Full wwPDB X-ray Structure Validation Report (i)

Jun 12, 2024 – 05:08 PM EDT

PDB ID	:	3E6A
Title	:	Crystal structure and Functional Analysis of Glyceraldehyde-3-phosphate Dehydrogenase from Oryza Sativa
Authors	:	Tien, Y.C.; Lin, Y.H.; Chang, S.L.; Chen, C.J.
Deposited on	:	2008-08-15
Resolution	:	3.77 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

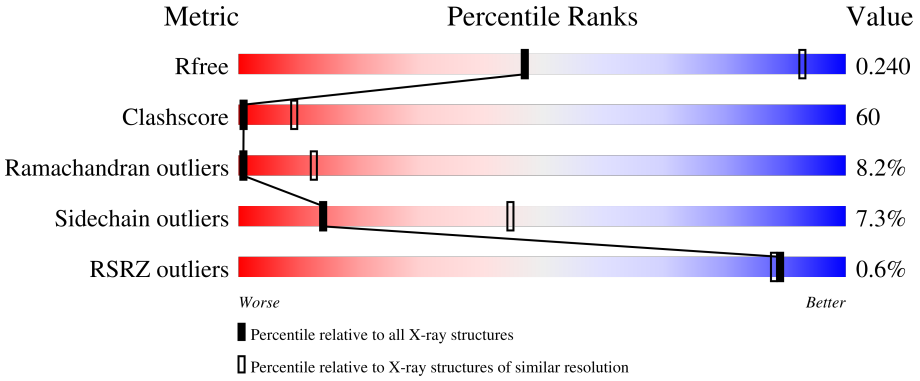
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.77 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1038 (3.96-3.60)
Clashscore	141614	1100 (3.96-3.60)
Ramachandran outliers	138981	1062 (3.96-3.60)
Sidechain outliers	138945	1058 (3.96-3.60)
RSRZ outliers	127900	1009 (3.98-3.58)

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

Mol	Chain	Length	Quality of chain
1	A	336	% 35% 54% 9% ••
1	B	336	% 31% 59% 10%
1	C	336	% 29% 60% 10% •
1	O	336	% 29% 60% 9% •

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
2	SO4	A	6923	-	-	X	-
2	SO4	C	6926	-	-	X	X

2 Entry composition (i)

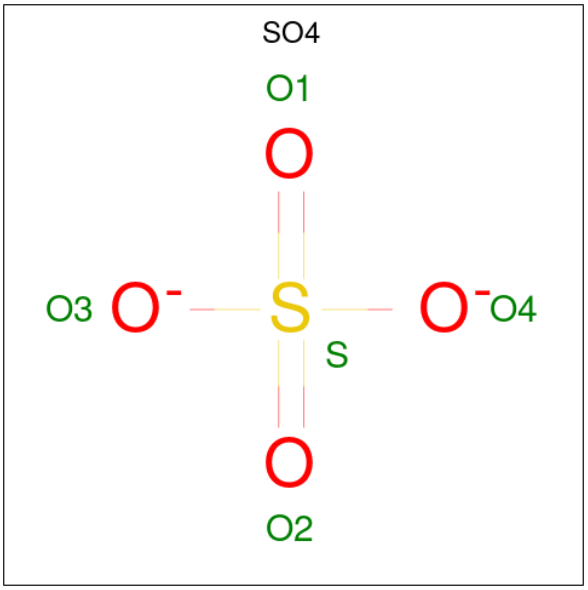
There are 3 unique types of molecules in this entry. The entry contains 10312 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Glyceraldehyde-3-phosphate dehydrogenase, cytosolic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	O	335	2544	1616	430	489	9	0	0	0
1	A	334	2539	1614	429	487	9	0	0	0
1	B	335	2544	1616	430	489	9	0	0	0
1	C	335	2544	1616	430	489	9	0	0	0

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
2	A	1	5	4	1	0	0
			Total	O	S		
2	A	1	5	4	1	0	0
			Total	O	S		
2	B	1	5	4	1	0	0
			Total	O	S		
2	B	1	5	4	1	0	0
			Total	O	S		
2	C	1	5	4	1	0	0
			Total	O	S		
2	C	1	5	4	1	0	0

- Molecule 3 is water.

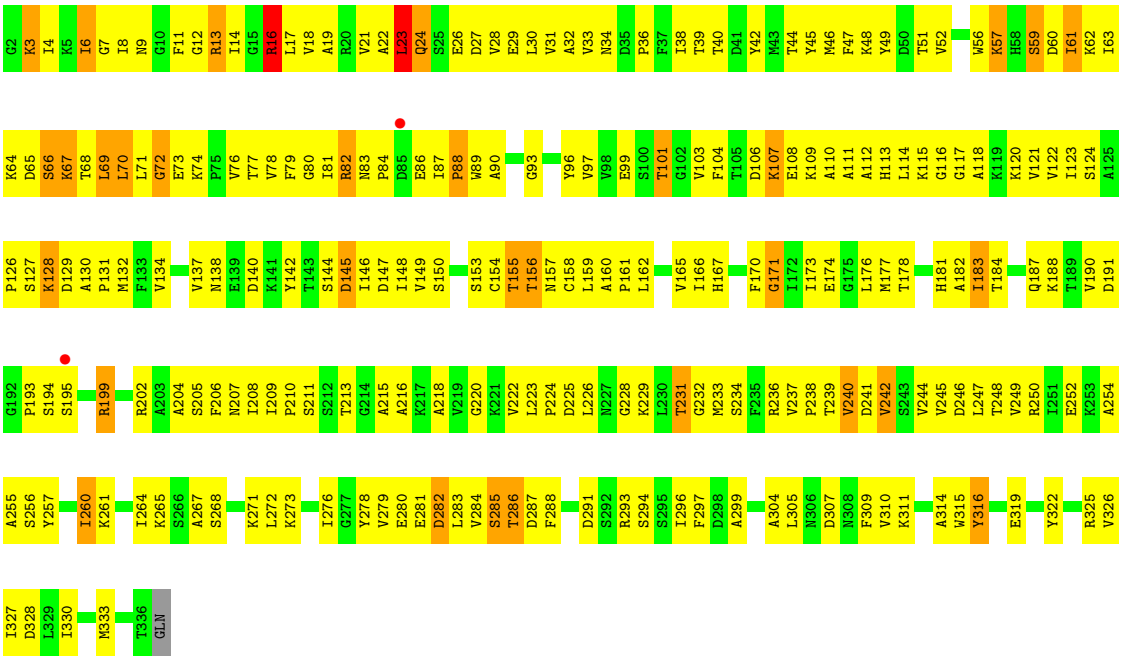
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	O	29	29	29	0	0
			Total	O		
3	A	23	23	23	0	0
			Total	O		
3	B	23	23	23	0	0
			Total	O		
3	C	26	26	26	0	0

3 Residue-property plots (i)

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

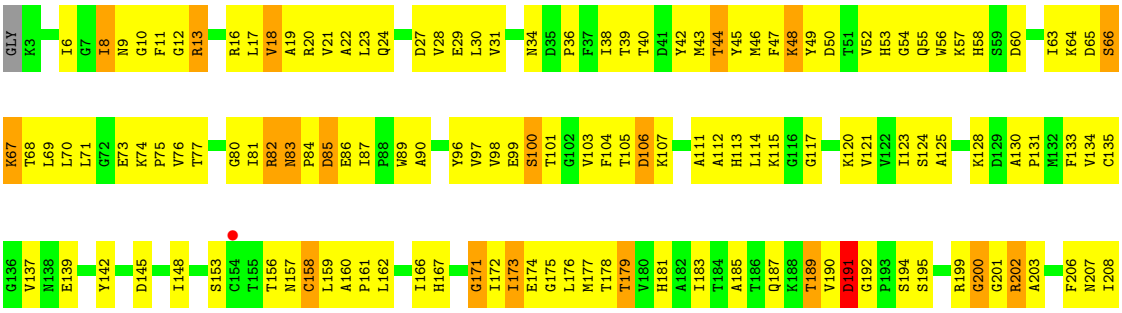
• Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase, cytosolic

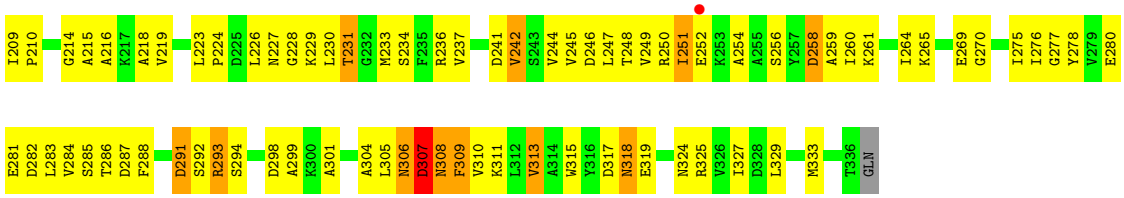
Chain O:



• Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase, cytosolic

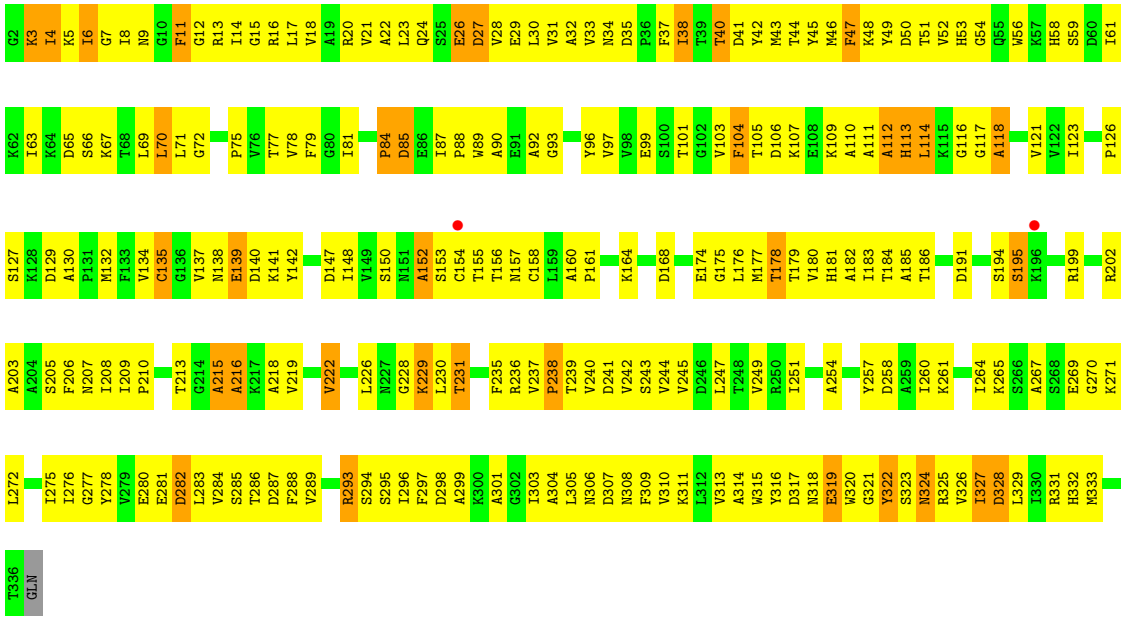
Chain A:





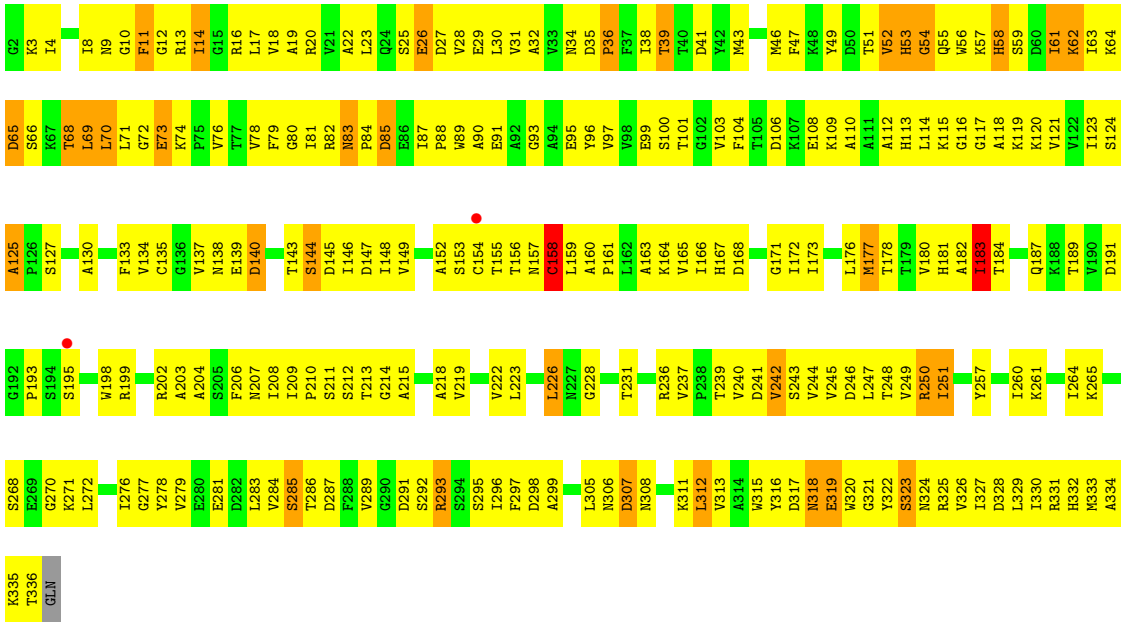
• Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase, cytosolic

Chain B:



• Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase, cytosolic

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	76.26Å 127.42Å 77.39Å 90.00° 118.05° 90.00°	Depositor
Resolution (Å)	30.00 – 3.77 26.61 – 3.51	Depositor EDS
% Data completeness (in resolution range)	99.1 (30.00-3.77) 98.8 (26.61-3.51)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.33	Depositor
$< I/\sigma(I) >$ [1]	4.60 (at 3.55Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.196 , 0.210 0.222 , 0.240	Depositor DCC
R_{free} test set	810 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	38.3	Xtriage
Anisotropy	1.061	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 34.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.010 for -h-l,k,h 0.010 for l,k,-h-l 0.037 for h,-k,-h-l 0.034 for -h-l,-k,l 0.033 for l,-k,h	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	10312	wwPDB-VP
Average B, all atoms (Å^2)	0.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.52% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.32	0/2586	0.60	0/3504
1	B	0.34	0/2591	0.62	0/3510
1	C	0.33	0/2591	0.64	0/3510
1	O	0.34	0/2591	0.72	6/3510 (0.2%)
All	All	0.33	0/10359	0.65	6/14034 (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	A	0	1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	O	16	ARG	O-C-N	8.49	136.28	122.70
1	O	16	ARG	CA-C-N	-7.60	100.47	117.20
1	O	195	SER	CA-C-O	-6.68	106.07	120.10
1	O	16	ARG	N-CA-C	6.62	128.88	111.00
1	O	195	SER	CA-C-N	5.81	129.98	117.20
1	O	16	ARG	C-N-CA	-5.54	107.84	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	13	ARG	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2539	0	2562	328	0
1	B	2544	0	2568	322	0
1	C	2544	0	2568	345	0
1	O	2544	0	2568	364	0
2	A	10	0	0	3	0
2	B	10	0	0	1	0
2	C	10	0	0	11	0
2	O	10	0	0	1	0
3	A	23	0	0	0	19
3	B	23	0	0	7	10
3	C	26	0	0	0	18
3	O	29	0	0	1	9
All	All	10312	0	10266	1227	29

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 60.

