3:C:860:VAL:N	2.30	0.45
3:C:900:ASP:OD1	3:C:992:MET:SD	2.74	0.45
3:C:976:LEU:O	3:C:980:LEU:HD23	2.16	0.45
3:C:1041:SER:HB3	3:C:1044:THR:O	2.16	0.45
4:D:952:LEU:HD12	4:D:952:LEU:HA	1.85	0.45
4:D:1032:VAL:HG23	4:D:1142:VAL:HG11	1.99	0.45
2:T:257:THR:O	2:T:260:SER:N	2.50	0.45
2:A:193:ILE:HD12	2:A:193:ILE:C	2.40	0.45
2:B:76:ILE:HG23	2:B:125:ILE:HD12	1.98	0.45
2:B:181:THR:HB	2:B:182:ARG:CB	2.47	0.45
3:C:169:GLN:HB2	3:C:427:LEU:HD21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:174:PRO:HB2	3:C:303:GLY:HA3	1.99	0.45
3:C:506:PRO:O	3:C:572:VAL:HG13	2.15	0.45
3:C:741:ILE:HG22	3:C:742:HIS:N	2.31	0.45
4:D:365:ILE:H	4:D:365:ILE:CD1	2.07	0.45
4:D:1106:VAL:HG13	4:D:1110:ASP:HB2	1.98	0.45
3:C:797:VAL:HG11	3:C:823:VAL:HG21	1.98	0.45
3:C:1037:THR:HG22	3:C:1038:GLY:N	2.32	0.45
4:D:633:ILE:O	4:D:665:THR:O	2.35	0.45
4:D:929:VAL:HG23	4:D:929:VAL:O	2.16	0.45
7:O:1:DG:C4'	7:O:1:DG:O5'	2.65	0.45
1:J:104:LEU:HD23	1:J:104:LEU:O	2.17	0.45
2:B:65:THR:N	2:B:73:VAL:HG23	2.31	0.45
2:B:99:LYS:HE2	2:B:99:LYS:HB3	1.64	0.45
3:C:747:GLU:HG3	3:C:859:LEU:HD21	1.98	0.45
4:D:376:GLU:OE2	6:F:165:SER:OG	2.26	0.45
6:F:253:MET:HE1	6:F:296:ALA:C	2.42	0.45
7:O:12:DG:H2'	7:O:13:DT:H71	1.98	0.45
2:B:192:LEU:C	2:B:193:ILE:HD13	2.41	0.45
3:C:1035:ARG:CZ	3:C:1047:PRO:HB3	2.46	0.45
4:D:285:LYS:HG3	4:D:289:LYS:CD	2.46	0.45
4:D:577:PRO:HB3	4:D:581:MET:HE2	1.99	0.45
4:D:591:LEU:HD23	4:D:630:ARG:O	2.17	0.45
4:D:693:ALA:O	4:D:697:ASN:HB2	2.17	0.45
4:D:1122:VAL:HG23	4:D:1126:GLN:HE21	1.80	0.45
2:A:10:SER:OG	2:A:22:VAL:HG13	2.17	0.45
3:C:154:LYS:O	3:C:443:LYS:HE3	2.17	0.45
4:D:102:THR:OG1	4:D:129:ILE:HD12	2.16	0.45
4:D:814:ARG:O	4:D:817:ALA:O	2.35	0.45
4:D:920:PHE:CZ	4:D:948:ILE:HG13	2.52	0.45
4:D:1191:ASN:OD1	4:D:1202:ALA:HB3	2.16	0.45
6:F:321:GLN:NE2	6:F:331:GLU:OE2	2.50	0.45
2:B:147:VAL:CG1	2:B:166:SER:HB2	2.47	0.45
3:C:154:LYS:HE2	3:C:630:GLY:O	2.17	0.45
3:C:203:LEU:HD22	3:C:217:ILE:HB	1.99	0.45
3:C:597:LEU:HD23	3:C:597:LEU:C	2.42	0.45
4:D:113:ARG:HB2	4:D:312:MET:HE1	1.98	0.45
4:D:269:ASP:OD2	4:D:272:ALA:N	2.50	0.45
4:D:956:ILE:CD1	4:D:956:ILE:O	2.65	0.45
4:D:1220:SER:HB3	4:D:1223:SER:HB3	1.99	0.45
7:O:2:DC:H2''	7:O:3:DT:C5'	2.47	0.45
3:C:103:PHE:CE2	3:C:124:LEU:HG	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:291:PHE:HA	3:C:297:TYR:HB2	1.98	0.44
3:C:390:VAL:HG11	3:C:394:ARG:HH21	1.83	0.44
3:C:723:GLU:HA	3:C:723:GLU:OE1	2.18	0.44
4:D:103:HIS:HB3	4:D:106:TYR:HD2	1.81	0.44
4:D:138:SER:HB3	4:D:253:THR:HG1	1.79	0.44
2:B:22:VAL:HG12	2:B:193:ILE:HG23	1.98	0.44
3:C:53:GLU:OE2	3:C:60:ARG:NH1	2.37	0.44
3:C:62:ARG:HG3	3:C:66:ILE:HD11	1.99	0.44
3:C:1126:VAL:HG23	3:C:1126:VAL:O	2.17	0.44
4:D:622:MET:CE	4:D:667:LEU:HD13	2.32	0.44
4:D:791:PHE:O	4:D:791:PHE:HD1	2.01	0.44
4:D:1110:ASP:N	4:D:1110:ASP:OD1	2.50	0.44
4:D:1129:ARG:O	4:D:1133:ILE:HG12	2.17	0.44
2:B:176:TYR:H	2:B:176:TYR:HD1	1.65	0.44
3:C:62:ARG:HG3	3:C:66:ILE:CD1	2.47	0.44
3:C:659:GLN:OE1	3:C:659:GLN:N	2.50	0.44
3:C:680:ILE:HD11	3:C:692:VAL:HG12	1.99	0.44
3:C:1011:PRO:HB2	3:C:1012:TYR:CD2	2.53	0.44
3:C:1043:ILE:HD12	3:C:1043:ILE:H	1.82	0.44
4:D:656:LYS:O	4:D:656:LYS:HE2	2.17	0.44
4:D:911:ARG:HG2	4:D:952:LEU:HD21	2.00	0.44
4:D:929:VAL:HG22	14:D:2112:HOH:O	2.16	0.44
5:E:53:TYR:CE1	5:E:101:LEU:HD12	2.53	0.44
6:F:462:ARG:HA	6:F:462:ARG:HD3	1.79	0.44
3:C:197:PRO:HB3	3:C:297:TYR:OH	2.16	0.44
3:C:445:ARG:C	3:C:446:LEU:HD23	2.42	0.44
3:C:627:ILE:HD12	3:C:628:ASP:N	2.33	0.44
4:D:467:GLN:NE2	4:D:467:GLN:HA	2.32	0.44
4:D:686:GLN:O	4:D:686:GLN:HG3	2.18	0.44
3:C:43:GLY:O	3:C:46:ASP:HB2	2.17	0.44
3:C:538:PRO:C	3:C:546:THR:OG1	2.61	0.44
3:C:1022:LEU:HD23	3:C:1022:LEU:N	2.32	0.44
3:C:1090:ARG:O	3:C:1093:VAL:HG12	2.18	0.44
4:D:525:HIS:O	4:D:528:VAL:HG22	2.17	0.44
4:D:599:TYR:CA	4:D:610:GLY:HA3	2.47	0.44
4:D:640:LEU:O	4:D:656:LYS:HE3	2.17	0.44
4:D:687:MET:CE	4:D:695:ILE:HD11	2.48	0.44
4:D:1190:GLU:O	4:D:1190:GLU:HG3	2.16	0.44
2:T:286:ILE:CG2	2:T:289:PHE:HB2	2.47	0.44
2:A:40:ARG:CZ	2:B:33:THR:HG22	2.47	0.44
2:A:44:SER:HB3	3:C:893:GLU:OE1	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:64:THR:O	2:A:73:VAL:HG23	2.18	0.44
3:C:197:PRO:HB3	3:C:297:TYR:CZ	2.53	0.44
3:C:369:LEU:HD12	3:C:369:LEU:HA	1.56	0.44
3:C:1003:ASP:OD1	3:C:1005:ARG:HB3	2.17	0.44
4:D:47:PHE:CD1	4:D:322:PRO:HB3	2.52	0.44
4:D:102:THR:HG23	4:D:258:ALA:CB	2.48	0.44