All (1227) 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)
1:O:240:VAL:HB	1:B:206:PHE:CE1	1.42	1.55
1:A:42:TYR:CZ	1:A:46:MET:HE2	1.66	1.31
1:O:206:PHE:CE2	1:B:240:VAL:HB	1.71	1.25
1:A:11:PHE:CE2	1:A:16:ARG:CD	2.21	1.24
1:A:42:TYR:CE2	1:A:46:MET:CE	2.20	1.23
1:C:215:ALA:HB2	2:C:6926:SO4:O3	1.37	1.20
1:O:240:VAL:CB	1:B:206:PHE:CE1	2.25	1.18
1:O:12:GLY:O	1:O:16:ARG:HD3	1.43	1.18
1:B:205:SER:O	1:B:206:PHE:CD2	1.97	1.17
1:A:158:CYS:SG	1:A:245:VAL:HG21	1.87	1.14
1:A:11:PHE:CE2	1:A:16:ARG:HD3	1.81	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:240:VAL:HB	1:B:206:PHE:CD1	1.84	1.13
1:A:46:MET:HE3	1:C:193:PRO:HA	1.21	1.12
1:A:42:TYR:CZ	1:A:46:MET:CE	2.32	1.11
1:A:11:PHE:CE2	1:A:16:ARG:HG2	1.86	1.10
1:O:288:PHE:HE1	1:O:315:TRP:CG	1.71	1.08
1:B:110:ALA:HB2	1:B:123:ILE:HD11	1.35	1.08
1:O:206:PHE:CE2	1:B:240:VAL:CB	2.39	1.04
1:A:11:PHE:CE2	1:A:16:ARG:CG	2.41	1.04
1:B:216:ALA:HB1	1:B:231:THR:HA	1.39	1.03
1:C:64:LYS:HB2	1:C:70:LEU:HD22	1.40	1.03
1:A:42:TYR:CE2	1:A:46:MET:HE3	1.94	1.03
1:O:288:PHE:CE1	1:O:315:TRP:CG	2.47	1.01
1:A:173:ILE:HD11	1:A:252:GLU:N	1.74	1.00
1:O:170:PHE:CE2	1:O:260:ILE:HD12	1.96	1.00
1:B:205:SER:O	1:B:206:PHE:HD2	1.37	0.99
1:B:35:ASP:OD1	1:B:38:ILE:HD13	1.61	0.99
1:C:23:LEU:HD11	1:C:71:LEU:HD23	1.45	0.99
1:A:42:TYR:HD1	1:C:198:TRP:CE2	1.81	0.98
1:O:288:PHE:HE1	1:O:315:TRP:CD1	1.81	0.98
1:A:13:ARG:NH1	1:A:50:ASP:OD2	1.96	0.98
1:B:288:PHE:HE2	1:B:315:TRP:CG	1.83	0.97
1:B:288:PHE:CE2	1:B:315:TRP:CG	2.52	0.97
1:O:48:LYS:CE	1:O:49:TYR:HE2	1.79	0.95
1:O:176:LEU:HD13	1:C:311:LYS:HB2	1.44	0.95
1:A:42:TYR:OH	1:A:46:MET:HE2	1.65	0.95
1:B:4:ILE:HD11	1:B:28:VAL:HG22	1.49	0.95
1:B:239:THR:HG21	3:B:6956:HOH:O	1.66	0.94
1:A:248:THR:HG23	1:B:176:LEU:HD12	1.49	0.94
1:O:206:PHE:CD2	1:B:240:VAL:HB	2.00	0.94
1:O:240:VAL:HB	1:B:206:PHE:HE1	1.13	0.94
1:A:42:TYR:OH	1:A:46:MET:CE	2.16	0.94
1:C:215:ALA:CB	2:C:6926:SO4:O3	2.16	0.94
1:O:48:LYS:HE2	1:O:49:TYR:HE2	1.29	0.94
1:O:64:LYS:HG3	1:O:70:LEU:HB2	1.49	0.93
1:A:42:TYR:CD1	1:C:198:TRP:CE2	2.56	0.93
1:B:103:VAL:HG23	1:B:104:PHE:H	1.34	0.93
1:A:11:PHE:CD2	1:A:16:ARG:HG2	2.05	0.92
1:A:114:LEU:HD11	1:A:148:ILE:HD11	1.52	0.91
1:B:160:ALA:HB3	1:B:161:PRO:HD3	1.52	0.91
1:O:48:LYS:CD	1:O:49:TYR:HE2	1.84	0.90
1:C:213:THR:OG1	2:C:6926:SO4:S	2.29	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:PHE:HE2	1:A:16:ARG:CD	1.76	0.90
1:A:24:GLN:HE21	1:A:58:HIS:CD2	1.90	0.89
1:C:38:ILE:HG12	1:C:46:MET:HE2	1.53	0.88
1:O:48:LYS:CD	1:O:49:TYR:CE2	2.56	0.88
1:O:99:GLU:HB2	1:O:123:ILE:HA	1.54	0.88
1:A:160:ALA:HB3	1:A:161:PRO:HD3	1.56	0.88
1:C:11:PHE:CZ	1:C:16:ARG:HG2	2.10	0.87
1:C:181:HIS:HB3	1:C:236:ARG:HE	1.38	0.87
1:O:44:THR:HG22	1:O:69:LEU:HD11	1.57	0.87
1:O:48:LYS:HE2	1:O:49:TYR:CE2	2.09	0.87
1:A:208:ILE:HG23	1:A:237:VAL:HG12	1.57	0.87
1:C:158:CYS:HA	1:C:295:SER:HB2	1.57	0.86
1:A:158:CYS:SG	1:A:245:VAL:CG2	2.62	0.86
1:C:272:LEU:HB3	1:C:276:ILE:HD13	1.54	0.86
1:O:57:LYS:NZ	1:O:61:ILE:CD1	2.38	0.86
1:A:42:TYR:HE2	1:A:46:MET:HE3	1.35	0.86
1:C:83:ASN:HD22	1:C:84:PRO:CD	1.89	0.86
1:O:162:LEU:O	1:O:166:ILE:HD13	1.75	0.86
1:A:55:GLN:OE1	1:A:57:LYS:HG2	1.75	0.86
1:O:206:PHE:HE2	1:B:240:VAL:CB	1.88	0.85
1:O:63:ILE:HD12	1:O:63:ILE:H	1.42	0.85
1:O:282:ASP:HA	1:C:199:ARG:HE	1.39	0.85
1:B:21:VAL:HB	1:B:327:ILE:HD12	1.58	0.85
1:O:140:ASP:OD2	3:O:6937:HOH:O	1.95	0.84
1:A:42:TYR:CE2	1:A:46:MET:SD	2.69	0.84
1:O:183:ILE:HD13	1:O:183:ILE:O	1.77	0.84
1:C:261:LYS:HE3	1:C:299:ALA:HB1	1.60	0.84
1:C:34:ASN:HB2	1:C:79:PHE:HB2	1.60	0.83
1:C:83:ASN:HD22	1:C:84:PRO:HD2	1.43	0.83
1:O:57:LYS:HZ1	1:O:61:ILE:HD11	1.40	0.83
1:B:138:ASN:HB2	1:B:141:LYS:HG3	1.61	0.83
1:C:249:VAL:HG22	1:C:250:ARG:H	1.42	0.82
1:B:110:ALA:CB	1:B:123:ILE:HD11	2.08	0.82
1:O:90:ALA:HB2	1:O:117:GLY:HA3	1.61	0.82
1:B:90:ALA:HB2	1:B:117:GLY:HA3	1.59	0.82
1:O:82:ARG:HH11	1:O:82:ARG:HB2	1.43	0.82
1:O:222:VAL:HG23	1:O:223:LEU:H	1.44	0.81
1:A:175:GLY:HA3	1:A:249:VAL:HG23	1.61	0.81
1:B:288:PHE:CE2	1:B:315:TRP:CB	2.62	0.81
1:A:24:GLN:HE21	1:A:58:HIS:CG	1.98	0.81
1:O:79:PHE:HB3	1:O:81:ILE:HD12	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:GLU:OE2	1:A:252:GLU:HA	1.80	0.80
1:A:233:MET:SD	1:B:311:LYS:HD3	2.21	0.80
1:O:57:LYS:HZ3	1:O:61:ILE:HD13	1.47	0.80
1:A:29:GLU:HG3	1:A:74:LYS:HZ1	1.47	0.80
1:O:264:ILE:HD12	1:O:297:PHE:CG	2.17	0.79
1:A:11:PHE:HE2	1:A:16:ARG:HD3	1.31	0.79
1:O:240:VAL:CB	1:B:206:PHE:HE1	1.77	0.79
1:C:88:PRO:HB2	1:C:91:GLU:HB3	1.64	0.79
1:B:134:VAL:HG23	1:B:222:VAL:HG11	1.64	0.79
1:B:324:ASN:HD22	1:B:324:ASN:N	1.81	0.79
1:A:46:MET:CE	1:C:193:PRO:HA	2.10	0.79
1:O:23:LEU:H	1:O:23:LEU:HD23	1.48	0.79
1:O:237:VAL:HG11	1:C:237:VAL:HG11	1.65	0.79
1:O:280:GLU:HG2	1:O:299:ALA:HB3	1.64	0.79
1:B:286:THR:HG21	1:C:51:THR:HG23	1.64	0.79
1:A:19:ALA:O	1:A:23:LEU:HD13	1.82	0.79
1:A:11:PHE:CD2	1:A:16:ARG:HD3	2.18	0.78
1:A:38:ILE:HD12	1:A:43:MET:HG2	1.63	0.78
1:O:97:VAL:HB	1:O:121:VAL:HG22	1.63	0.78
1:O:272:LEU:HB3	1:O:276:ILE:HG22	1.64	0.78
1:O:48:LYS:HD3	1:O:49:TYR:CE2	2.17	0.78
1:A:81:ILE:HD12	1:A:81:ILE:H	1.47	0.78
1:A:29:GLU:HG3	1:A:74:LYS:NZ	1.99	0.78
1:A:64:LYS:HB2	1:A:70:LEU:HD21	1.66	0.78
1:O:61:ILE:N	1:O:61:ILE:HD12	1.99	0.77
1:C:61:ILE:HD13	1:C:71:LEU:HD12	1.66	0.77
1:C:161:PRO:O	1:C:165:VAL:HG23	1.84	0.77
1:O:48:LYS:CE	1:O:49:TYR:CE2	2.64	0.77
1:O:34:ASN:HB2	1:O:79:PHE:HB2	1.66	0.77
1:O:81:ILE:HD13	1:O:88:PRO:HD2	1.66	0.77
1:A:100:SER:HA	1:A:124:SER:OG	1.85	0.77
1:C:14:ILE:H	1:C:14:ILE:HD12	1.50	0.77
1:O:51:THR:HG23	1:A:286:THR:HG21	1.67	0.77
1:B:294:SER:OG	1:B:325:ARG:HD2	1.85	0.77
1:A:11:PHE:CD2	1:A:16:ARG:CG	2.66	0.76
1:O:68:THR:O	1:O:69:LEU:HB2	1.85	0.76
1:O:48:LYS:HG2	1:O:49:TYR:CD2	2.21	0.76
1:A:251:ILE:HD13	1:A:251:ILE:H	1.50	0.76
1:A:206:PHE:CE2	1:C:240:VAL:HB	2.21	0.76
1:A:281:GLU:HB2	1:A:283:LEU:HD21	1.68	0.76
1:O:199:ARG:HG3	1:O:199:ARG:HH11	1.51	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:ILE:CD1	1:A:173:ILE:N	2.49	0.76
1:B:257:TYR:HA	1:B:260:ILE:HD12	1.66	0.76
1:C:29:GLU:HG3	1:C:31:VAL:HG13	1.68	0.76
1:O:82:ARG:HH11	1:O:82:ARG:CB	1.99	0.75
1:A:101:THR:OG1	1:A:103:VAL:HG22	1.86	0.75
1:A:284:VAL:HG11	1:B:209:ILE:HG12	1.68	0.75
1:C:62:LYS:HG3	1:C:70:LEU:HD23	1.69	0.75
1:C:153:SER:CB	2:C:6926:SO4:O1	2.35	0.75
1:O:112:ALA:HA	1:O:115:LYS:NZ	2.01	0.75
1:C:73:GLU:HB3	1:C:74:LYS:HE3	1.68	0.75
1:A:305:LEU:HB2	1:B:176:LEU:HD21	1.67	0.75
1:A:305:LEU:HD13	1:B:231:THR:HG22	1.68	0.75
1:A:11:PHE:CZ	1:A:16:ARG:HG2	2.22	0.74
1:A:18:VAL:HG13	1:A:327:ILE:HD11	1.68	0.74
1:O:240:VAL:CA	1:B:206:PHE:HE1	1.98	0.74
1:C:181:HIS:HB3	1:C:236:ARG:NE	2.01	0.74
1:B:182:ALA:HB1	1:B:239:THR:O	1.86	0.74
1:C:38:ILE:HG12	1:C:46:MET:CE	2.18	0.74
1:O:84:PRO:HA	1:O:87:ILE:HD12	1.67	0.74
1:O:48:LYS:HG2	1:O:49:TYR:CE2	2.23	0.73
1:O:245:VAL:HG23	1:O:316:TYR:CE2	2.23	0.73
1:C:158:CYS:SG	1:C:245:VAL:HG21	2.28	0.73
1:B:177:MET:HG2	1:B:178:THR:N	2.01	0.73
1:A:177:MET:HG2	1:A:178:THR:N	2.03	0.73
1:O:193:PRO:CG	1:B:38:ILE:HD11	2.17	0.73
1:O:206:PHE:HE2	1:B:240:VAL:CA	2.01	0.73
1:O:57:LYS:HZ1	1:O:61:ILE:CD1	1.99	0.73
1:A:13:ARG:NH2	1:A:52:VAL:HG12	2.04	0.73
1:A:233:MET:SD	1:B:311:LYS:CD	2.77	0.73
1:B:288:PHE:CD2	1:B:315:TRP:HB3	2.23	0.72
1:C:161:PRO:HB3	1:C:276:ILE:HD11	1.72	0.72
1:O:96:TYR:HA	1:O:120:LYS:O	1.89	0.72
1:B:63:ILE:HD12	1:B:63:ILE:H	1.54	0.72
1:O:31:VAL:HG21	1:O:93:GLY:O	1.90	0.72
1:A:203:ALA:HB3	1:A:207:ASN:OD1	1.90	0.72
1:A:305:LEU:HD11	1:B:228:GLY:O	1.90	0.72
1:C:35:ASP:OD1	1:C:38:ILE:HD12	1.89	0.72
1:A:24:GLN:NE2	1:A:58:HIS:CD2	2.58	0.72
1:B:59:SER:HB2	1:B:72:GLY:HA3	1.71	0.72
1:O:19:ALA:O	1:O:23:LEU:HD23	1.90	0.71
1:O:183:ILE:HD12	1:O:183:ILE:H	1.55	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:ASN:O	1:A:294:SER:HB3	1.89	0.71
1:A:100:SER:O	1:A:100:SER:OG	2.07	0.71
1:A:215:ALA:HB2	2:A:6923:SO4:O3	1.90	0.71
1:B:42:TYR:O	1:B:46:MET:HG3	1.91	0.71
1:O:57:LYS:NZ	1:O:61:ILE:HD13	2.01	0.71
1:B:215:ALA:O	1:B:219:VAL:HG23	1.90	0.71
1:C:4:ILE:HG21	1:C:330:ILE:HG22	1.72	0.71
1:A:11:PHE:CE2	1:A:16:ARG:HD2	2.23	0.71
1:A:64:LYS:HB2	1:A:70:LEU:CD2	2.20	0.71
1:A:64:LYS:HD3	1:A:68:THR:HG21	1.72	0.71
1:A:173:ILE:N	1:A:173:ILE:HD12	2.05	0.71
1:C:16:ARG:O	1:C:19:ALA:HB3	1.91	0.71
1:C:213:THR:OG1	2:C:6926:SO4:O2	2.05	0.71
1:O:240:VAL:CA	1:B:206:PHE:CE1	2.73	0.71
1:C:68:THR:HA	1:C:78:VAL:HG23	1.71	0.70
1:C:199:ARG:HH11	1:C:210:PRO:HB2	1.56	0.70
1:C:23:LEU:CD1	1:C:71:LEU:HD23	2.21	0.70
1:A:172:ILE:HD12	1:A:226:LEU:HD21	1.73	0.70
1:B:127:SER:HB3	1:B:130:ALA:HB3	1.71	0.70
1:B:288:PHE:HE2	1:B:315:TRP:CD1	2.09	0.70
1:C:11:PHE:CE1	1:C:16:ARG:HG2	2.27	0.70
1:B:81:ILE:HD13	1:B:87:ILE:HA	1.72	0.70
1:O:206:PHE:CE2	1:B:240:VAL:CA	2.74	0.70
1:O:208:ILE:HD12	1:C:315:TRP:HZ3	1.55	0.70
1:O:16:ARG:O	1:O:19:ALA:HB3	1.92	0.70
1:O:104:PHE:HD1	1:O:109:LYS:HB3	1.56	0.70
1:O:228:GLY:O	1:C:305:LEU:HD11	1.92	0.69
1:A:83:ASN:N	1:A:83:ASN:HD22	1.89	0.69
1:O:57:LYS:NZ	1:O:61:ILE:HD11	2.01	0.69
1:O:285:SER:HB3	1:C:208:ILE:HB	1.74	0.69
1:O:127:SER:CB	1:O:130:ALA:HB3	2.22	0.69
1:O:199:ARG:HG3	1:O:199:ARG:NH1	2.07	0.69
1:A:176:LEU:HD21	1:B:305:LEU:HB2	1.73	0.69
1:A:183:ILE:HD12	1:C:189:THR:HB	1.75	0.69
1:C:153:SER:OG	2:C:6926:SO4:O1	2.09	0.69
1:A:285:SER:HA	1:A:315:TRP:CZ3	2.28	0.69
1:C:199:ARG:NH1	1:C:210:PRO:HB2	2.08	0.69
1:B:205:SER:HA	1:B:238:PRO:HG3	1.75	0.68
1:B:6:ILE:HG22	1:B:96:TYR:HB2	1.75	0.68
1:C:213:THR:OG1	2:C:6926:SO4:O3	2.10	0.68
1:O:288:PHE:CE1	1:O:315:TRP:CD1	2.73	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:TYR:HE2	1:A:333:MET:HA	1.58	0.68
1:A:202:ARG:HH21	1:C:51:THR:N	1.92	0.68
1:O:81:ILE:HD13	1:O:87:ILE:HA	1.75	0.68
1:C:264:ILE:HD12	1:C:297:PHE:CG	2.28	0.68
1:O:222:VAL:HG23	1:O:223:LEU:N	2.09	0.67
1:B:4:ILE:CD1	1:B:28:VAL:HG22	2.24	0.67
1:B:38:ILE:CD1	1:B:38:ILE:N	2.57	0.67
1:O:57:LYS:HA	1:O:57:LYS:HE3	1.76	0.67
1:A:309:PHE:HE2	1:B:175:GLY:H	1.41	0.67
1:O:23:LEU:HD11	1:O:47:PHE:CZ	2.30	0.67
1:O:59:SER:O	1:O:72:GLY:HA3	1.94	0.67
1:O:183:ILE:HD12	1:O:239:THR:O	1.94	0.67
1:B:6:ILE:CG2	1:B:96:TYR:HB2	2.24	0.67
1:C:69:LEU:O	1:C:70:LEU:HB2	1.94	0.67
1:A:84:PRO:HB2	1:A:112:ALA:HB3	1.76	0.67
1:C:81:ILE:HD13	1:C:87:ILE:HA	1.76	0.67
1:C:134:VAL:HG22	1:C:152:ALA:HB2	1.76	0.67
1:C:158:CYS:O	1:C:161:PRO:HD2	1.94	0.67
1:O:256:SER:O	1:O:260:ILE:HD13	1.94	0.67
1:A:84:PRO:HA	1:A:87:ILE:HD11	1.76	0.67
1:O:59:SER:O	1:O:60:ASP:HB3	1.95	0.67
1:O:208:ILE:H	1:C:285:SER:HB2	1.60	0.66
1:C:88:PRO:HB2	1:C:91:GLU:CB	2.24	0.66
1:O:215:ALA:O	1:O:218:ALA:HB3	1.95	0.66
1:O:254:ALA:HA	1:O:307:ASP:O	1.95	0.66
1:C:172:ILE:HG23	1:C:249:VAL:CG2	2.25	0.66
1:A:142:TYR:CE2	1:A:333:MET:HG2	2.31	0.66
1:C:215:ALA:HB2	2:C:6926:SO4:S	2.35	0.66
1:O:68:THR:O	1:O:69:LEU:CB	2.42	0.66
1:O:288:PHE:CE1	1:O:315:TRP:CB	2.78	0.66
1:C:159:LEU:HD11	1:C:247:LEU:HD22	1.76	0.66
1:C:159:LEU:HD13	1:C:245:VAL:HG11	1.75	0.66
1:B:111:ALA:HA	1:B:148:ILE:HD11	1.78	0.66
1:B:205:SER:C	1:B:206:PHE:CD2	2.68	0.66
1:O:211:SER:O	1:O:234:SER:HB3	1.94	0.66
1:B:216:ALA:HB1	1:B:231:THR:CA	2.20	0.66
1:A:69:LEU:O	1:A:75:PRO:HA	1.95	0.66
1:A:258:ASP:HA	1:A:261:LYS:HD3	1.77	0.66
1:B:243:SER:HB2	1:B:316:TYR:CE1	2.30	0.66
1:O:176:LEU:HD23	1:O:231:THR:HG23	1.77	0.65
1:O:264:ILE:HD12	1:O:297:PHE:CD2	2.31	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:90:ALA:HB2	1:C:117:GLY:O	1.96	0.65
1:O:48:LYS:CG	1:O:49:TYR:CE2	2.80	0.65
1:O:18:VAL:HG13	1:O:327:ILE:HD11	1.79	0.65
1:O:9:ASN:ND2	1:O:87:ILE:HD13	2.12	0.65
1:C:31:VAL:HG21	1:C:93:GLY:O	1.96	0.65
1:A:305:LEU:HD23	1:A:309:PHE:HD2	1.61	0.64
1:C:251:ILE:HD13	1:C:251:ILE:H	1.62	0.64
1:A:44:THR:CG2	1:A:69:LEU:HD11	2.28	0.64
1:A:176:LEU:O	1:A:247:LEU:HD12	1.97	0.64
1:A:237:VAL:HG11	1:B:237:VAL:HG11	1.77	0.64
1:A:260:ILE:O	1:A:264:ILE:HG12	1.97	0.64
1:A:30:LEU:HD23	1:A:31:VAL:N	2.12	0.64
1:O:161:PRO:O	1:O:165:VAL:HG23	1.96	0.64
1:O:12:GLY:O	1:O:16:ARG:CD	2.35	0.64
1:A:208:ILE:O	1:A:210:PRO:HD3	1.97	0.64
1:C:83:ASN:ND2	1:C:84:PRO:HD2	2.13	0.64
1:O:166:ILE:HD12	1:O:166:ILE:H	1.63	0.64
1:O:260:ILE:HD13	1:O:260:ILE:N	2.13	0.64
1:O:296:ILE:HB	1:O:315:TRP:HB2	1.80	0.64
1:O:284:VAL:HG11	1:C:209:ILE:HG12	1.80	0.63
1:A:131:PRO:HD2	1:A:148:ILE:O	1.97	0.63
1:A:246:ASP:OD1	1:B:178:THR:HG21	1.97	0.63
1:B:56:TRP:HD1	1:B:61:ILE:HD11	1.64	0.63
1:C:11:PHE:CE1	1:C:16:ARG:HA	2.33	0.63
1:O:194:SER:H	1:B:42:TYR:HE2	1.41	0.63
1:B:59:SER:HB2	1:B:72:GLY:CA	2.28	0.63
1:B:158:CYS:HG	1:B:316:TYR:HD2	1.45	0.63
1:C:251:ILE:HD13	1:C:308:ASN:O	1.99	0.63
1:C:327:ILE:HA	1:C:330:ILE:HD12	1.78	0.63
1:C:4:ILE:HG21	1:C:330:ILE:CG2	2.27	0.63
1:C:83:ASN:HD22	1:C:84:PRO:N	1.97	0.63
1:B:327:ILE:HG22	1:B:327:ILE:O	1.97	0.63
1:C:161:PRO:HB3	1:C:276:ILE:CD1	2.28	0.63
1:O:205:SER:O	1:O:206:PHE:HD1	1.82	0.63
1:A:66:SER:C	1:A:68:THR:H	2.01	0.63
1:A:67:LYS:O	1:A:77:THR:HA	1.99	0.63
1:B:103:VAL:HG23	1:B:104:PHE:N	2.11	0.63
1:O:247:LEU:HG	1:O:249:VAL:HG13	1.80	0.63
1:O:257:TYR:CD2	1:O:261:LYS:HD2	2.34	0.62
1:O:282:ASP:HB3	1:C:199:ARG:HG3	1.81	0.62
1:A:42:TYR:HE2	1:A:46:MET:CE	1.88	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:ILE:CD1	1:A:252:GLU:N	2.57	0.62
1:B:89:TRP:NE1	1:B:113:HIS:ND1	2.43	0.62
1:B:325:ARG:HG2	1:B:325:ARG:HH11	1.63	0.62
1:C:249:VAL:HG22	1:C:250:ARG:N	2.11	0.62
1:O:64:LYS:HG3	1:O:70:LEU:CB	2.28	0.62
1:A:90:ALA:HB2	1:A:117:GLY:HA3	1.82	0.62
1:B:126:PRO:HD3	1:B:153:SER:HB3	1.81	0.62
1:B:285:SER:CB	3:B:6956:HOH:O	2.48	0.62
1:A:43:MET:C	1:A:45:TYR:H	2.02	0.62
1:C:11:PHE:H	1:C:35:ASP:HB2	1.63	0.62
1:O:84:PRO:HA	1:O:87:ILE:CD1	2.29	0.61
1:O:288:PHE:CD1	1:O:315:TRP:CB	2.83	0.61
1:O:113:HIS:O	1:O:118:ALA:HB3	2.00	0.61
1:A:42:TYR:CE1	1:C:198:TRP:CD1	2.88	0.61
1:B:85:ASP:H	1:B:112:ALA:HB1	1.66	0.61
1:B:177:MET:HG2	1:B:178:THR:H	1.65	0.61
1:O:122:VAL:HG13	1:O:149:VAL:HG23	1.82	0.61
1:O:248:THR:HG23	1:C:176:LEU:HD12	1.82	0.61
1:C:219:VAL:HG12	1:C:223:LEU:HB2	1.82	0.61
1:B:142:TYR:CZ	1:B:333:MET:HG2	2.34	0.61
1:B:181:HIS:O	1:B:236:ARG:HA	2.00	0.61
1:B:288:PHE:CD2	1:B:315:TRP:CB	2.83	0.61
1:O:111:ALA:O	1:O:114:LEU:HD23	2.00	0.61
1:O:288:PHE:CD1	1:O:315:TRP:HB3	2.35	0.61
1:C:272:LEU:HD13	1:C:276:ILE:CD1	2.30	0.61
1:O:99:GLU:HA	1:O:99:GLU:OE2	2.01	0.61
1:A:265:LYS:HG2	1:A:269:GLU:OE2	2.00	0.61
1:A:158:CYS:HG	1:A:245:VAL:CG2	2.13	0.61
1:O:213:THR:HG22	1:O:233:MET:HA	1.82	0.61
1:A:42:TYR:HD1	1:C:198:TRP:CZ2	2.19	0.61
1:C:208:ILE:O	1:C:210:PRO:HD3	2.01	0.60
1:C:306:ASN:O	1:C:308:ASN:N	2.33	0.60
1:C:137:VAL:HG21	1:C:160:ALA:HB1	1.82	0.60
1:O:18:VAL:HG13	1:O:327:ILE:CD1	2.32	0.60
1:O:178:THR:O	1:O:246:ASP:HB3	2.02	0.60
1:O:310:VAL:HG22	1:O:311:LYS:N	2.16	0.60
1:A:43:MET:O	1:A:45:TYR:N	2.34	0.60
1:B:324:ASN:O	1:B:328:ASP:HB2	2.00	0.60
1:C:138:ASN:C	1:C:140:ASP:H	2.04	0.60
1:O:245:VAL:HG12	1:O:246:ASP:N	2.16	0.60