4:D:579:LEU:HD23	4:D:807:THR:HB	1.99	0.44
3:C:31:SER:O	3:C:954:LEU:HD11	2.18	0.44
3:C:370:ARG:HG2	3:C:374:GLU:CD	2.43	0.44
3:C:895:MET:HE2	3:C:895:MET:HB2	1.62	0.44
4:D:91:ARG:O	4:D:321:PRO:HG3	2.18	0.44
4:D:1140:GLN:NE2	4:D:1155:ILE:HD12	2.33	0.44
5:E:76:VAL:CG1	5:E:77:GLY:N	2.81	0.44
8:P:11:DA:H2'	8:P:12:DA:H8	1.83	0.44
1:J:57:ARG:HG3	4:D:25:TYR:HA	2.00	0.44
2:B:170:PRO:CB	2:B:202:ILE:HD11	2.42	0.44
3:C:478:GLU:OE1	3:C:579:SER:OG	2.25	0.44
3:C:1049:GLY:HA3	4:D:421:ARG:CZ	2.48	0.44
4:D:740:GLN:H	4:D:740:GLN:NE2	2.01	0.44
4:D:878:ASP:OD1	14:D:2108:HOH:O	2.21	0.44
4:D:1034:GLU:OE2	4:D:1041:PRO:HA	2.17	0.44
8:P:4:DA:H2''	8:P:5:DC:H6	1.82	0.44
2:A:187:THR:O	2:A:187:THR:HG23	2.18	0.44
3:C:77:LEU:HD23	3:C:77:LEU:HA	1.76	0.44
3:C:167:VAL:HG13	3:C:445:ARG:O	2.18	0.44
3:C:1138:MET:C	3:C:1139:ARG:HG3	2.43	0.44
4:D:781:THR:CG2	4:D:814:ARG:HD2	2.47	0.44
4:D:1171:SER:O	4:D:1174:THR:HG22	2.18	0.44
4:D:1174:THR:OG1	4:D:1175:GLU:CB	2.66	0.44
6:F:406:SER:HB3	6:F:409:GLU:HG3	2.00	0.44
6:F:465:LEU:HD23	6:F:466:ASP:HB2	2.00	0.44
2:A:175:THR:HG22	2:A:195:ASP:HB3	2.00	0.43
3:C:70:GLU:N	3:C:70:GLU:OE1	2.51	0.43
3:C:89:ASP:OD1	3:C:89:ASP:N	2.51	0.43
3:C:346:MET:HB2	3:C:356:VAL:CG2	2.48	0.43
3:C:523:THR:HG22	3:C:526:GLU:OE2	2.18	0.43
3:C:1118:GLU:OE1	4:D:412:ARG:HG3	2.19	0.43
4:D:475:MET:HE3	4:D:475:MET:HB2	1.80	0.43
4:D:1162:MET:HE2	4:D:1211:ILE:HG23	2.00	0.43
6:F:373:LEU:C	6:F:373:LEU:CD2	2.91	0.43
6:F:394:LEU:HB2	6:F:464:TYR:CE1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:58:ASN:HD21	1:J:60:LEU:CG	2.31	0.43
2:A:78:LEU:CD1	3:C:611:ARG:HH11	2.31	0.43
3:C:174:PRO:O	3:C:303:GLY:HA2	2.18	0.43
3:C:365:GLY:HA3	3:C:525:ASP:OD1	2.18	0.43
3:C:873:GLY:HA3	3:C:1028:VAL:CG1	2.47	0.43
3:C:1074:TYR:CZ	4:D:1258:LEU:HD21	2.53	0.43
4:D:555:ALA:HA	4:D:559:MET:HE3	1.99	0.43
4:D:739:PRO:HD3	4:D:791:PHE:CE2	2.53	0.43
4:D:1041:PRO:HB3	4:D:1116:ALA:CB	2.48	0.43
4:D:1056:LEU:HD23	4:D:1057:GLU:N	2.33	0.43
6:F:359:ILE:HG22	6:F:360:SER:N	2.32	0.43
2:A:48:GLY:HA3	2:A:168:TYR:HB3	2.01	0.43
3:C:215:VAL:CG2	3:C:225:VAL:HA	2.30	0.43
3:C:221:ARG:O	3:C:223:GLN:NE2	2.34	0.43
3:C:291:PHE:O	3:C:297:TYR:HB3	2.18	0.43
3:C:494:TYR:CD2	3:C:572:VAL:HG21	2.46	0.43
3:C:529:ARG:CZ	3:C:529:ARG:HB3	2.48	0.43
3:C:809:GLU:O	3:C:813:ARG:HG2	2.18	0.43
4:D:277:LEU:HD21	4:D:292:ALA:O	2.18	0.43
4:D:536:PHE:C	4:D:538:GLY:H	2.25	0.43
4:D:1081:LEU:HB3	4:D:1113:MET:SD	2.58	0.43
6:F:171:LYS:HB3	6:F:171:LYS:HE2	1.77	0.43
6:F:173:ILE:HG22	6:F:238:LEU:HD13	2.00	0.43
6:F:263:ASN:O	6:F:267:ILE:HG13	2.18	0.43
3:C:45:LEU:CD2	3:C:443:LYS:HD2	2.48	0.43
3:C:562:VAL:HG12	3:C:563:SER:N	2.33	0.43
3:C:706:LEU:N	14:C:1311:HOH:O	2.23	0.43
3:C:710:LEU:HD23	3:C:732:LEU:HD11	2.01	0.43
3:C:751:ARG:CD	3:C:856:VAL:HG22	2.48	0.43
4:D:67:ARG:NH1	6:F:423:GLN:HA	2.33	0.43
4:D:133:ALA:C	4:D:256:MET:HE3	2.44	0.43
4:D:281:ILE:HD12	4:D:281:ILE:C	2.43	0.43
4:D:493:GLU:HA	4:D:513:GLU:OE1	2.18	0.43
2:A:63:PHE:HE1	3:C:741:ILE:HD13	1.83	0.43
2:A:146:TYR:OH	3:C:869:LYS:NZ	2.52	0.43
2:B:147:VAL:HG13	2:B:147:VAL:O	2.19	0.43
3:C:510:VAL:HG12	3:C:568:ASP:O	2.19	0.43
3:C:729:SER:HA	3:C:895:MET:HE1	2.00	0.43
3:C:1103:ILE:HD13	4:D:547:LEU:HB3	2.00	0.43
4:D:452:PHE:CE1	4:D:491:ILE:HG12	2.53	0.43
4:D:740:GLN:O	4:D:744:ILE:HG13	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:859:LEU:HD12	4:D:862:THR:HG21	2.01	0.43
2:T:254:LEU:HB2	2:T:256:LEU:HG	2.01	0.43
1:J:69:VAL:N	1:J:70:PRO:HD3	2.34	0.43
2:A:18:ARG:HA	2:A:204:PRO:CG	2.49	0.43
2:A:219:PHE:HE1	2:B:38:LEU:HD21	1.81	0.43
2:B:28:PRO:HA	2:B:29:GLY:HA2	1.79	0.43
3:C:619:THR:OG1	3:C:620:GLY:N	2.50	0.43
4:D:177:LEU:HD23	4:D:177:LEU:C	2.43	0.43
4:D:788:LEU:HD21	4:D:792:TYR:CE2	2.53	0.43
4:D:863:ALA:O	4:D:866:THR:HG22	2.18	0.43
4:D:900:LEU:HD11	4:D:948:ILE:HD12	2.01	0.43
4:D:1036:PHE:O	4:D:1211:ILE:HG23	2.18	0.43
1:J:48:ALA:HB2	4:D:65:TYR:OH	2.18	0.43
1:J:85:LEU:HD21	6:F:192:GLU:HB3	2.01	0.43
2:A:11:GLU:OE2	2:B:225:LEU:HD22	2.18	0.43
2:A:214:THR:HG23	2:B:231:HIS:CG	2.54	0.43
3:C:228:LEU:HD23	3:C:228:LEU:HA	1.70	0.43
3:C:623:LEU:HD12	3:C:703:GLU:OE1	2.19	0.43
3:C:984:LEU:HD13	3:C:989:GLY:HA2	2.00	0.43
4:D:910:ILE:O	4:D:910:ILE:HG12	2.19	0.43
6:F:394:LEU:HD13	6:F:464:TYR:CG	2.54	0.43
3:C:591:ASP:OD2	3:C:880:HIS:ND1	2.41	0.43
4:D:633:ILE:HD13	4:D:635:VAL:HG13	2.00	0.43