1:B:215:ALA:HA	1:B:218:ALA:HB3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:8:ILE:HG22	1:C:10:GLY:H	1.66	0.60
1:B:140:ASP:C	1:B:142:TYR:H	2.03	0.60
1:O:309:PHE:CZ	1:C:176:LEU:HG	2.36	0.60
1:A:18:VAL:HG13	1:A:327:ILE:CD1	2.31	0.60
1:B:261:LYS:HE3	1:B:299:ALA:HB1	1.84	0.60
1:O:177:MET:SD	1:O:177:MET:C	2.79	0.60
1:A:55:GLN:OE1	1:A:57:LYS:CG	2.50	0.60
1:B:16:ARG:HD2	1:B:47:PHE:HA	1.84	0.59
1:B:121:VAL:HB	1:B:148:ILE:HD13	1.83	0.59
1:B:244:VAL:CG2	1:B:313:VAL:HG13	2.32	0.59
1:O:160:ALA:HB3	1:O:161:PRO:HD3	1.84	0.59
1:C:38:ILE:CG1	1:C:46:MET:HE2	2.29	0.59
1:O:284:VAL:HB	1:C:207:ASN:HD22	1.67	0.59
1:A:175:GLY:CA	1:A:249:VAL:HG23	2.31	0.59
1:O:106:ASP:OD1	1:O:128:LYS:HE2	2.03	0.59
1:A:11:PHE:HZ	1:A:47:PHE:HD2	1.50	0.59
1:C:64:LYS:O	1:C:68:THR:HG23	2.03	0.59
1:A:244:VAL:CG2	1:A:313:VAL:HG23	2.32	0.59
1:A:251:ILE:HD13	1:A:251:ILE:N	2.16	0.59
1:B:281:GLU:O	1:B:283:LEU:N	2.35	0.59
1:C:154:CYS:SG	1:C:181:HIS:CE1	2.95	0.59
1:C:264:ILE:HD12	1:C:297:PHE:CD1	2.38	0.59
1:O:202:ARG:HG3	1:C:284:VAL:HG11	1.84	0.59
1:O:288:PHE:CD1	1:O:315:TRP:CG	2.88	0.59
1:A:254:ALA:HB2	1:A:308:ASN:ND2	2.16	0.59
1:B:56:TRP:CD1	1:B:61:ILE:HD11	2.38	0.59
1:O:191:ASP:HA	1:O:202:ARG:HA	1.83	0.59
1:O:190:VAL:CG2	1:B:185:ALA:HB2	2.32	0.59
1:O:226:LEU:HA	1:O:229:LYS:HD2	1.85	0.59
1:B:324:ASN:HD22	1:B:324:ASN:H	1.50	0.59
1:C:127:SER:CB	1:C:130:ALA:HB3	2.33	0.59
1:C:199:ARG:HB3	1:C:209:ILE:HG23	1.84	0.59
1:O:187:GLN:HB3	1:O:204:ALA:HB2	1.85	0.59
1:A:230:LEU:O	1:A:231:THR:HB	2.02	0.59
1:O:72:GLY:O	1:O:73:GLU:HB2	2.01	0.59
1:O:79:PHE:HB3	1:O:81:ILE:CD1	2.33	0.59
1:A:298:ASP:OD1	1:A:301:ALA:HB2	2.03	0.59
1:C:65:ASP:OD2	1:C:65:ASP:C	2.42	0.59
1:C:329:LEU:O	1:C:333:MET:N	2.34	0.59
1:O:170:PHE:CZ	1:O:260:ILE:HD12	2.37	0.58
1:O:202:ARG:NH1	1:C:284:VAL:HG22	2.17	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:261:LYS:HE3	1:O:299:ALA:HB1	1.84	0.58
1:B:16:ARG:O	1:B:20:ARG:HG3	2.02	0.58
1:C:9:ASN:O	1:C:101:THR:HG23	2.03	0.58
1:O:157:ASN:O	1:O:294:SER:HB3	2.03	0.58
1:O:166:ILE:H	1:O:166:ILE:CD1	2.16	0.58
1:A:48:LYS:HE2	1:A:49:TYR:CE1	2.39	0.58
1:B:230:LEU:O	1:B:231:THR:HB	2.02	0.58
1:C:215:ALA:CA	2:C:6926:SO4:O3	2.50	0.58
1:O:183:ILE:HG23	1:O:237:VAL:O	2.03	0.58
1:B:257:TYR:O	1:B:261:LYS:HG3	2.03	0.58
1:C:172:ILE:HG12	1:C:249:VAL:HG21	1.84	0.58
1:A:44:THR:HG23	1:A:69:LEU:HD11	1.84	0.58
1:O:315:TRP:O	1:O:316:TYR:HB3	2.04	0.58
1:B:40:THR:OG1	1:B:78:VAL:HG21	2.04	0.58
1:C:14:ILE:O	1:C:18:VAL:HG23	2.04	0.58
1:O:205:SER:O	1:O:206:PHE:CD1	2.57	0.58
1:A:172:ILE:C	1:A:173:ILE:HD12	2.24	0.58
1:B:22:ALA:HB2	1:B:327:ILE:HD13	1.85	0.58
1:O:178:THR:HG23	1:O:233:MET:HG3	1.86	0.58
1:O:305:LEU:HD11	1:C:228:GLY:O	2.04	0.58
1:B:11:PHE:CD2	1:B:16:ARG:HG2	2.39	0.58
1:O:278:TYR:OH	1:O:280:GLU:OE1	2.13	0.58
1:B:27:ASP:OD2	1:B:331:ARG:HG3	2.03	0.58
1:B:152:ALA:HB1	1:B:156:THR:HB	1.86	0.58
1:C:61:ILE:HD13	1:C:71:LEU:CD1	2.33	0.58
1:O:155:THR:O	1:O:157:ASN:N	2.37	0.57
1:C:241:ASP:OD1	1:C:319:GLU:HG3	2.04	0.57
1:O:155:THR:HG22	1:O:156:THR:N	2.20	0.57
1:O:193:PRO:HB3	1:B:38:ILE:CD1	2.33	0.57
1:A:42:TYR:CD1	1:C:198:TRP:NE1	2.71	0.57
1:A:162:LEU:O	1:A:166:ILE:HD13	2.04	0.57
1:B:275:ILE:O	1:B:275:ILE:HG22	2.03	0.57
1:B:325:ARG:HA	1:B:325:ARG:NE	2.20	0.57
1:C:16:ARG:NH1	1:C:16:ARG:HG3	2.18	0.57
1:O:9:ASN:HD22	1:O:89:TRP:HZ2	1.52	0.57
1:O:57:LYS:HE3	1:O:57:LYS:CA	2.34	0.57
1:A:111:ALA:HB1	1:A:114:LEU:HD12	1.86	0.57
1:A:208:ILE:HD11	3:B:6956:HOH:O	2.03	0.57
1:C:110:ALA:CB	1:C:123:ILE:HD11	2.35	0.57
1:O:81:ILE:CD1	1:O:88:PRO:HD2	2.32	0.57
1:A:179:THR:HG23	1:A:234:SER:CB	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:158:CYS:C	1:C:161:PRO:HD2	2.23	0.57
1:O:48:LYS:CG	1:O:49:TYR:HE2	2.17	0.57
1:O:57:LYS:HE3	1:O:57:LYS:H	1.69	0.57
1:O:81:ILE:HD13	1:O:88:PRO:CD	2.35	0.57
1:A:107:LYS:HA	1:A:148:ILE:HG21	1.87	0.57
1:O:106:ASP:CB	1:O:128:LYS:HE2	2.35	0.57
1:A:16:ARG:O	1:A:19:ALA:HB3	2.05	0.57
1:A:66:SER:O	1:A:68:THR:N	2.38	0.57
1:O:260:ILE:N	1:O:260:ILE:CD1	2.68	0.57
1:B:160:ALA:HB3	1:B:161:PRO:CD	2.30	0.57
1:O:166:ILE:HD12	1:O:166:ILE:N	2.20	0.56
1:O:281:GLU:O	1:O:283:LEU:HG	2.05	0.56
1:A:23:LEU:HD21	1:A:71:LEU:HG	1.85	0.56
1:B:181:HIS:O	1:B:236:ARG:HD3	2.05	0.56
1:C:16:ARG:HG3	1:C:16:ARG:HH11	1.70	0.56
1:C:34:ASN:CB	1:C:79:PHE:HB2	2.34	0.56
1:C:176:LEU:HD22	1:C:231:THR:HG23	1.87	0.56
1:A:24:GLN:HG3	1:A:56:TRP:CH2	2.39	0.56
1:C:213:THR:HG23	1:C:213:THR:O	2.06	0.56
1:O:82:ARG:HB2	1:O:82:ARG:NH1	2.17	0.56
1:O:206:PHE:HE2	1:B:240:VAL:HA	1.67	0.56
1:O:240:VAL:HG22	1:O:241:ASP:N	2.19	0.56
1:A:31:VAL:C	1:A:76:VAL:HG13	2.25	0.56
1:C:106:ASP:HB2	1:C:109:LYS:HB2	1.87	0.56
1:C:211:SER:OG	1:C:212:SER:N	2.39	0.56
1:A:113:HIS:HB2	1:A:121:VAL:CG2	2.36	0.56
1:A:173:ILE:HD13	1:A:251:ILE:HA	1.87	0.56
1:O:199:ARG:HD3	1:C:283:LEU:O	2.06	0.56
1:O:239:THR:HG21	1:C:208:ILE:HG13	1.86	0.56
1:O:240:VAL:HA	1:B:206:PHE:HE1	1.70	0.56
1:O:286:THR:OG1	1:C:207:ASN:ND2	2.39	0.56
1:O:68:THR:HG22	1:O:69:LEU:N	2.21	0.56
1:O:182:ALA:HB1	1:O:239:THR:O	2.06	0.56
1:A:42:TYR:HE1	1:C:198:TRP:CG	2.23	0.56
1:A:282:ASP:HB3	1:B:199:ARG:HG2	1.87	0.56
1:A:24:GLN:HG3	1:A:56:TRP:HH2	1.71	0.56
1:B:6:ILE:HD12	1:B:28:VAL:HG12	1.86	0.56
1:C:81:ILE:CD1	1:C:87:ILE:HA	2.36	0.56
1:C:173:ILE:HD12	1:C:250:ARG:HD2	1.88	0.56
1:C:264:ILE:HD12	1:C:297:PHE:CD2	2.41	0.56
1:C:272:LEU:CB	1:C:276:ILE:HD13	2.29	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:83:ASN:HB2	1:O:86:GLU:HG3	1.87	0.56
1:A:22:ALA:HA	1:A:28:VAL:HG13	1.88	0.56
1:A:216:ALA:HB3	1:A:231:THR:HA	1.88	0.56
1:C:181:HIS:HB3	1:C:236:ARG:CD	2.36	0.56
1:O:206:PHE:CE2	1:B:240:VAL:CG2	2.88	0.56
1:B:272:LEU:O	1:B:276:ILE:HG22	2.06	0.56
1:O:112:ALA:HA	1:O:115:LYS:HZ3	1.69	0.55
1:A:9:ASN:HD22	1:A:113:HIS:HE1	1.54	0.55
1:A:245:VAL:O	1:A:313:VAL:HA	2.06	0.55
1:B:49:TYR:CD1	1:C:283:LEU:HD11	2.41	0.55
1:C:242:VAL:HA	1:C:317:ASP:HA	1.88	0.55
1:O:245:VAL:CG1	1:O:246:ASP:N	2.68	0.55
1:C:13:ARG:NH2	1:C:319:GLU:OE1	2.39	0.55
1:C:134:VAL:HG23	1:C:222:VAL:HG11	1.88	0.55
1:A:21:VAL:HG11	1:A:327:ILE:HG13	1.88	0.55
1:A:207:ASN:HD22	1:B:284:VAL:CG2	2.19	0.55
1:B:20:ARG:O	1:B:24:GLN:HB2	2.06	0.55
1:C:25:SER:OG	1:C:28:VAL:HB	2.06	0.55
1:C:101:THR:O	1:C:103:VAL:HG23	2.06	0.55
1:C:178:THR:O	1:C:246:ASP:HB3	2.06	0.55
1:C:276:ILE:HD12	1:C:276:ILE:N	2.21	0.55
1:O:256:SER:O	1:O:260:ILE:CD1	2.55	0.55
1:B:280:GLU:HG2	1:B:299:ALA:HB3	1.89	0.55
1:C:137:VAL:HG12	1:C:138:ASN:N	2.21	0.55
1:O:44:THR:HG22	1:O:69:LEU:CD1	2.34	0.55
1:O:134:VAL:CG2	1:O:222:VAL:HG11	2.36	0.55
1:O:242:VAL:HG21	1:O:285:SER:O	2.06	0.55
1:A:9:ASN:O	1:A:101:THR:HG22	2.05	0.55
1:B:156:THR:HG23	1:B:219:VAL:HG22	1.89	0.55
1:B:158:CYS:HA	1:B:295:SER:HB2	1.89	0.55
1:A:42:TYR:CE1	1:C:198:TRP:CG	2.95	0.55
1:C:134:VAL:HG22	1:C:152:ALA:CB	2.36	0.55
1:O:115:LYS:H	1:O:115:LYS:HD2	1.70	0.55
1:A:318:ASN:ND2	1:A:319:GLU:HG3	2.20	0.55
1:B:17:LEU:CD1	1:B:319:GLU:HB3	2.37	0.55
1:B:265:LYS:O	1:B:269:GLU:HG3	2.07	0.55
1:C:11:PHE:N	1:C:35:ASP:HB2	2.22	0.55
1:A:97:VAL:HG11	1:A:113:HIS:CG	2.42	0.55
1:A:153:SER:HB2	2:A:6923:SO4:O4	2.07	0.55
1:A:167:HIS:HB2	1:A:172:ILE:CD1	2.37	0.55
1:B:49:TYR:CE1	1:C:283:LEU:HD11	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:283:LEU:HG	1:C:287:ASP:OD2	2.06	0.55
1:O:8:ILE:O	1:O:33:VAL:HA	2.07	0.54
1:O:48:LYS:CG	1:O:49:TYR:CD2	2.90	0.54
1:O:181:HIS:O	1:O:237:VAL:HG22	2.07	0.54