4:D:796:ASN:ND2	4:D:798:ILE:HB	2.28	0.43
4:D:799:ILE:HD13	4:D:799:ILE:HA	1.73	0.43
7:O:6:DA:H2"	7:O:7:DC:OP2	2.17	0.43
2:A:93:VAL:CG2	2:A:113:PRO:HG3	2.48	0.43
2:B:111:VAL:O	2:B:111:VAL:HG13	2.18	0.43
3:C:178:PHE:CE1	3:C:193:VAL:HG21	2.54	0.43
3:C:394:ARG:HG3	3:C:398:GLN:CG	2.48	0.43
3:C:404:THR:HG23	3:C:407:THR:HG23	1.99	0.43
4:D:110:VAL:O	4:D:110:VAL:HG13	2.19	0.43
4:D:590:THR:HG23	4:D:630:ARG:HE	1.84	0.43
4:D:676:LEU:N	4:D:676:LEU:CD1	2.81	0.43
4:D:813:THR:O	4:D:813:THR:HG22	2.18	0.43
4:D:1258:LEU:HD12	4:D:1258:LEU:HA	1.90	0.43
1:J:28:GLN:N	1:J:44:PHE:O	2.50	0.43
2:A:34:LEU:HD23	2:A:34:LEU:HA	1.77	0.43
2:A:98:ARG:O	2:A:99:LYS:HD2	2.18	0.43
2:B:34:LEU:CD1	2:B:192:LEU:HD22	2.37	0.43
2:B:191:LYS:HG2	2:B:193:ILE:HD11	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:239:ILE:HG22	3:C:253:LEU:HD22	1.99	0.43
3:C:265:LEU:HD21	3:C:284:GLN:HA	2.01	0.43
3:C:1025:HIS:CD2	3:C:1025:HIS:O	2.72	0.43
4:D:23:TRP:HB3	4:D:92:MET:HE3	2.01	0.43
4:D:51:ILE:H	4:D:51:ILE:HG12	1.64	0.43
4:D:612:TYR:OH	4:D:627:LEU:HG	2.19	0.43
4:D:1272:GLN:OE1	4:D:1272:GLN:HA	2.19	0.43
6:F:320:ILE:O	6:F:324:LEU:HB2	2.18	0.43
6:F:373:LEU:O	6:F:373:LEU:HD23	2.18	0.43
2:B:226:ASN:O	2:B:227:ALA:HB3	2.19	0.42
3:C:51:SER:HB2	3:C:371:THR:OG1	2.19	0.42
3:C:94:MET:HE3	3:C:395:MET:HB3	2.01	0.42
3:C:454:LEU:HD12	3:C:454:LEU:O	2.19	0.42
3:C:1105:GLU:HG3	3:C:1106:PRO:HD2	2.00	0.42
4:D:58:TRP:HA	4:D:82:VAL:HG23	2.01	0.42
4:D:735:VAL:CG1	4:D:816:LEU:HD22	2.49	0.42
4:D:1247:ASN:O	4:D:1260:PRO:HG3	2.19	0.42
4:D:1279:ALA:HB1	5:E:79:LEU:HD13	2.00	0.42
8:P:3:DC:H2"	8:P:4:DA:H8	1.82	0.42
3:C:31:SER:HA	3:C:964:ALA:O	2.19	0.42
3:C:114:LYS:HG2	3:C:161:GLY:O	2.19	0.42
3:C:344:THR:O	3:C:344:THR:HG22	2.19	0.42
3:C:698:CYS:O	3:C:705:ALA:N	2.49	0.42
3:C:781:VAL:CG2	3:C:838:VAL:HG21	2.48	0.42
4:D:237:ASP:O	4:D:238:GLU:HB3	2.18	0.42
4:D:1100:LEU:HD23	4:D:1100:LEU:C	2.44	0.42
4:D:1165:ARG:HG2	4:D:1183:GLU:HA	2.01	0.42
5:E:28:THR:HG23	5:E:28:THR:O	2.19	0.42
2:T:269:VAL:O	2:T:269:VAL:HG23	2.19	0.42
1:J:69:VAL:N	1:J:70:PRO:CD	2.83	0.42
1:J:106:LYS:HE2	1:J:106:LYS:HB3	1.77	0.42
2:A:46:ILE:HA	2:A:47:PRO:HD3	1.89	0.42
2:A:96:TYR:O	2:A:111:VAL:HG13	2.18	0.42
2:B:68:GLY:O	2:B:129:ASN:N	2.41	0.42
3:C:640:VAL:CG2	3:C:641:ILE:N	2.82	0.42
3:C:728:LEU:HD22	3:C:906:ILE:HG22	1.97	0.42
3:C:851:GLU:C	3:C:852:LEU:HD12	2.44	0.42
3:C:946:TRP:CE2	3:C:978:GLY:HA3	2.55	0.42
4:D:934:ASN:OD1	4:D:934:ASN:N	2.53	0.42
5:E:80:VAL:CG1	5:E:81:GLU:N	2.82	0.42
6:F:186:GLU:OE1	6:F:186:GLU:HA	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:306:ILE:CG2	6:F:310:MET:HB3	2.49	0.42
6:F:345:PRO:HA	6:F:348:VAL:HG13	2.00	0.42
4:D:901:ALA:HB2	4:D:912:ASP:N	2.35	0.42
4:D:1174:THR:CG2	4:D:1176:PHE:N	2.76	0.42
5:E:53:TYR:HE1	5:E:101:LEU:HD12	1.84	0.42
1:J:85:LEU:O	1:J:85:LEU:HD12	2.19	0.42
3:C:963:VAL:HG12	3:C:964:ALA:N	2.35	0.42
4:D:653:ASN:HB2	4:D:654:GLY:HA2	1.99	0.42
6:F:447:LYS:N	6:F:447:LYS:HD3	2.35	0.42
6:F:454:HIS:CD2	6:F:456:SER:OG	2.73	0.42
2:T:286:ILE:HG23	2:T:289:PHE:HB2	2.01	0.42
2:A:174:VAL:O	3:C:901:GLY:HA3	2.20	0.42
3:C:467:HIS:HD2	3:C:469:SER:OG	2.02	0.42
3:C:510:VAL:HG11	3:C:567:VAL:CB	2.50	0.42
3:C:691:GLN:HG2	3:C:692:VAL:H	1.84	0.42
3:C:919:ILE:HD12	3:C:920:GLY:H	1.84	0.42
4:D:214:ARG:NH1	14:D:2118:HOH:O	2.47	0.42
4:D:584:GLY:HA3	4:D:719:GLY:O	2.19	0.42
6:F:408:ARG:HH21	11:F:506:EDO:H22	1.85	0.42
1:J:28:GLN:CD	1:J:46:ASP:HA	2.45	0.42
2:B:97:LEU:HD23	2:B:136:VAL:CG1	2.50	0.42
2:B:104:VAL:O	2:B:104:VAL:HG13	2.20	0.42
3:C:85:SER:HA	3:C:86:PRO:HA	1.69	0.42
3:C:118:MET:HE2	3:C:118:MET:HB3	1.81	0.42
4:D:64:LYS:NZ	4:D:76:GLU:OE2	2.47	0.42
4:D:412:ARG:HA	4:D:416:ASN:HD22	1.85	0.42
4:D:735:VAL:HG11	4:D:816:LEU:CD2	2.50	0.42
4:D:1171:SER:O	4:D:1174:THR:CG2	2.67	0.42
7:O:2:DC:H2''	7:O:3:DT:H5'	2.02	0.42
2:T:256:LEU:HB3	2:T:260:SER:HB2	2.00	0.42
2:A:42:LEU:O	2:A:46:ILE:HG12	2.20	0.42
3:C:33:ALA:HB2	3:C:966:PRO:CG	2.49	0.42
3:C:595:ARG:HA	3:C:595:ARG:HD2	1.91	0.42
3:C:780:ILE:O	3:C:780:ILE:HG13	2.18	0.42
4:D:799:ILE:CG2	4:D:803:LYS:HE2	2.50	0.42
5:E:80:VAL:CG2	5:E:100:LEU:HD22	2.50	0.42
6:F:332:PRO:HA	6:F:336:GLU:OE1	2.20	0.42
6:F:349:LEU:HD12	6:F:349:LEU:HA	1.79	0.42
2:A:40:ARG:HH11	2:B:33:THR:HG22	1.81	0.42
2:B:4:SER:OG	2:B:27:GLU:OE2	2.27	0.42
3:C:180:GLU:HB3	3:C:191:HIS:CD2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:310:LYS:O	3:C:354:VAL:HG21	2.20	0.42
3:C:808:GLU:H	3:C:808:GLU:CD	2.24	0.42
4:D:448:ALA:HB1	4:D:491:ILE:HD11	2.01	0.42
4:D:831:ILE:HA	4:D:831:ILE:HD12	1.74	0.42
3:C:583:ALA:HB3	3:C:621:MET:HG3	2.00	0.42
3:C:788:ARG:O	3:C:830:VAL:CG1	2.68	0.42
4:D:83:THR:OG1	4:D:84:ARG:N	2.53	0.42
4:D:250:GLU:HG3	4:D:251:TYR:CE2	2.55	0.42
4:D:647:GLU:OE1	4:D:655:TRP:HH2	2.03	0.42
1:J:71:GLU:HG2	1:J:72:PRO:HD2	2.01	0.41
2:B:38:LEU:HA	2:B:38:LEU:HD22	1.79	0.41
2:B:134:LEU:HD23	2:B:134:LEU:C	2.45	0.41
3:C:193:VAL:CG1	3:C:205:PHE:HB2	2.50	0.41
3:C:649:ILE:CD1	3:C:693:ILE:HG22	2.50	0.41
3:C:801:GLY:HA2	3:C:802:GLU:C	2.45	0.41
3:C:973:GLU:CB	4:D:732:MET:HE3	2.50	0.41
3:C:1015:THR:OG1	4:D:731:SER:OG	2.39	0.41
4:D:130:TYR:O	4:D:372:ARG:HD3	2.20	0.41
4:D:229:LEU:HA	4:D:233:GLN:OE1	2.20	0.41
4:D:278:ARG:HH11	4:D:278:ARG:HG3	1.85	0.41
4:D:676:LEU:H	4:D:676:LEU:CD1	2.33	0.41
4:D:742:GLN:O	4:D:746:GLU:HG2	2.19	0.41
4:D:755:ILE:HD13	4:D:772:SER:OG	2.19	0.41
4:D:884:ILE:HD11	4:D:886:ARG:NE	2.35	0.41
4:D:1132:GLN:HG3	4:D:1163:LEU:CD1	2.50	0.41
1:J:89:ARG:HH21	6:F:276:THR:HG23	1.83	0.41
3:C:602:MET:HA	3:C:605:GLN:HB2	2.03	0.41
3:C:885:VAL:HG22	4:D:536:PHE:O	2.20	0.41
3:C:947:ALA:O	3:C:951:PRO:HD2	2.21	0.41
3:C:952:GLU:C	3:C:954:LEU:H	2.28	0.41
3:C:1100:GLY:CA	4:D:458:LYS:HE3	2.45	0.41
4:D:339:ASP:CG	4:D:397:ARG:HH22	2.28	0.41
4:D:581:MET:HE3	4:D:716:LYS:CB	2.50	0.41
4:D:683:VAL:N	14:D:2103:HOH:O	2.53	0.41
4:D:818:GLY:C	4:D:838:SER:HB3	2.45	0.41
4:D:860:ALA:O	4:D:863:ALA:HB3	2.20	0.41
4:D:901:ALA:O	4:D:902:GLU:CB	2.68	0.41
4:D:1181:LEU:CD1	4:D:1213:LYS:HE2	2.50	0.41
6:F:465:LEU:O	6:F:466:ASP:HB2	2.19	0.41
1:J:58:ASN:HD21	1:J:60:LEU:HG	1.84	0.41
2:A:212:GLY:O	2:A:216:VAL:N	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:165:VAL:HG23	3:C:431:MET:HB2	2.02	0.41
3:C:361:ILE:H	3:C:361:ILE:CD1	2.30	0.41
3:C:466:VAL:HG12	4:D:856:ARG:CZ	2.51	0.41
3:C:479:THR:OG1	3:C:480:PRO:CD	2.68	0.41
3:C:575:ARG:HE	3:C:967:VAL:CG2	2.28	0.41
3:C:614:ALA:HA	3:C:705:ALA:CB	2.50	0.41
3:C:1117:LYS:NZ	3:C:1120:GLN:HE22	2.18	0.41
4:D:52:PHE:O	4:D:91:ARG:HD2	2.20	0.41
4:D:224:ASN:O	4:D:228:LYS:HG3	2.19	0.41
4:D:815:THR:CG2	4:D:820:LYS:HA	2.34	0.41
2:A:147:VAL:CG1	2:A:166:SER:HB2	2.50	0.41
2:B:152:ASN:CA	2:B:154:ALA:HA	2.49	0.41
3:C:263:GLU:HA	3:C:266:LEU:HD12	2.02	0.41
3:C:400:VAL:O	3:C:401:GLU:HB3	2.20	0.41
3:C:570:MET:HG2	3:C:571:ASP:N	2.36	0.41
4:D:20:ILE:HD13	4:D:318:PRO:HD3	2.03	0.41
4:D:433:GLY:HA3	4:D:436:LEU:HD12	2.02	0.41
4:D:1168:ILE:HD13	4:D:1176:PHE:CG	2.54	0.41
6:F:179:LEU:CD1	6:F:187:LEU:HD12	2.51	0.41
6:F:337:LEU:HD12	6:F:337:LEU:HA	1.80	0.41
7:O:31:DT:C6	7:O:31:DT:H5'	2.55	0.41
2:B:151:GLN:HG2	2:B:151:GLN:O	2.19	0.41
3:C:154:LYS:NZ	3:C:664:ARG:HH12	2.18	0.41
3:C:265:LEU:HD11	3:C:287:LEU:CD1	2.45	0.41
3:C:572:VAL:HG22	3:C:576:GLN:NE2	2.35	0.41
3:C:632:VAL:HG13	3:C:694:ALA:O	2.20	0.41
3:C:783:ILE:H	3:C:783:ILE:CD1	2.06	0.41
4:D:173:ARG:NH2	4:D:201:GLY:HA2	2.35	0.41
6:F:173:ILE:HG22	6:F:238:LEU:HD12	2.01	0.41
6:F:310:MET:O	6:F:314:ILE:HG13	2.21	0.41
2:T:279:THR:CG2	2:T:282:ASP:HB2	2.44	0.41
2:T:283:LEU:HD23	2:T:283:LEU:HA	1.85	0.41
1:J:108:LYS:HE2	1:J:108:LYS:HB3	1.88	0.41
2:A:84:VAL:HG13	2:A:84:VAL:O	2.21	0.41
3:C:574:PRO:HB2	3:C:968:PHE:HB2	2.03	0.41
3:C:764:ILE:HB	3:C:767:VAL:CG2	2.50	0.41
3:C:918:ASN:O	3:C:920:GLY:N	2.54	0.41
4:D:1044:LYS:HE3	4:D:1118:ASP:HB2	2.02	0.41
2:A:62:GLU:OE2	3:C:867:LYS:HE3	2.21	0.41
2:A:207:ALA:O	2:A:210:SER:OG	2.12	0.41
3:C:523:THR:OG1	3:C:524:ALA:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:754:LYS:HD3	4:D:39:LEU:HD12	2.01	0.41
3:C:1066:ALA:CB	4:D:506:ARG:HA	2.51	0.41
5:E:84:LEU:HB2	5:E:85:GLN:NE2	2.36	0.41
6:F:344:THR:O	6:F:348:VAL:HG12	2.21	0.41
1:J:102:LEU:C	1:J:105:ILE:HG22	2.45	0.41
2:A:147:VAL:CG1	2:A:168:TYR:HE2	2.33	0.41
2:B:71:GLU:OE2	2:B:127:THR:HG23	2.20	0.41
2:B:89:ASP:O	2:B:90:ASP:HB2	2.20	0.41
3:C:590:HIS:O	3:C:919:ILE:CD1	2.68	0.41
3:C:758:GLU:CG	3:C:798:THR:HG22	2.38	0.41
4:D:31:PRO:HB3	4:D:348:ILE:HG23	2.03	0.41
4:D:245:GLN:O	4:D:249:GLY:HA3	2.21	0.41
4:D:277:LEU:HD23	4:D:277:LEU:O	2.21	0.41
4:D:629:VAL:HG13	4:D:671:MET:HE1	2.02	0.41
4:D:1171:SER:HA	4:D:1174:THR:CG2	2.48	0.41
6:F:176:VAL:HG21	6:F:235:GLU:HB3	2.02	0.41
1:J:58:ASN:HD21	1:J:60:LEU:CD1	2.32	0.41
2:A:12:GLU:HB2	2:A:20:ARG:O	2.20	0.41