1:O:267:ALA:O	1:O:272:LEU:HB2	2.07	0.54
1:A:66:SER:C	1:A:68:THR:N	2.61	0.54
1:B:23:LEU:CD1	1:B:71:LEU:HG	2.38	0.54
1:C:3:LYS:HE2	1:C:26:GLU:O	2.06	0.54
1:C:17:LEU:HD23	1:C:20:ARG:HD2	1.89	0.54
1:O:288:PHE:HD1	1:O:315:TRP:HB3	1.72	0.54
1:C:177:MET:HG3	1:C:245:VAL:HG13	1.90	0.54
1:O:49:TYR:N	1:O:49:TYR:HD2	2.06	0.54
1:A:265:LYS:HB2	1:A:278:TYR:CD1	2.41	0.54
1:C:73:GLU:CB	1:C:74:LYS:HE3	2.35	0.54
1:A:294:SER:OG	1:A:325:ARG:HD2	2.07	0.54
1:B:325:ARG:HG2	1:B:325:ARG:NH1	2.19	0.54
1:C:61:ILE:CD1	1:C:71:LEU:HD12	2.35	0.54
1:O:287:ASP:OD1	1:A:49:TYR:HB3	2.07	0.54
1:B:38:ILE:HD13	1:B:38:ILE:N	2.23	0.54
1:B:103:VAL:O	1:B:105:THR:N	2.39	0.54
1:O:62:LYS:HE2	1:O:70:LEU:HD23	1.87	0.54
1:O:205:SER:C	1:O:206:PHE:CD1	2.80	0.54
1:O:208:ILE:HD12	1:C:315:TRP:CZ3	2.41	0.54
1:B:71:LEU:HD22	1:B:71:LEU:N	2.22	0.54
1:B:17:LEU:HD21	1:B:53:HIS:CD2	2.42	0.54
1:C:84:PRO:HA	1:C:87:ILE:CD1	2.37	0.54
1:C:276:ILE:HG22	1:C:277:GLY:N	2.23	0.54
1:O:40:THR:O	1:O:44:THR:HG23	2.07	0.54
1:A:173:ILE:HD11	1:A:252:GLU:CA	2.37	0.54
1:B:132:MET:HA	1:B:150:SER:O	2.08	0.54
1:O:284:VAL:CG1	1:C:209:ILE:HG12	2.37	0.54
1:O:309:PHE:CE2	1:C:176:LEU:HG	2.43	0.54
1:A:38:ILE:HG13	1:A:43:MET:HE2	1.90	0.54
1:B:61:ILE:HD12	1:B:61:ILE:N	2.23	0.54
1:O:48:LYS:HG2	1:O:49:TYR:HD2	1.72	0.54
1:O:120:LYS:HD3	1:O:147:ASP:OD1	2.08	0.54
1:A:42:TYR:CZ	1:A:46:MET:HE3	2.26	0.54
1:A:87:ILE:HD13	1:A:89:TRP:CZ2	2.43	0.54
1:A:208:ILE:CD1	3:B:6956:HOH:O	2.55	0.54
1:C:159:LEU:HD22	1:C:177:MET:SD	2.48	0.54
1:B:152:ALA:HB3	1:B:157:ASN:ND2	2.22	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:158:CYS:SG	1:C:245:VAL:CG2	2.96	0.53
1:A:60:ASP:OD2	1:A:60:ASP:N	2.41	0.53
1:C:148:ILE:N	1:C:148:ILE:HD12	2.23	0.53
1:O:32:ALA:HA	1:O:77:THR:O	2.08	0.53
1:O:84:PRO:HB2	1:O:112:ALA:HB3	1.88	0.53
1:O:120:LYS:HE2	1:O:146:ILE:O	2.08	0.53
1:C:272:LEU:HD13	1:C:276:ILE:HD13	1.88	0.53
1:O:131:PRO:HD2	1:O:148:ILE:O	2.08	0.53
1:O:99:GLU:CB	1:O:123:ILE:HA	2.31	0.53
1:O:282:ASP:HA	1:C:199:ARG:NE	2.18	0.53
1:A:9:ASN:ND2	1:A:34:ASN:HD22	2.07	0.53
1:A:308:ASN:O	1:A:309:PHE:HB2	2.08	0.53
1:O:106:ASP:HB3	1:O:128:LYS:HE2	1.91	0.53
1:O:165:VAL:HG21	1:O:276:ILE:HD13	1.91	0.53
1:O:241:ASP:O	1:O:242:VAL:HB	2.08	0.53
1:O:271:LYS:HG3	1:O:272:LEU:N	2.24	0.53
1:A:114:LEU:HD11	1:A:148:ILE:CD1	2.32	0.53
1:A:124:SER:O	1:A:125:ALA:HB2	2.09	0.53
1:A:252:GLU:OE2	1:A:252:GLU:CA	2.55	0.53
1:C:87:ILE:HG21	1:C:89:TRP:CZ2	2.44	0.53
1:O:144:SER:O	1:O:146:ILE:N	2.42	0.53
1:B:8:ILE:HD12	1:B:8:ILE:N	2.24	0.53
1:B:322:TYR:O	1:B:325:ARG:HB2	2.08	0.53
1:A:49:TYR:HD1	1:A:55:GLN:HG3	1.74	0.53
1:A:173:ILE:HD11	1:A:252:GLU:H	1.70	0.53
1:A:183:ILE:HG22	1:A:187:GLN:NE2	2.24	0.53
1:A:202:ARG:HH21	1:C:51:THR:H	1.57	0.53
1:B:288:PHE:CE2	1:B:315:TRP:HB2	2.40	0.53
1:B:329:LEU:O	1:B:333:MET:HB2	2.08	0.53
1:C:36:PRO:HA	1:C:80:GLY:HA2	1.90	0.53
1:O:44:THR:OG1	1:O:45:TYR:N	2.42	0.53
1:O:49:TYR:CE1	1:A:283:LEU:HD22	2.44	0.53
1:O:206:PHE:CD2	1:B:240:VAL:CB	2.81	0.53
1:B:52:VAL:HG11	1:B:241:ASP:HB2	1.90	0.53
1:A:39:THR:HG22	1:A:40:THR:N	2.24	0.53
1:A:85:ASP:HA	1:A:112:ALA:O	2.08	0.53
1:B:105:THR:HA	1:B:123:ILE:HD12	1.91	0.53
1:O:65:ASP:OD1	1:O:65:ASP:O	2.26	0.52
1:A:17:LEU:HD23	1:A:20:ARG:HD2	1.91	0.52
1:A:285:SER:HA	1:A:315:TRP:HZ3	1.72	0.52
1:B:265:LYS:HE2	1:B:269:GLU:OE1	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:215:ALA:N	2:C:6926:SO4:O3	2.42	0.52
1:O:296:ILE:O	1:O:314:ALA:HA	2.09	0.52
1:A:42:TYR:CE2	1:A:46:MET:HE2	2.01	0.52
1:B:219:VAL:HA	1:B:222:VAL:HG22	1.90	0.52
1:B:261:LYS:HB3	1:B:278:TYR:OH	2.09	0.52
1:C:35:ASP:CG	1:C:38:ILE:HD12	2.29	0.52
1:A:189:THR:HB	1:C:183:ILE:HD12	1.91	0.52
1:B:160:ALA:CB	1:B:161:PRO:HD3	2.33	0.52
1:A:207:ASN:HB2	1:A:209:ILE:HD11	1.92	0.52
1:B:6:ILE:HD12	1:B:28:VAL:CG1	2.40	0.52
1:B:251:ILE:HG13	1:B:308:ASN:HA	1.91	0.52
1:B:303:ILE:HG22	1:B:311:LYS:HB3	1.91	0.52
1:C:18:VAL:HG12	1:C:327:ILE:HD11	1.92	0.52
1:C:97:VAL:HB	1:C:121:VAL:HG22	1.92	0.52
1:C:176:LEU:HD22	1:C:231:THR:CG2	2.39	0.52
1:O:113:HIS:CB	1:O:121:VAL:HG21	2.39	0.52
1:A:42:TYR:CD1	1:C:198:TRP:CD2	2.97	0.52
1:B:134:VAL:CG2	1:B:222:VAL:HG11	2.37	0.52
1:A:36:PRO:CB	1:A:82:ARG:HE	2.23	0.52
1:A:42:TYR:OH	1:A:46:MET:HE3	2.05	0.52
1:A:48:LYS:HG2	1:A:49:TYR:CD1	2.45	0.52
1:A:265:LYS:HB2	1:A:278:TYR:CE1	2.45	0.52
1:C:127:SER:HB3	1:C:130:ALA:HB3	1.91	0.52
1:O:9:ASN:HD21	1:O:87:ILE:HD13	1.75	0.52
1:O:36:PRO:HG3	1:O:80:GLY:C	2.30	0.52
1:O:123:ILE:HD11	1:O:148:ILE:CG2	2.40	0.52
1:O:132:MET:HA	1:O:150:SER:O	2.10	0.52
1:O:153:SER:O	1:O:154:CYS:C	2.48	0.52
1:A:167:HIS:HB2	1:A:172:ILE:HD12	1.91	0.52
1:O:23:LEU:O	1:O:24:GLN:HB2	2.09	0.52
1:O:40:THR:CG2	1:O:69:LEU:HD13	2.39	0.52
1:O:49:TYR:CD2	1:O:49:TYR:N	2.76	0.52
1:O:142:TYR:CE1	1:O:146:ILE:HB	2.45	0.52
1:O:193:PRO:CB	1:B:38:ILE:HD11	2.40	0.52
1:B:63:ILE:HD12	1:B:63:ILE:N	2.24	0.52
1:A:207:ASN:HB2	1:A:209:ILE:CD1	2.40	0.52
1:C:10:GLY:HA3	1:C:100:SER:C	2.30	0.52
1:C:63:ILE:N	1:C:63:ILE:HD12	2.24	0.52
1:C:167:HIS:ND1	1:C:226:LEU:HD21	2.25	0.52
1:O:52:VAL:HG11	1:O:241:ASP:OD1	2.10	0.51
1:B:24:GLN:NE2	1:B:58:HIS:HB3	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:285:SER:HB2	3:B:6956:HOH:O	2.07	0.51
1:C:138:ASN:C	1:C:140:ASP:N	2.62	0.51
1:C:264:ILE:O	1:C:268:SER:HB3	2.10	0.51
1:O:162:LEU:O	1:O:166:ILE:CD1	2.53	0.51
1:O:184:THR:HG23	1:O:236:ARG:NH2	2.25	0.51
1:O:311:LYS:HB2	1:C:176:LEU:CD1	2.41	0.51
1:A:254:ALA:HA	1:A:307:ASP:O	2.09	0.51
1:B:161:PRO:O	1:B:164:LYS:HB3	2.10	0.51
1:B:324:ASN:N	1:B:324:ASN:ND2	2.53	0.51
1:C:173:ILE:HB	1:C:250:ARG:O	2.11	0.51
1:C:250:ARG:HD3	1:C:308:ASN:O	2.10	0.51
1:C:327:ILE:O	1:C:330:ILE:N	2.40	0.51
1:O:66:SER:O	1:O:67:LYS:HG3	2.11	0.51
1:A:13:ARG:NH2	1:A:52:VAL:CG1	2.72	0.51
1:B:107:LYS:O	1:B:111:ALA:HB2	2.09	0.51
1:C:81:ILE:HD12	1:C:87:ILE:HG23	1.91	0.51
1:O:261:LYS:HA	1:O:297:PHE:HE2	1.75	0.51
1:O:310:VAL:HG22	1:O:311:LYS:H	1.75	0.51
1:B:219:VAL:HA	1:B:222:VAL:CG2	2.41	0.51
1:B:332:HIS:C	1:B:332:HIS:ND1	2.64	0.51
1:C:172:ILE:HG23	1:C:249:VAL:HG23	1.91	0.51
1:O:57:LYS:HZ3	1:O:61:ILE:CD1	2.08	0.51
1:O:176:LEU:HB3	1:C:311:LYS:HE2	1.93	0.51
1:B:126:PRO:CD	1:B:153:SER:HB3	2.41	0.51
1:B:228:GLY:O	1:B:230:LEU:N	2.44	0.51
1:O:104:PHE:O	1:O:110:ALA:HB2	2.10	0.51
1:O:202:ARG:NH1	1:B:45:TYR:OH	2.42	0.51
1:O:250:ARG:HH11	1:O:250:ARG:HB2	1.76	0.51
1:B:121:VAL:HB	1:B:148:ILE:CD1	2.40	0.51
1:C:143:THR:O	1:C:145:ASP:N	2.44	0.51
1:O:57:LYS:HE3	1:O:57:LYS:N	2.26	0.51
1:O:113:HIS:HB2	1:O:121:VAL:HG21	1.92	0.51
1:C:17:LEU:HD22	1:C:320:TRP:HE3	1.75	0.51
1:O:63:ILE:H	1:O:63:ILE:CD1	2.19	0.51
1:A:207:ASN:ND2	1:B:286:THR:OG1	2.43	0.51
1:B:164:LYS:HG3	1:B:168:ASP:OD2	2.11	0.51
1:C:166:ILE:HG13	1:C:312:LEU:CD1	2.41	0.51
1:O:6:ILE:HA	1:O:96:TYR:O	2.10	0.51
1:B:272:LEU:HD23	1:B:275:ILE:HG22	1.92	0.51
1:A:63:ILE:N	1:A:63:ILE:HD12	2.26	0.50
1:B:51:THR:O	1:B:51:THR:HG22	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:177:MET:CE	1:B:179:THR:HG23	2.42	0.50
1:C:328:ASP:HA	1:C:331:ARG:HD2	1.93	0.50
1:C:31:VAL:C	1:C:76:VAL:HG13	2.32	0.50
1:C:181:HIS:CB	1:C:236:ARG:HE	2.16	0.50
1:C:264:ILE:HG21	1:C:297:PHE:HB2	1.92	0.50
1:O:49:TYR:HE1	1:A:283:LEU:HD13	1.76	0.50
1:O:294:SER:OG	1:O:325:ARG:HD2	2.11	0.50
1:A:276:ILE:HG13	1:A:277:GLY:N	2.26	0.50
1:B:24:GLN:HE21	1:B:58:HIS:HB3	1.76	0.50
1:C:181:HIS:HB3	1:C:236:ARG:HD3	1.92	0.50
1:O:176:LEU:CD2	1:O:231:THR:HG23	2.41	0.50