2:A:106:THR:HB	2:A:123:MET:O	2.21	0.41
2:B:30:PHE:CA	2:B:33:THR:HG23	2.47	0.41
2:B:125:ILE:HG23	2:B:126:ALA:H	1.85	0.41
3:C:41:VAL:HG22	3:C:494:TYR:HE1	1.86	0.41
3:C:169:GLN:HB2	3:C:427:LEU:CD2	2.51	0.41
3:C:228:LEU:O	3:C:231:ALA:N	2.54	0.41
3:C:270:ARG:O	3:C:274:PRO:HG3	2.20	0.41
3:C:387:MET:HE2	3:C:387:MET:HB3	1.95	0.41
3:C:393:GLU:CD	6:F:247:ARG:HD3	2.46	0.41
3:C:447:SER:HB3	3:C:488:ILE:HG12	2.02	0.41
3:C:610:VAL:HG23	3:C:611:ARG:N	2.36	0.41
3:C:1048:LEU:N	3:C:1048:LEU:CD2	2.81	0.41
4:D:52:PHE:CD2	4:D:322:PRO:HD3	2.55	0.41
4:D:155:MET:HE1	4:D:219:LEU:CB	2.51	0.41
4:D:365:ILE:HD11	6:F:235:GLU:OE2	2.21	0.41
4:D:507:LEU:HD12	4:D:507:LEU:HA	1.84	0.41
4:D:640:LEU:O	4:D:656:LYS:CE	2.69	0.41
4:D:1069:PRO:HB2	4:D:1071:ASP:OD1	2.21	0.41
5:E:29:PRO:CB	5:E:33:THR:HG23	2.50	0.41
5:E:86:GLU:OE1	5:E:91:ILE:HG12	2.20	0.41
6:F:244:LEU:HD12	6:F:289:ILE:HG21	2.03	0.41
6:F:452:LEU:HD12	6:F:452:LEU:HA	1.86	0.41
2:A:40:ARG:NH2	2:B:32:TYR:HD2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:40:ARG:CD	2:B:33:THR:HG22	2.43	0.41
2:B:139:VAL:CG2	2:B:161:ARG:HH21	2.35	0.41
3:C:556:GLY:N	3:C:557:GLY:CA	2.83	0.41
4:D:26:GLY:HA3	4:D:51:ILE:HG21	1.98	0.41
4:D:34:ILE:O	6:F:304:ILE:HG23	2.21	0.41
4:D:271:ASP:HA	4:D:303:GLN:NE2	2.36	0.41
4:D:826:PRO:HD3	4:D:853:HIS:CE1	2.54	0.41
4:D:938:GLU:OE1	4:D:938:GLU:N	2.36	0.41
2:A:146:TYR:CE2	3:C:734:GLU:HA	2.57	0.40
2:A:216:VAL:HG13	2:B:216:VAL:HG23	2.02	0.40
3:C:34:LYS:C	3:C:35:LEU:HD12	2.45	0.40
3:C:166:VAL:CG1	3:C:372:VAL:HG23	2.49	0.40
3:C:538:PRO:O	3:C:546:THR:OG1	2.38	0.40
3:C:1001:LEU:HB2	3:C:1010:PHE:HD2	1.86	0.40
4:D:117:LEU:O	4:D:117:LEU:HD22	2.19	0.40
4:D:157:VAL:HG12	14:D:2114:HOH:O	2.22	0.40
4:D:899:THR:O	4:D:957:THR:O	2.39	0.40
4:D:1004:GLU:HB3	4:D:1005:PRO:HD3	2.04	0.40
4:D:1208:LEU:HD23	4:D:1208:LEU:HA	1.87	0.40
2:T:279:THR:O	2:T:282:ASP:N	2.50	0.40
2:B:161:ARG:HD3	2:B:161:ARG:HA	1.53	0.40
3:C:132:ASN:O	3:C:136:GLY:N	2.52	0.40
3:C:273:ARG:N	3:C:274:PRO:HD3	2.35	0.40
3:C:614:ALA:HB2	3:C:700:GLN:HB3	2.03	0.40
3:C:709:ASN:C	3:C:710:LEU:HD12	2.46	0.40
4:D:119:ASP:O	4:D:120:LEU:HD12	2.22	0.40
4:D:228:LYS:HG3	4:D:228:LYS:H	1.75	0.40
4:D:243:GLU:HG2	4:D:247:ARG:HH21	1.85	0.40
4:D:556:ARG:O	4:D:560:LEU:HB2	2.20	0.40
4:D:566:LEU:N	4:D:566:LEU:HD23	2.37	0.40
4:D:920:PHE:HE1	4:D:945:ASP:HA	1.85	0.40
6:F:188:ALA:O	6:F:192:GLU:HG3	2.20	0.40
3:C:493:VAL:HG23	3:C:578:VAL:O	2.21	0.40
4:D:262:LYS:HG3	4:D:310:MET:CE	2.50	0.40
4:D:1004:GLU:N	4:D:1005:PRO:HD2	2.35	0.40
4:D:1090:ILE:N	4:D:1098:GLY:O	2.30	0.40
6:F:324:LEU:CD2	6:F:328:LEU:HD22	2.52	0.40
6:F:437:THR:OG1	7:O:3:DT:OP2	2.40	0.40
2:A:18:ARG:CB	2:A:197:GLU:HA	2.51	0.40
2:A:149:ALA:HB2	2:A:164:VAL:C	2.47	0.40
2:B:151:GLN:CG	2:B:151:GLN:O	2.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:584:MET:HE3	3:C:622:GLU:HG3	2.03	0.40
3:C:598:MET:O	3:C:602:MET:HG3	2.22	0.40
3:C:602:MET:CE	3:C:1024:LEU:HD21	2.51	0.40
3:C:644:VAL:O	3:C:644:VAL:HG23	2.21	0.40
3:C:754:LYS:HD3	4:D:39:LEU:CD1	2.52	0.40
3:C:967:VAL:HG23	3:C:968:PHE:N	2.34	0.40
4:D:12:ILE:HD13	4:D:12:ILE:HG21	1.79	0.40
4:D:81:GLU:HG2	4:D:83:THR:HG22	2.04	0.40
4:D:776:ILE:HG13	4:D:776:ILE:H	1.70	0.40
4:D:1165:ARG:HE	4:D:1209:MET:HE1	1.85	0.40
6:F:310:MET:HA	6:F:313:VAL:CG1	2.51	0.40
1:J:48:ALA:HB2	4:D:65:TYR:HH	1.85	0.40
1:J:57:ARG:HG3	4:D:25:TYR:C	2.45	0.40
2:A:2:LEU:HD12	2:B:143:GLY:CA	2.52	0.40
2:A:2:LEU:CD1	2:B:142:ARG:HB3	2.51	0.40
3:C:54:TRP:HD1	3:C:61:TRP:CZ2	2.39	0.40
3:C:943:VAL:HA	3:C:944:PRO:HD3	1.98	0.40
3:C:966:PRO:O	3:C:967:VAL:C	2.65	0.40
4:D:35:ASN:OD1	4:D:37:ARG:N	2.48	0.40
4:D:581:MET:HE3	4:D:716:LYS:HB2	2.04	0.40
4:D:633:ILE:C	4:D:633:ILE:HD12	2.47	0.40
4:D:972:GLY:HA2	10:D:2005:SO4:O2	2.21	0.40
4:D:1004:GLU:HB3	4:D:1005:PRO:CD	2.52	0.40
6:F:359:ILE:HG22	6:F:360:SER:H	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	J	81/114 (71%)	75 (93%)	6 (7%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	A	214/350 (61%)	202 (94%)	12 (6%)	0	100	100
2	B	231/350 (66%)	216 (94%)	14 (6%)	1 (0%)	30	50
2	T	33/350 (9%)	33 (100%)	0	0	100	100
3	C	1093/1169 (94%)	1038 (95%)	51 (5%)	4 (0%)	30	50
4	D	1238/1317 (94%)	1189 (96%)	46 (4%)	3 (0%)	43	64
5	E	72/107 (67%)	65 (90%)	5 (7%)	2 (3%)	4	6
6	F	298/466 (64%)	294 (99%)	4 (1%)	0	100	100
All	All	3260/4223 (77%)	3112 (96%)	138 (4%)	10 (0%)	36	56