1:B:77:THR:HG22	1:B:78:VAL:N	2.25	0.50
1:O:60:ASP:C	1:O:61:ILE:HD12	2.31	0.50
1:O:159:LEU:HD13	1:O:177:MET:HG3	1.92	0.50
1:B:17:LEU:HD22	1:B:320:TRP:HE3	1.76	0.50
1:B:112:ALA:O	1:B:113:HIS:C	2.50	0.50
1:C:52:VAL:HG22	1:C:240:VAL:HG21	1.93	0.50
1:A:137:VAL:HG21	1:A:160:ALA:HB1	1.92	0.50
1:A:215:ALA:O	1:A:219:VAL:HG23	2.11	0.50
1:A:305:LEU:HD13	1:B:231:THR:CG2	2.40	0.50
1:B:29:GLU:O	1:B:31:VAL:HG13	2.12	0.50
1:B:288:PHE:CE2	1:B:315:TRP:CD1	2.92	0.50
1:C:244:VAL:HG12	1:C:245:VAL:N	2.26	0.50
1:C:324:ASN:O	1:C:325:ARG:C	2.50	0.50
1:A:30:LEU:HD22	1:A:76:VAL:HG11	1.93	0.50
1:B:228:GLY:C	1:B:230:LEU:H	2.14	0.50
1:C:244:VAL:HG22	1:C:315:TRP:CD2	2.47	0.50
1:C:289:VAL:HA	1:C:317:ASP:OD2	2.12	0.50
1:C:296:ILE:N	1:C:296:ILE:HD12	2.25	0.50
1:O:222:VAL:CG2	1:O:223:LEU:H	2.21	0.50
1:A:97:VAL:O	1:A:121:VAL:HG13	2.12	0.50
1:B:30:LEU:HD23	1:B:31:VAL:N	2.26	0.50
1:C:96:TYR:OH	1:C:334:ALA:HB2	2.11	0.50
1:C:156:THR:O	1:C:158:CYS:N	2.40	0.50
1:O:9:ASN:O	1:O:101:THR:HG22	2.11	0.50
1:B:18:VAL:CG1	1:B:327:ILE:HD11	2.42	0.50
1:B:81:ILE:CD1	1:B:87:ILE:HA	2.41	0.50
1:C:291:ASP:OD1	1:C:293:ARG:HB2	2.11	0.50
1:A:159:LEU:HD22	1:A:177:MET:SD	2.52	0.49
1:C:148:ILE:HD12	1:C:148:ILE:H	1.76	0.49
1:O:231:THR:OG1	1:O:232:GLY:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:255:ALA:N	1:O:307:ASP:HB3	2.27	0.49
1:A:304:ALA:HB1	1:A:310:VAL:HG12	1.93	0.49
1:B:33:VAL:HG12	1:B:34:ASN:N	2.27	0.49
1:B:107:LYS:HA	1:B:148:ILE:HG21	1.94	0.49
1:O:137:VAL:HG11	1:O:223:LEU:HD22	1.93	0.49
1:A:291:ASP:OD1	1:A:293:ARG:NE	2.45	0.49
1:C:323:SER:O	1:C:326:VAL:HB	2.13	0.49
1:A:174:GLU:OE1	1:B:306:ASN:ND2	2.32	0.49
1:A:203:ALA:HB1	1:A:206:PHE:HB2	1.93	0.49
1:C:95:GLU:O	1:C:119:LYS:HB2	2.12	0.49
1:C:250:ARG:HG2	1:C:250:ARG:HH21	1.78	0.49
1:O:193:PRO:HB3	1:B:38:ILE:HD11	1.93	0.49
1:O:193:PRO:HG3	1:B:38:ILE:HD11	1.94	0.49
1:C:176:LEU:O	1:C:247:LEU:HD12	2.11	0.49
1:O:126:PRO:HG3	1:O:153:SER:HB3	1.94	0.49
1:O:282:ASP:HB3	1:C:199:ARG:CG	2.42	0.49
1:A:158:CYS:O	1:A:161:PRO:HD2	2.12	0.49
1:B:296:ILE:O	1:B:314:ALA:HA	2.12	0.49
1:B:322:TYR:C	1:B:322:TYR:CD2	2.85	0.49
1:C:180:VAL:HG12	1:C:237:VAL:HG22	1.94	0.49
1:O:155:THR:O	1:O:158:CYS:N	2.43	0.49
1:A:158:CYS:HB2	1:A:294:SER:O	2.13	0.49
1:B:106:ASP:O	1:B:107:LYS:C	2.50	0.49
1:C:244:VAL:CG1	1:C:245:VAL:N	2.76	0.49
1:O:22:ALA:O	1:O:24:GLN:N	2.44	0.49
1:O:106:ASP:OD1	1:O:128:LYS:HG2	2.13	0.49
1:A:84:PRO:HA	1:A:87:ILE:CD1	2.43	0.49
1:A:200:GLY:HA2	1:A:209:ILE:HG21	1.94	0.49
1:B:158:CYS:SG	1:B:316:TYR:CD2	3.06	0.49
1:B:199:ARG:HH11	1:B:210:PRO:CG	2.24	0.49
1:B:276:ILE:HG13	1:B:295:SER:O	2.12	0.49
1:B:303:ILE:HG12	1:B:304:ALA:N	2.27	0.49
1:C:250:ARG:HA	1:C:308:ASN:O	2.12	0.49
1:A:29:GLU:CG	1:A:74:LYS:HZ1	2.23	0.49
1:A:135:CYS:HB2	1:A:325:ARG:HD3	1.94	0.49
1:A:142:TYR:CZ	1:A:333:MET:HG2	2.48	0.49
1:C:153:SER:HB2	2:C:6926:SO4:O1	2.13	0.49
1:O:244:VAL:HG22	1:O:245:VAL:O	2.12	0.48
1:B:226:LEU:HA	1:B:229:LYS:HD2	1.94	0.48
1:B:254:ALA:HA	1:B:307:ASP:O	2.13	0.48
1:O:48:LYS:C	1:O:49:TYR:HD2	2.17	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:257:TYR:CE2	1:O:261:LYS:HD2	2.48	0.48
1:B:18:VAL:HG13	1:B:327:ILE:HD11	1.94	0.48
1:O:103:VAL:HG23	1:O:104:PHE:CE2	2.47	0.48
1:B:117:GLY:O	1:B:118:ALA:C	2.52	0.48
1:O:283:LEU:HD13	1:O:288:PHE:CE2	2.48	0.48
1:A:208:ILE:HG13	3:B:6956:HOH:O	2.13	0.48
1:A:256:SER:O	1:A:259:ALA:HB3	2.13	0.48
1:A:265:LYS:HD2	1:A:278:TYR:CE2	2.48	0.48
1:A:285:SER:CA	1:A:315:TRP:CZ3	2.97	0.48
1:B:49:TYR:HE2	1:C:281:GLU:OE2	1.96	0.48
1:C:62:LYS:O	1:C:70:LEU:HB3	2.14	0.48
1:B:14:ILE:O	1:B:18:VAL:HG23	2.12	0.48
1:B:101:THR:OG1	1:B:103:VAL:HG22	2.13	0.48
1:C:38:ILE:HG21	1:C:46:MET:HE2	1.96	0.48
1:A:139:GLU:H	1:A:139:GLU:CD	2.17	0.48
1:A:284:VAL:HG12	1:B:209:ILE:HA	1.95	0.48
1:B:77:THR:CG2	1:B:78:VAL:N	2.76	0.48
1:B:139:GLU:HG2	1:B:139:GLU:O	2.12	0.48
1:B:219:VAL:HG12	1:B:219:VAL:O	2.14	0.48
1:B:272:LEU:HD23	1:B:275:ILE:CG2	2.43	0.48
1:O:13:ARG:HG2	1:O:319:GLU:OE2	2.13	0.48
1:O:36:PRO:HG2	1:O:82:ARG:HG2	1.94	0.48
1:O:115:LYS:O	1:O:116:GLY:C	2.51	0.48
1:A:305:LEU:O	1:A:306:ASN:HB3	2.14	0.48
1:C:14:ILE:HD12	1:C:14:ILE:N	2.26	0.48
1:C:160:ALA:HB3	1:C:161:PRO:HD3	1.94	0.48
1:O:7:GLY:O	1:O:97:VAL:HG13	2.14	0.48
1:A:130:ALA:CB	1:A:148:ILE:HG22	2.44	0.48
1:A:233:MET:CE	1:B:301:ALA:O	2.62	0.48
1:A:309:PHE:HE2	1:B:175:GLY:N	2.07	0.48
1:B:40:THR:O	1:B:43:MET:HB3	2.12	0.48
1:C:11:PHE:CE2	1:C:43:MET:HG3	2.48	0.48
1:A:84:PRO:C	1:A:86:GLU:H	2.17	0.48
1:C:110:ALA:HB3	1:C:123:ILE:HD11	1.95	0.48
1:C:180:VAL:O	1:C:243:SER:HB3	2.13	0.48
1:C:322:TYR:O	1:C:324:ASN:N	2.47	0.48
1:O:245:VAL:HG23	1:O:316:TYR:HE2	1.75	0.47
1:A:49:TYR:CD1	1:A:55:GLN:HG3	2.49	0.47
1:A:84:PRO:HB2	1:A:112:ALA:CB	2.43	0.47
1:A:166:ILE:HD11	1:A:264:ILE:HD11	1.95	0.47
1:B:107:LYS:O	1:B:111:ALA:N	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:283:LEU:HD21	1:C:49:TYR:CZ	2.49	0.47
1:C:82:ARG:O	1:C:82:ARG:HG2	2.14	0.47
1:C:292:SER:HA	1:C:321:GLY:HA2	1.96	0.47
1:O:65:ASP:O	1:O:66:SER:C	2.51	0.47
1:A:171:GLY:O	1:A:251:ILE:HA	2.14	0.47
1:A:175:GLY:HA2	1:B:309:PHE:CE2	2.49	0.47
1:B:65:ASP:O	1:B:67:LYS:N	2.47	0.47
1:C:34:ASN:CG	1:C:34:ASN:O	2.51	0.47
1:O:183:ILE:O	1:O:183:ILE:CD1	2.55	0.47
1:A:90:ALA:HB2	1:A:117:GLY:O	2.14	0.47
1:C:322:TYR:O	1:C:323:SER:C	2.53	0.47
1:O:21:VAL:HG12	1:O:21:VAL:O	2.13	0.47
1:O:112:ALA:HA	1:O:115:LYS:HZ2	1.76	0.47
1:A:11:PHE:HZ	1:A:47:PHE:CD2	2.31	0.47
1:A:287:ASP:CG	1:B:202:ARG:HH22	2.17	0.47
1:C:244:VAL:CG2	1:C:315:TRP:CE3	2.98	0.47
1:C:247:LEU:HD12	1:C:248:THR:N	2.29	0.47
1:C:334:ALA:C	1:C:336:THR:H	2.18	0.47
1:O:215:ALA:HB2	2:O:6921:SO4:O4	2.14	0.47
1:A:113:HIS:HB2	1:A:121:VAL:HG21	1.96	0.47
1:B:22:ALA:C	1:B:24:GLN:H	2.18	0.47
1:O:79:PHE:CB	1:O:81:ILE:HD12	2.40	0.47
1:O:206:PHE:HE2	1:B:240:VAL:CG2	2.26	0.47
1:O:250:ARG:NH1	1:O:250:ARG:CB	2.78	0.47
1:A:23:LEU:CD2	1:A:71:LEU:HG	2.44	0.47
1:A:84:PRO:O	1:A:86:GLU:N	2.48	0.47
1:A:162:LEU:O	1:A:166:ILE:CD1	2.63	0.47
1:B:49:TYR:HB3	1:C:287:ASP:OD1	2.15	0.47
1:B:229:LYS:O	1:B:230:LEU:HD23	2.14	0.47
1:C:199:ARG:O	1:C:202:ARG:HG2	2.15	0.47
1:O:19:ALA:O	1:O:23:LEU:CD2	2.63	0.47
1:B:44:THR:HG21	1:B:63:ILE:HD11	1.97	0.47
1:B:49:TYR:CZ	1:C:283:LEU:HD11	2.49	0.47
1:B:264:ILE:HG21	1:B:297:PHE:CD2	2.50	0.47
1:B:275:ILE:O	1:B:275:ILE:CG2	2.63	0.47
1:C:257:TYR:CE2	1:C:261:LYS:HD2	2.49	0.47
1:C:135:CYS:HB2	1:C:325:ARG:HD3	1.97	0.47
1:O:193:PRO:HB3	1:B:38:ILE:HD12	1.96	0.47
1:A:173:ILE:HD13	1:A:251:ILE:CA	2.45	0.47
1:C:114:LEU:C	1:C:116:GLY:H	2.18	0.47
1:C:279:VAL:HG23	1:C:298:ASP:HA	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:291:ASP:OD1	1:C:293:ARG:HD3	2.15	0.47
1:O:264:ILE:O	1:O:267:ALA:HB3	2.16	0.46
1:A:181:HIS:O	1:A:236:ARG:HA	2.15	0.46
1:B:287:ASP:OD1	1:C:49:TYR:HB3	2.14	0.46
1:C:28:VAL:HG12	1:C:29:GLU:N	2.30	0.46
1:O:106:ASP:CG	1:O:128:LYS:HE2	2.35	0.46
1:A:178:THR:HB	1:A:246:ASP:HB3	1.97	0.46
1:A:189:THR:HB	1:C:183:ILE:CD1	2.45	0.46
1:O:28:VAL:HG22	1:O:29:GLU:N	2.29	0.46
1:A:81:ILE:H	1:A:81:ILE:CD1	2.22	0.46
1:A:283:LEU:N	1:A:283:LEU:HD23	2.31	0.46
1:A:43:MET:C	1:A:45:TYR:N	2.69	0.46
1:A:83:ASN:N	1:A:83:ASN:ND2	2.57	0.46
1:A:87:ILE:HB	1:A:89:TRP:NE1	2.30	0.46
1:C:12:GLY:HA2	1:C:16:ARG:HH12	1.81	0.46
1:C:99:GLU:OE2	1:C:104:PHE:HB2	2.16	0.46
1:O:138:ASN:OD1	1:O:222:VAL:HG12	2.15	0.46
1:A:158:CYS:HG	1:A:245:VAL:HG23	1.78	0.46
1:A:329:LEU:O	1:A:333:MET:HG3	2.15	0.46
1:A:134:VAL:HG21	1:A:156:THR:HG22	1.97	0.46
1:B:215:ALA:HB2	2:B:6924:SO4:O3	2.16	0.46
1:C:206:PHE:O	1:C:207:ASN:OD1	2.34	0.46
1:A:16:ARG:NE	1:A:46:MET:O	2.49	0.46
1:A:70:LEU:N	1:A:70:LEU:HD22	2.30	0.46
1:A:73:GLU:HA	1:A:73:GLU:OE2	2.15	0.46
1:A:99:GLU:HB3	1:A:123:ILE:HA	1.98	0.46
1:C:17:LEU:HA	1:C:20:ARG:HD2	1.98	0.46
1:C:39:THR:O	1:C:43:MET:HB2	2.16	0.46
1:C:99:GLU:HA	1:C:99:GLU:OE1	2.15	0.46
1:C:265:LYS:O	1:C:268:SER:N	2.49	0.46
1:O:9:ASN:HD21	1:O:87:ILE:CD1	2.29	0.46
1:A:87:ILE:HD13	1:A:89:TRP:HZ2	1.80	0.46
1:A:114:LEU:CD1	1:A:148:ILE:HD11	2.37	0.46
1:C:49:TYR:CE1	1:C:55:GLN:NE2	2.84	0.46
1:O:61:ILE:CD1	1:O:61:ILE:N	2.71	0.46
1:O:158:CYS:O	1:O:161:PRO:HD2	2.15	0.46
1:O:206:PHE:CD2	1:B:240:VAL:CG2	2.99	0.46
1:O:218:ALA:C	1:O:220:GLY:N	2.69	0.46
1:A:203:ALA:O	1:A:209:ILE:HD11	2.16	0.46
1:A:203:ALA:CB	1:A:206:PHE:HB2	2.46	0.46
1:A:230:LEU:O	1:A:231:THR:CB	2.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:140:ASP:C	1:B:142:TYR:N	2.69	0.46
1:O:170:PHE:CE2	1:O:260:ILE:CD1	2.86	0.46
1:A:115:LYS:C	1:A:117:GLY:H	2.20	0.46
1:A:191:ASP:OD1	1:C:51:THR:HB	2.16	0.46
1:A:199:ARG:C	1:A:201:GLY:H	2.20	0.46
1:B:49:TYR:CE2	1:C:281:GLU:OE2	2.69	0.46
1:B:210:PRO:HB3	1:B:235:PHE:CD1	2.51	0.46
1:B:286:THR:O	1:B:289:VAL:HG23	2.16	0.46
1:C:187:GLN:NE2	1:C:204:ALA:CB	2.79	0.46
1:A:96:TYR:HA	1:A:120:LYS:O	2.16	0.45
1:B:46:MET:O	1:B:48:LYS:N	2.49	0.45
1:B:184:THR:C	1:B:186:THR:H	2.20	0.45
1:B:277:GLY:HA3	1:B:293:ARG:NH2	2.30	0.45
1:B:296:ILE:HD12	1:B:296:ILE:N	2.31	0.45
1:B:322:TYR:C	1:B:322:TYR:HD2	2.20	0.45
1:C:139:GLU:HG3	1:C:332:HIS:CD2	2.51	0.45
1:C:260:ILE:O	1:C:264:ILE:HG13	2.16	0.45
1:O:333:MET:HE2	1:O:333:MET:HB3	1.81	0.45
1:A:42:TYR:HD1	1:C:198:TRP:CD2	2.29	0.45
1:A:166:ILE:CD1	1:A:264:ILE:HD11	2.47	0.45
1:B:4:ILE:HG13	1:B:28:VAL:HA	1.98	0.45
1:B:49:TYR:CG	1:C:283:LEU:HD11	2.52	0.45
1:C:85:ASP:OD1	1:C:112:ALA:HB1	2.15	0.45
1:C:279:VAL:HG22	1:C:297:PHE:O	2.16	0.45
1:O:142:TYR:HE1	1:O:146:ILE:HB	1.79	0.45
1:A:85:ASP:N	1:A:85:ASP:OD2	2.47	0.45
1:O:49:TYR:CD1	1:A:283:LEU:HD22	2.52	0.45
1:O:173:ILE:HG13	1:O:252:GLU:HB3	1.98	0.45
1:O:209:ILE:HA	1:O:210:PRO:HD3	1.76	0.45
1:A:12:GLY:O	1:A:16:ARG:HG3	2.16	0.45
1:A:248:THR:HG1	1:A:311:LYS:HZ3	1.63	0.45
1:A:291:ASP:O	1:A:293:ARG:N	2.50	0.45
1:O:255:ALA:O	1:O:307:ASP:HA	2.15	0.45
1:A:130:ALA:HB2	1:A:148:ILE:HG22	1.99	0.45
1:A:284:VAL:O	1:A:287:ASP:HB2	2.17	0.45
1:B:5:LYS:HB2	1:B:93:GLY:O	2.16	0.45
1:B:44:THR:HG21	1:B:63:ILE:HG13	1.99	0.45
1:B:174:GLU:HA	1:B:229:LYS:O	2.16	0.45
1:C:278:TYR:CE1	1:C:299:ALA:HB2	2.51	0.45
1:O:127:SER:HB3	1:O:130:ALA:HB3	1.96	0.45
1:O:183:ILE:HD11	1:O:240:VAL:HA	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:276:ILE:HG23	1:O:276:ILE:O	2.16	0.45
1:O:284:VAL:HG22	1:C:202:ARG:NH1	2.32	0.45
1:A:97:VAL:HG21	1:A:113:HIS:HB3	1.98	0.45
1:B:79:PHE:CZ	1:B:88:PRO:HG2	2.52	0.45
1:C:11:PHE:HE1	1:C:16:ARG:HA	1.81	0.45
1:C:243:SER:HB2	1:C:316:TYR:CZ	2.51	0.45
1:O:184:THR:HG23	1:O:236:ARG:HH22	1.82	0.45
1:A:106:ASP:OD2	1:A:128:LYS:HE2	2.17	0.45
1:A:283:LEU:HD12	1:A:288:PHE:CE1	2.52	0.45
1:B:213:THR:HG23	1:B:213:THR:O	2.17	0.45
1:B:247:LEU:HD11	1:B:249:VAL:HB	1.99	0.45
1:C:123:ILE:HG22	1:C:125:ALA:O	2.17	0.45
1:C:138:ASN:O	1:C:140:ASP:N	2.50	0.45
1:A:55:GLN:HG2	1:A:56:TRP:N	2.31	0.45
1:A:207:ASN:HD22	1:B:284:VAL:HG23	1.80	0.45
1:B:228:GLY:C	1:B:230:LEU:N	2.71	0.45
1:A:13:ARG:HH21	1:A:52:VAL:HG12	1.79	0.45
1:B:265:LYS:C	1:B:267:ALA:H	2.19	0.45
1:B:320:TRP:O	1:B:323:SER:HB2	2.17	0.45
1:C:35:ASP:HA	1:C:36:PRO:HD2	1.77	0.45
1:C:89:TRP:NE1	1:C:113:HIS:ND1	2.65	0.45
1:O:206:PHE:CE2	1:B:240:VAL:HG23	2.52	0.44
1:A:281:GLU:CB	1:A:283:LEU:HD21	2.42	0.44
1:B:65:ASP:C	1:B:67:LYS:H	2.20	0.44
1:B:183:ILE:HG12	1:B:239:THR:O	2.16	0.44
1:C:9:ASN:HB3	1:C:99:GLU:OE1	2.16	0.44
1:C:82:ARG:HG3	1:C:82:ARG:HH11	1.82	0.44
1:O:8:ILE:HB	1:O:33:VAL:HG12	1.98	0.44
1:O:97:VAL:O	1:O:121:VAL:HG13	2.18	0.44
1:A:38:ILE:HG22	1:A:42:TYR:CD2	2.52	0.44
1:A:173:ILE:CD1	1:A:252:GLU:HG2	2.47	0.44
1:A:306:ASN:C	1:A:308:ASN:H	2.20	0.44
1:B:286:THR:CG2	1:C:51:THR:HG23	2.39	0.44
1:C:95:GLU:HG2	1:C:119:LYS:HG3	1.99	0.44
1:C:124:SER:O	1:C:125:ALA:HB2	2.17	0.44
1:C:198:TRP:O	1:C:199:ARG:C	2.56	0.44
1:C:219:VAL:O	1:C:223:LEU:N	2.48	0.44
1:A:106:ASP:CG	1:A:128:LYS:HE2	2.37	0.44
1:C:38:ILE:CG2	1:C:46:MET:HE2	2.47	0.44
1:C:154:CYS:SG	1:C:155:THR:N	2.91	0.44
1:O:4:ILE:HD13	1:O:330:ILE:HG22	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:107:LYS:O	1:O:111:ALA:HB2	2.17	0.44
1:O:174:GLU:HB2	1:C:305:LEU:HD23	1.99	0.44
1:O:283:LEU:HD13	1:O:288:PHE:HE2	1.82	0.44
1:A:11:PHE:CD2	1:A:16:ARG:CD	2.79	0.44
1:A:36:PRO:HB3	1:A:80:GLY:O	2.17	0.44
1:A:281:GLU:HB2	1:A:283:LEU:CD2	2.43	0.44
1:B:107:LYS:N	1:B:129:ASP:OD1	2.41	0.44
1:C:264:ILE:HG21	1:C:297:PHE:CB	2.47	0.44
1:O:40:THR:HG23	1:O:69:LEU:HD13	1.98	0.44
1:C:56:TRP:CZ2	1:C:58:HIS:HB3	2.53	0.44
1:C:325:ARG:NE	1:C:325:ARG:HA	2.32	0.44
1:O:191:ASP:OD1	1:O:202:ARG:NE	2.50	0.44
1:A:244:VAL:HG22	1:A:313:VAL:HG23	1.99	0.44
1:B:70:LEU:HD12	1:B:75:PRO:N	2.33	0.44
1:B:152:ALA:HB3	1:B:157:ASN:HD21	1.82	0.44
1:C:30:LEU:O	1:C:76:VAL:HG22	2.18	0.44
1:C:293:ARG:HB2	1:C:296:ILE:HD11	2.00	0.44
1:O:124:SER:C	1:O:322:TYR:OH	2.56	0.44
1:A:242:VAL:HA	1:A:317:ASP:HA	1.99	0.44
1:A:291:ASP:OD1	1:A:293:ARG:HB2	2.18	0.44
1:B:7:GLY:O	1:B:97:VAL:HA	2.18	0.44
1:B:147:ASP:N	1:B:147:ASP:OD2	2.50	0.44
1:C:17:LEU:HD22	1:C:320:TRP:CE3	2.52	0.44
1:O:77:THR:HG21	1:O:79:PHE:CZ	2.53	0.44
1:A:153:SER:CB	2:A:6923:SO4:O4	2.66	0.44
1:C:13:ARG:HH21	1:C:52:VAL:HG21	1.83	0.44
1:O:165:VAL:HB	1:O:166:ILE:HD12	1.99	0.44
1:O:183:ILE:H	1:O:183:ILE:CD1	2.26	0.44
1:O:250:ARG:HG3	1:O:309:PHE:CD1	2.53	0.44
1:A:241:ASP:CG	1:A:242:VAL:H	2.21	0.44
1:B:9:ASN:ND2	1:B:99:GLU:OE1	2.51	0.44
1:B:284:VAL:HG22	1:B:287:ASP:OD2	2.18	0.44
1:C:63:ILE:HG22	1:C:65:ASP:O	2.18	0.44
1:O:81:ILE:HB	1:O:87:ILE:HG12	1.99	0.43
1:O:162:LEU:CD1	1:O:264:ILE:HD11	2.48	0.43
1:O:264:ILE:O	1:O:268:SER:N	2.51	0.43
1:B:257:TYR:CD2	1:B:261:LYS:HD2	2.52	0.43
1:C:72:GLY:O	1:C:73:GLU:HB2	2.17	0.43
1:C:83:ASN:ND2	1:C:84:PRO:N	2.65	0.43
1:C:152:ALA:HB1	1:C:156:THR:HB	2.00	0.43
1:C:159:LEU:CD1	1:C:247:LEU:HD22	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:30:LEU:HD12	1:O:31:VAL:N	2.33	0.43
1:A:285:SER:HB3	1:B:208:ILE:HB	2.00	0.43
1:B:298:ASP:OD2	1:B:315:TRP:NE1	2.52	0.43
1:O:153:SER:O	1:O:155:THR:N	2.51	0.43
1:C:61:ILE:HG23	1:C:61:ILE:O	2.18	0.43
1:O:145:ASP:OD2	1:O:145:ASP:N	2.52	0.43
1:O:199:ARG:O	1:O:202:ARG:HG2	2.17	0.43
1:O:240:VAL:CG1	1:B:206:PHE:CE1	2.99	0.43
1:A:90:ALA:HB2	1:A:117:GLY:CA	2.47	0.43
1:A:137:VAL:HG12	1:A:223:LEU:HD21	1.99	0.43
1:B:112:ALA:O	1:B:114:LEU:N	2.52	0.43
1:O:23:LEU:HD11	1:O:47:PHE:HZ	1.78	0.43
1:O:268:SER:O	1:O:273:LYS:HA	2.17	0.43
1:O:284:VAL:HG12	1:C:209:ILE:HA	2.00	0.43
1:A:153:SER:O	1:A:157:ASN:HB2	2.17	0.43
1:B:27:ASP:OD1	1:B:28:VAL:HG23	2.19	0.43
1:B:111:ALA:HA	1:B:148:ILE:CD1	2.47	0.43
1:B:326:VAL:C	1:B:328:ASP:H	2.22	0.43
1:C:52:VAL:O	1:C:54:GLY:N	2.44	0.43
1:C:65:ASP:OD2	1:C:66:SER:N	2.51	0.43
1:C:84:PRO:HA	1:C:87:ILE:HD12	2.01	0.43
1:O:296:ILE:N	1:O:296:ILE:HD12	2.33	0.43
1:A:6:ILE:HD13	1:A:28:VAL:HG21	2.01	0.43
1:A:48:LYS:HE2	1:A:49:TYR:CZ	2.53	0.43
1:B:84:PRO:O	1:B:87:ILE:HG13	2.19	0.43
1:B:243:SER:HB2	1:B:316:TYR:CZ	2.53	0.43