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	E	76	VAL
3	C	982	SER
3	C	1134	ALA
4	D	902	GLU
4	D	1194	VAL
3	C	544	ARG
5	E	78	PRO
2	B	183	VAL
4	D	935	VAL
3	C	967	VAL

5.3.2 Protein sidechains ⓘ

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%)	62 (87%)	9 (13%)	4	8
2	A	178/297 (60%)	159 (89%)	19 (11%)	6	12
2	B	171/297 (58%)	150 (88%)	21 (12%)	4	8
2	T	35/297 (12%)	29 (83%)	6 (17%)	2	3
3	C	857/984 (87%)	762 (89%)	95 (11%)	6	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	D	994/1095 (91%)	894 (90%)	100 (10%)	7	14
5	E	62/86 (72%)	51 (82%)	11 (18%)	2	3
6	F	252/379 (66%)	227 (90%)	25 (10%)	7	15
All	All	2620/3533 (74%)	2334 (89%)	286 (11%)	6	12

All (286) 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	66	GLU
1	J	71	GLU
1	J	91	VAL
1	J	104	LEU
1	J	105	ILE
2	A	14	VAL
2	A	40	ARG
2	A	71	GLU
2	A	74	THR
2	A	91	GLU
2	A	111	VAL
2	A	117	THR
2	A	127	THR
2	A	129	ASN
2	A	130	ASP
2	A	134	LEU
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	194	ILE
2	B	17	ASN
2	B	33	THR
2	B	38	LEU
2	B	43	LEU
2	B	51	VAL

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Mol	Chain	Res	Type
2	B	60	LEU
2	B	63	PHE
2	B	84	VAL
2	B	85	VAL
2	B	99	LYS
2	B	110	ILE
2	B	125	ILE
2	B	144	ARG
2	B	161	ARG
2	B	176	TYR
2	B	177	LYS
2	B	178	VAL
2	B	200	ASN
2	B	215	LEU
2	B	218	LEU
2	B	231	HIS
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	204	GLU
3	C	227	VAL
3	C	241	GLU
3	C	248	ILE
3	C	253	LEU
3	C	268	ILE
3	C	280	LYS
3	C	299	LEU
3	C	301	ARG
3	C	336	LEU
3	C	347	THR
3	C	364	PHE
3	C	404	THR
3	C	434	ASN

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Mol	Chain	Res	Type
3	C	437	LEU
3	C	441	THR
3	C	443	LYS
3	C	446	LEU
3	C	449	LEU
3	C	454	LEU
3	C	462	GLU
3	C	466	VAL
3	C	491	LEU
3	C	531	VAL
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
3	C	640	VAL
3	C	664	ARG
3	C	703	GLU
3	C	727	ILE
3	C	737	VAL
3	C	753	THR
3	C	754	LYS
3	C	763	ASP
3	C	775	LEU
3	C	777	GLU
3	C	778	ARG
3	C	780	ILE
3	C	783	ILE
3	C	823	VAL
3	C	830	VAL
3	C	839	ILE
3	C	848	ASP
3	C	859	LEU
3	C	872	ASP
3	C	876	LEU
3	C	895	MET
3	C	919	ILE

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Mol	Chain	Res	Type
3	C	927	LEU
3	C	936	ASN
3	C	954	LEU
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	1001	LEU
3	C	1008	GLU
3	C	1021	ILE
3	C	1022	LEU
3	C	1028	VAL
3	C	1032	ILE
3	C	1045	GLN
3	C	1048	LEU
3	C	1084	SER
3	C	1088	VAL
3	C	1091	VAL
3	C	1108	ILE
3	C	1116	LEU
3	C	1122	LEU
3	C	1128	VAL
3	C	1129	LEU
3	C	1132	ASP
3	C	1138	MET
4	D	7	PHE
4	D	12	ILE
4	D	14	LEU
4	D	28	VAL
4	D	51	ILE
4	D	55	THR
4	D	70	PHE
4	D	101	VAL
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

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Mol	Chain	Res	Type
4	D	234	LEU
4	D	238	GLU
4	D	239	VAL
4	D	240	LEU
4	D	243	GLU
4	D	246	ASP
4	D	259	GLU
4	D	298	VAL
4	D	304	GLN
4	D	314	LEU
4	D	360	LEU
4	D	365	ILE
4	D	406	LEU
4	D	417	LEU
4	D	449	LEU
4	D	451	LEU
4	D	456	VAL
4	D	467	GLN
4	D	489	GLU
4	D	504	LEU
4	D	507	LEU
4	D	513	GLU
4	D	518	GLU
4	D	558	LEU
4	D	562	SER
4	D	566	LEU
4	D	567	SER
4	D	574	LEU
4	D	576	MET
4	D	588	LEU
4	D	591	LEU
4	D	599	TYR
4	D	600	GLN
4	D	603	THR
4	D	627	LEU
4	D	629	VAL
4	D	635	VAL
4	D	647	GLU
4	D	653	ASN
4	D	655	TRP
4	D	656	LYS
4	D	666	THR

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Mol	Chain	Res	Type
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	741	LYS
4	D	743	GLU
4	D	746	GLU
4	D	767	THR
4	D	769	ARG
4	D	784	VAL
4	D	799	ILE
4	D	830	PHE
4	D	831	ILE
4	D	853	HIS
4	D	876	LEU
4	D	900	LEU
4	D	914	HIS
4	D	923	THR
4	D	945	ASP
4	D	952	LEU
4	D	956	ILE
4	D	961	VAL
4	D	1009	LEU
4	D	1039	ARG
4	D	1042	ARG
4	D	1056	LEU
4	D	1079	ASP
4	D	1086	ARG
4	D	1112	LEU
4	D	1122	VAL
4	D	1150	ILE
4	D	1183	GLU
4	D	1186	GLU
4	D	1208	LEU
4	D	1215	SER
4	D	1222	LEU
4	D	1234	LEU
4	D	1241	CYS
4	D	1258	LEU

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Mol	Chain	Res	Type
4	D	1278	GLU
5	E	27	ASP
5	E	37	ILE
5	E	50	LEU
5	E	59	ARG
5	E	76	VAL
5	E	84	LEU
5	E	85	GLN
5	E	89	LEU
5	E	101	LEU
5	E	102	GLU
5	E	104	THR
6	F	166	VAL
6	F	172	GLN
6	F	182	GLU
6	F	216	ARG
6	F	268	ARG
6	F	291	GLN
6	F	310	MET
6	F	313	VAL
6	F	317	LEU
6	F	324	LEU
6	F	325	LEU
6	F	337	LEU
6	F	348	VAL
6	F	349	LEU
6	F	373	LEU
6	F	383	VAL
6	F	402	LEU
6	F	412	VAL
6	F	420	THR
6	F	433	VAL
6	F	437	THR
6	F	452	LEU
6	F	462	ARG
6	F	465	LEU
6	F	466	ASP
2	T	254	LEU
2	T	255	ASP
2	T	260	SER
2	T	275	LEU
2	T	279	THR

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Mol	Chain	Res	Type
2	T	284	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) 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	534	GLN
3	C	576	GLN
3	C	590	HIS
3	C	603	GLN
3	C	685	GLN
3	C	700	GLN
3	C	720	HIS
3	C	742	HIS
3	C	936	ASN
3	C	1068	GLN
3	C	1120	GLN
4	D	165	GLN
4	D	287	GLN
4	D	303	GLN
4	D	368	ASN
4	D	416	ASN
4	D	467	GLN
4	D	515	GLN
4	D	544	HIS
4	D	564	ASN
4	D	600	GLN
4	D	684	ASN
4	D	740	GLN
4	D	748	HIS
4	D	765	ASN
4	D	766	HIS
4	D	778	GLN
4	D	796	ASN

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Mol	Chain	Res	Type
4	D	853	HIS
4	D	881	GLN
4	D	932	ASN
4	D	1126	GLN
4	D	1146	GLN
5	E	34	ASN
5	E	85	GLN
5	E	103	HIS
6	F	199	GLN
6	F	214	GLN
6	F	309	HIS
6	F	395	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 oligosaccharides 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	F	505	-	4,4,4	0.24	0	6,6,6	0.15	0
11	EDO	F	506	-	3,3,3	0.45	0	2,2,2	0.29	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	SO4	F	501	-	4,4,4	0.25	0	6,6,6	0.09	0
10	SO4	D	2007	-	4,4,4	0.23	0	6,6,6	0.14	0
11	EDO	D	2009	-	3,3,3	0.42	0	2,2,2	0.35	0
10	SO4	C	1202	-	4,4,4	0.23	0	6,6,6	0.16	0
10	SO4	F	504	-	4,4,4	0.25	0	6,6,6	0.13	0
11	EDO	C	1205	-	3,3,3	0.48	0	2,2,2	0.27	0
11	EDO	C	1204	-	3,3,3	0.40	0	2,2,2	0.45	0
11	EDO	D	2008	-	3,3,3	0.45	0	2,2,2	0.29	0
11	EDO	D	2010	-	3,3,3	0.47	0	2,2,2	0.18	0
10	SO4	D	2004	-	4,4,4	0.24	0	6,6,6	0.30	0
10	SO4	F	502	-	4,4,4	0.23	0	6,6,6	0.25	0
10	SO4	F	503	-	4,4,4	0.24	0	6,6,6	0.16	0
10	SO4	C	1203	-	4,4,4	0.22	0	6,6,6	0.17	0
10	SO4	C	1201	-	4,4,4	0.23	0	6,6,6	0.13	0
10	SO4	D	2005	-	4,4,4	0.20	0	6,6,6	0.15	0
10	SO4	D	2006	-	4,4,4	0.23	0	6,6,6	0.25	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	C	1204	-	-	1/1/1/1	-
11	EDO	D	2008	-	-	1/1/1/1	-
11	EDO	D	2010	-	-	0/1/1/1	-

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
11	C	1205	EDO	1	0
11	D	2008	EDO	3	0
10	F	502	SO4	1	0
10	C	1203	SO4	2	0
10	D	2005	SO4	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	0.48	3 (3%) 46 44	64, 97, 141, 158	0
2	A	218/350 (62%)	0.54	12 (5%) 30 30	59, 86, 118, 137	0
2	B	233/350 (66%)	1.00	31 (13%) 7 6	80, 110, 134, 148	0
2	T	53/350 (15%)	1.35	15 (28%) 1 1	113, 149, 165, 169	0
3	C	1099/1169 (94%)	0.47	53 (4%) 35 35	42, 85, 147, 163	0
4	D	1248/1317 (94%)	0.20	30 (2%) 59 57	39, 73, 125, 156	0
5	E	76/107 (71%)	0.28	2 (2%) 57 55	51, 78, 113, 117	0
6	F	302/466 (64%)	0.00	0 100 100	38, 72, 122, 137	0
7	O	31/31 (100%)	-0.50	0 100 100	51, 64, 83, 89	0
8	P	26/26 (100%)	-0.44	0 100 100	59, 68, 83, 93	0
9	G	0/17	-	-	-	-
All	All	3369/4297 (78%)	0.36	146 (4%) 40 38	38, 82, 141, 169	0

All (146) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	155	SER	5.5
2	T	275	LEU	5.4
3	C	228	LEU	4.8
3	C	229	LEU	4.4
2	A	2	LEU	4.0
2	B	157	ALA	4.0
2	B	1	MET	3.8
2	A	218	LEU	3.8
3	C	562	VAL	3.8
1	J	26	PRO	3.8
2	T	288	ASN	3.6
3	C	277	PRO	3.6

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Mol	Chain	Res	Type	RSRZ
3	C	481	GLU	3.4
3	C	330	VAL	3.4
2	B	64	THR	3.4
2	B	171	VAL	3.3
3	C	311	LEU	3.3
3	C	968	PHE	3.2
3	C	299	LEU	3.2
2	A	90	ASP	3.2
2	B	43	LEU	3.2
2	B	183	VAL	3.1
3	C	324	LEU	3.1
2	B	152	ASN	3.1
4	D	663	ALA	3.1
4	D	111	PRO	3.1
4	D	901	ALA	3.0
3	C	201	ALA	3.0
2	T	269	VAL	3.0
2	T	283	LEU	3.0
3	C	287	LEU	3.0
3	C	248	ILE	3.0
4	D	4	VAL	3.0
3	C	455	SER	2.9
4	D	728	VAL	2.9
2	B	177	LYS	2.9
3	C	252	THR	2.9
3	C	240	VAL	2.8
3	C	329	VAL	2.8
3	C	21	ASN	2.8
4	D	1179	GLY	2.8
3	C	227	VAL	2.8
4	D	817	ALA	2.8
1	J	72	PRO	2.8
1	J	69	VAL	2.8
2	B	140	VAL	2.8
4	D	611	VAL	2.7
2	T	251	ILE	2.7
2	B	61	HIS	2.7
3	C	218	ASP	2.7
4	D	903	ARG	2.6
2	T	276	VAL	2.6
3	C	459	ALA	2.6
3	C	323	THR	2.6

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Mol	Chain	Res	Type	RSRZ
3	C	938	ASP	2.6
2	B	172	LEU	2.6
3	C	190	LEU	2.6
4	D	65	TYR	2.6
2	B	21	PHE	2.6
3	C	361	ILE	2.5
2	A	30	PHE	2.5
4	D	1009	LEU	2.5
2	B	178	VAL	2.5
4	D	849	PHE	2.5
5	E	24	SER	2.5
4	D	633	ILE	2.5
2	B	107	ALA	2.5
3	C	594	ASN	2.5
4	D	991	GLY	2.5
4	D	607	PRO	2.5
3	C	225	VAL	2.5
3	C	535	ALA	2.5
3	C	675	ALA	2.5
2	B	44	SER	2.4
2	B	7	PRO	2.4
4	D	1178	PRO	2.4
4	D	924	LEU	2.4
3	C	145	MET	2.4
4	D	1283	ALA	2.4
3	C	203	LEU	2.4
2	B	163	PRO	2.4
2	T	270	HIS	2.4
3	C	196	ILE	2.3
4	D	1173	SER	2.3
2	T	272	VAL	2.3
2	T	294	ILE	2.3
2	B	227	ALA	2.3
2	A	3	ILE	2.3
2	B	65	THR	2.3
3	C	572	VAL	2.3
2	A	221	LEU	2.3
4	D	6	PHE	2.3
2	B	154	ALA	2.3
2	B	32	TYR	2.3
2	B	229	SER	2.3
3	C	1053	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	164	VAL	2.3
2	B	153	LYS	2.2
3	C	765	PRO	2.2
2	A	26	LEU	2.2
2	T	297	VAL	2.2
3	C	550	VAL	2.2
3	C	623	LEU	2.2
2	B	63	PHE	2.2
3	C	205	PHE	2.2
4	D	813	THR	2.2
3	C	1011	PRO	2.2
3	C	267	ASP	2.2
3	C	671	HIS	2.2
3	C	1043	ILE	2.2
3	C	882	ASN	2.2
4	D	727	GLY	2.2
3	C	823	VAL	2.2
5	E	26	TYR	2.2
2	B	60	LEU	2.2
2	T	264	LEU	2.2
3	C	946	TRP	2.1
4	D	1169	ILE	2.1
3	C	952	GLU	2.1
4	D	66	LYS	2.1
2	A	83	LEU	2.1
2	B	194	ILE	2.1
3	C	234	TRP	2.1
2	T	271	THR	2.1
2	A	51	VAL	2.1
4	D	197	VAL	2.1
4	D	635	VAL	2.1
3	C	573	SER	2.1
2	B	62	GLU	2.1
3	C	254	GLU	2.1
4	D	729	THR	2.1
2	T	254	LEU	2.1
2	A	220	GLY	2.1
2	B	231	HIS	2.1
4	D	284	GLY	2.1
4	D	281	ILE	2.1
2	B	66	VAL	2.1
3	C	463	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
2	A	50	ALA	2.0
2	T	281	SER	2.0
3	C	331	ALA	2.0
2	T	301	LEU	2.0
3	C	1048	LEU	2.0
3	C	239	ILE	2.0
4	D	412	ARG	2.0
2	A	180	ALA	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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(Å ²)	Q<0.9
10	SO4	D	2007	5/5	0.68	0.09	93,98,113,141	0
10	SO4	F	504	5/5	0.73	0.07	112,114,117,128	0
10	SO4	C	1203	5/5	0.76	0.08	103,113,139,197	0
13	MG	D	2003	1/1	0.76	0.28	82,82,82,82	0
10	SO4	C	1202	5/5	0.77	0.08	105,111,115,178	0
10	SO4	C	1201	5/5	0.79	0.07	111,114,124,138	0
11	EDO	D	2009	4/4	0.80	0.12	71,86,103,103	0
11	EDO	C	1205	4/4	0.81	0.15	74,93,101,112	0
11	EDO	F	506	4/4	0.82	0.12	73,88,95,95	0
11	EDO	C	1204	4/4	0.84	0.11	53,63,75,77	0
11	EDO	D	2008	4/4	0.86	0.10	74,89,105,105	0
10	SO4	F	501	5/5	0.88	0.09	97,98,116,122	0
10	SO4	D	2006	5/5	0.88	0.09	80,103,121,126	0
10	SO4	F	505	5/5	0.88	0.11	80,84,117,167	0
10	SO4	D	2004	5/5	0.89	0.11	69,72,83,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
10	SO4	F	502	5/5	0.89	0.09	84,86,102,108	0
10	SO4	F	503	5/5	0.90	0.10	85,92,98,113	0
11	EDO	D	2010	4/4	0.92	0.20	62,75,77,89	0
10	SO4	D	2005	5/5	0.93	0.14	80,85,97,125	0
12	ZN	D	2002	1/1	0.97	0.12	222,222,222,222	0
12	ZN	D	2001	1/1	0.99	0.04	66,66,66,66	0

6.5 Other polymers [i](#)

There are no such residues in this entry.