1:C:97:VAL:O	1:C:121:VAL:HG13	2.19	0.43
1:C:317:ASP:O	1:C:318:ASN:C	2.56	0.43
1:B:85:ASP:N	1:B:112:ALA:HB1	2.32	0.43
1:C:249:VAL:CG2	1:C:250:ARG:H	2.21	0.43
1:O:3:LYS:HG2	1:O:26:GLU:O	2.18	0.43
1:A:233:MET:SD	1:B:311:LYS:HD2	2.57	0.43
1:A:241:ASP:OD1	1:A:318:ASN:OD1	2.37	0.43
1:A:285:SER:CA	1:A:315:TRP:HZ3	2.32	0.43
1:B:21:VAL:HG21	1:B:324:ASN:ND2	2.33	0.43
1:B:87:ILE:O	1:B:116:GLY:HA3	2.18	0.43
1:B:180:VAL:HG12	1:B:180:VAL:O	2.18	0.43
1:C:96:TYR:CD2	1:C:120:LYS:HB2	2.53	0.43
1:C:164:LYS:HG2	1:C:168:ASP:OD2	2.18	0.43
1:O:166:ILE:CD1	1:O:166:ILE:N	2.80	0.43
1:O:206:PHE:C	1:O:207:ASN:OD1	2.57	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:LEU:HD23	1:A:226:LEU:HA	1.88	0.43
1:B:161:PRO:HB3	1:B:272:LEU:HD22	2.01	0.43
1:B:260:ILE:HG22	1:B:264:ILE:HD12	2.00	0.43
1:C:13:ARG:NH2	1:C:52:VAL:HG21	2.34	0.43
1:C:133:PHE:HA	1:C:138:ASN:HD21	1.83	0.43
1:O:38:ILE:HG23	1:O:42:TYR:CD2	2.54	0.43
1:O:279:VAL:HG11	1:O:283:LEU:HD12	2.00	0.43
1:A:9:ASN:ND2	1:A:87:ILE:HD11	2.34	0.43
1:A:57:LYS:O	1:A:58:HIS:C	2.57	0.43
1:B:44:THR:HG21	1:B:63:ILE:CD1	2.49	0.43
1:O:250:ARG:HH11	1:O:250:ARG:CB	2.32	0.42
1:O:279:VAL:HG11	1:O:283:LEU:CD1	2.49	0.42
1:O:322:TYR:O	1:O:326:VAL:HG23	2.19	0.42
1:A:206:PHE:HZ	1:C:239:THR:O	2.01	0.42
1:A:284:VAL:CG2	1:B:207:ASN:ND2	2.82	0.42
1:A:305:LEU:O	1:A:306:ASN:CB	2.67	0.42
1:B:22:ALA:C	1:B:24:GLN:N	2.71	0.42
1:B:283:LEU:O	1:B:284:VAL:HG13	2.19	0.42
1:C:57:LYS:HA	1:C:57:LYS:HD3	1.77	0.42
1:C:241:ASP:O	1:C:242:VAL:HB	2.18	0.42
1:O:8:ILE:HG12	1:O:30:LEU:HD13	2.01	0.42
1:A:175:GLY:O	1:B:305:LEU:HD22	2.19	0.42
1:B:11:PHE:CE2	1:B:16:ARG:HG2	2.54	0.42
1:B:13:ARG:NH1	1:B:50:ASP:OD2	2.44	0.42
1:C:19:ALA:HB1	1:C:30:LEU:HD22	2.01	0.42
1:C:84:PRO:HB2	1:C:112:ALA:HB3	2.00	0.42
1:C:244:VAL:CG1	1:C:313:VAL:HG13	2.49	0.42
1:O:3:LYS:NZ	1:O:74:LYS:NZ	2.67	0.42
1:O:283:LEU:HD21	1:A:49:TYR:CD2	2.54	0.42
1:O:294:SER:OG	1:O:325:ARG:NH1	2.52	0.42
1:A:50:ASP:HB3	1:A:54:GLY:O	2.18	0.42
1:A:199:ARG:HG3	1:B:282:ASP:HB3	2.00	0.42
1:A:251:ILE:N	1:A:251:ILE:CD1	2.82	0.42
1:A:298:ASP:CG	1:A:301:ALA:HB2	2.39	0.42
1:B:303:ILE:CG1	1:B:304:ALA:N	2.81	0.42
1:C:53:HIS:HE1	1:C:241:ASP:OD2	2.02	0.42
1:C:153:SER:H	1:C:157:ASN:ND2	2.16	0.42
1:C:260:ILE:HG21	1:C:312:LEU:HD22	2.02	0.42
1:O:304:ALA:HB2	1:O:310:VAL:HG23	2.02	0.42
1:A:11:PHE:HE2	1:A:16:ARG:HD2	1.63	0.42
1:B:244:VAL:HG21	1:B:313:VAL:HG13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:90:ALA:HB3	1:C:117:GLY:HA3	2.01	0.42
1:C:154:CYS:HA	1:C:322:TYR:CD1	2.55	0.42
1:C:272:LEU:HD13	1:C:276:ILE:HD11	2.02	0.42
1:O:17:LEU:CD1	1:O:319:GLU:HB3	2.49	0.42
1:O:187:GLN:HB3	1:O:204:ALA:CB	2.49	0.42
1:A:207:ASN:ND2	1:B:284:VAL:CG2	2.82	0.42
1:B:107:LYS:O	1:B:111:ALA:CB	2.67	0.42
1:B:135:CYS:HB2	1:B:325:ARG:HD3	2.01	0.42
1:C:22:ALA:HA	1:C:25:SER:OG	2.20	0.42
1:O:68:THR:O	1:O:76:VAL:O	2.36	0.42
1:O:213:THR:HG22	1:O:233:MET:CA	2.47	0.42
1:A:9:ASN:CG	1:A:34:ASN:HD22	2.22	0.42
1:A:249:VAL:HG22	1:A:250:ARG:N	2.34	0.42
1:B:51:THR:HG23	1:C:286:THR:HG21	2.02	0.42
1:B:71:LEU:HD22	1:B:71:LEU:H	1.84	0.42
1:B:110:ALA:HB1	1:B:121:VAL:HG11	2.00	0.42
1:C:39:THR:O	1:C:43:MET:N	2.41	0.42
1:C:52:VAL:CG2	1:C:240:VAL:HG21	2.49	0.42
1:O:45:TYR:OH	1:B:202:ARG:NH1	2.53	0.42
1:B:244:VAL:HG22	1:B:245:VAL:N	2.35	0.42
1:C:32:ALA:N	1:C:76:VAL:HG13	2.34	0.42
1:C:293:ARG:HH21	1:C:293:ARG:CG	2.33	0.42
1:C:306:ASN:C	1:C:308:ASN:H	2.21	0.42
1:O:137:VAL:CG1	1:O:223:LEU:HD22	2.49	0.42
1:A:42:TYR:HA	1:C:198:TRP:CH2	2.54	0.42
1:A:158:CYS:SG	1:A:159:LEU:N	2.93	0.42
1:A:231:THR:HG22	1:B:305:LEU:HD13	2.01	0.42
1:A:298:ASP:HB3	1:A:301:ALA:CB	2.50	0.42
1:B:84:PRO:HB2	1:B:112:ALA:CB	2.50	0.42
1:C:95:GLU:HG2	1:C:119:LYS:HB2	2.01	0.42
1:C:149:VAL:HG21	1:C:333:MET:SD	2.60	0.42
1:C:293:ARG:NH2	1:C:293:ARG:HG2	2.35	0.42
1:O:223:LEU:CB	1:O:226:LEU:HD12	2.50	0.42
1:B:9:ASN:HD22	1:B:99:GLU:CD	2.22	0.42
1:B:32:ALA:HB2	1:B:92:ALA:CB	2.50	0.42
1:B:113:HIS:O	1:B:116:GLY:N	2.52	0.42
1:B:321:GLY:O	1:B:322:TYR:C	2.57	0.42
1:C:120:LYS:HA	1:C:147:ASP:O	2.20	0.42
1:O:9:ASN:ND2	1:O:113:HIS:HE1	2.17	0.42
1:A:229:LYS:O	1:A:230:LEU:HD23	2.19	0.42
1:C:104:PHE:O	1:C:110:ALA:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:106:ASP:O	1:O:108:GLU:N	2.53	0.41
1:A:71:LEU:HD13	1:A:71:LEU:HA	1.90	0.41
1:A:173:ILE:HG13	1:A:252:GLU:CD	2.40	0.41
1:A:285:SER:OG	1:B:207:ASN:HA	2.19	0.41
1:C:270:GLY:C	1:C:272:LEU:H	2.24	0.41
1:C:276:ILE:CG2	1:C:277:GLY:N	2.83	0.41
1:O:128:LYS:HE3	1:O:129:ASP:CG	2.40	0.41
1:O:188:LYS:HE3	1:O:193:PRO:O	2.21	0.41
1:A:137:VAL:CG1	1:A:223:LEU:HD21	2.50	0.41
1:A:190:VAL:O	1:A:192:GLY:N	2.53	0.41
1:A:291:ASP:OD2	1:A:293:ARG:NH2	2.54	0.41
1:B:89:TRP:HB2	1:B:118:ALA:H	1.84	0.41
1:B:111:ALA:O	1:B:114:LEU:HD12	2.20	0.41
1:C:65:ASP:OD2	1:C:68:THR:HG22	2.20	0.41
1:C:184:THR:HG23	1:C:236:ARG:CZ	2.50	0.41
1:O:199:ARG:HH11	1:O:199:ARG:CG	2.21	0.41
1:O:208:ILE:HG13	1:C:285:SER:HB2	2.03	0.41
1:O:247:LEU:CG	1:O:249:VAL:HG13	2.47	0.41
1:A:183:ILE:HG22	1:A:187:GLN:HE22	1.84	0.41
1:B:278:TYR:CE1	1:B:299:ALA:HB2	2.54	0.41
1:C:16:ARG:HH11	1:C:16:ARG:CG	2.32	0.41
1:C:25:SER:C	1:C:27:ASP:H	2.23	0.41
1:C:69:LEU:HD22	1:C:78:VAL:CG2	2.50	0.41
1:C:219:VAL:O	1:C:223:LEU:HB2	2.20	0.41
1:B:37:PHE:C	1:B:38:ILE:HD12	2.40	0.41
1:B:85:ASP:HB3	1:B:112:ALA:HB1	2.01	0.41
1:B:208:ILE:O	1:B:210:PRO:HD3	2.21	0.41
1:B:317:ASP:O	1:B:318:ASN:C	2.58	0.41
1:B:324:ASN:H	1:B:324:ASN:ND2	2.14	0.41
1:O:120:LYS:NZ	1:O:142:TYR:OH	2.51	0.41
1:A:39:THR:O	1:A:43:MET:HG3	2.21	0.41
1:A:284:VAL:HB	1:A:285:SER:H	1.70	0.41
1:B:81:ILE:HB	1:B:87:ILE:HG12	2.01	0.41
1:C:10:GLY:HA3	1:C:100:SER:O	2.20	0.41
1:O:167:HIS:ND1	1:O:171:GLY:HA2	2.35	0.41
1:O:173:ILE:HB	1:O:250:ARG:O	2.21	0.41
1:O:264:ILE:HD12	1:O:297:PHE:CD1	2.55	0.41
1:A:11:PHE:HB3	1:A:38:ILE:HD11	2.03	0.41
1:A:208:ILE:CG1	3:B:6956:HOH:O	2.68	0.41
1:B:12:GLY:O	1:B:15:GLY:N	2.53	0.41
1:B:26:GLU:H	1:B:26:GLU:CD	2.24	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:153:SER:O	1:B:155:THR:N	2.53	0.41
1:C:214:GLY:O	1:C:218:ALA:N	2.54	0.41
1:O:156:THR:C	1:O:158:CYS:H	2.23	0.41
1:A:307:ASP:OD1	1:A:307:ASP:N	2.54	0.41
1:B:113:HIS:O	1:B:114:LEU:C	2.59	0.41
1:C:182:ALA:O	1:C:183:ILE:C	2.59	0.41
1:C:334:ALA:O	1:C:336:THR:N	2.53	0.41
1:A:9:ASN:ND2	1:A:113:HIS:HE1	2.17	0.41
1:A:227:ASN:C	1:A:229:LYS:H	2.24	0.41
1:C:81:ILE:HG22	1:C:83:ASN:H	1.85	0.41
1:O:265:LYS:O	1:O:268:SER:N	2.53	0.41
1:O:310:VAL:CG2	1:O:311:LYS:N	2.82	0.41
1:A:8:ILE:HG23	1:A:98:VAL:HB	2.03	0.41
1:A:133:PHE:CE2	1:A:142:TYR:HB2	2.55	0.41
1:A:291:ASP:C	1:A:293:ARG:H	2.23	0.41
1:B:3:LYS:HE3	1:B:26:GLU:C	2.42	0.41
1:B:114:LEU:HD23	1:B:118:ALA:O	2.20	0.41
1:B:296:ILE:HG22	1:B:297:PHE:N	2.35	0.41
1:C:69:LEU:CD2	1:C:78:VAL:HG22	2.51	0.41
1:C:292:SER:HB2	1:C:324:ASN:ND2	2.35	0.41
1:O:285:SER:HA	1:O:315:TRP:CZ3	2.56	0.41
1:A:111:ALA:HA	1:A:148:ILE:HD11	2.02	0.41
1:B:265:LYS:C	1:B:267:ALA:N	2.75	0.41
1:B:327:ILE:O	1:B:327:ILE:CG2	2.68	0.41
1:C:23:LEU:HD12	1:C:47:PHE:HZ	1.85	0.41
1:C:53:HIS:NE2	1:C:319:GLU:OE1	2.40	0.41
1:C:181:HIS:HD2	1:C:243:SER:OG	2.04	0.41
1:O:68:THR:O	1:O:78:VAL:HG23	2.20	0.40
1:O:89:TRP:NE1	1:O:113:HIS:ND1	2.65	0.40
1:O:183:ILE:CD1	1:O:240:VAL:HA	2.51	0.40
1:O:239:THR:HG21	1:C:208:ILE:CG1	2.49	0.40
1:A:214:GLY:O	1:A:218:ALA:N	2.51	0.40
1:B:106:ASP:OD1	1:B:109:LYS:HD2	2.21	0.40
1:B:304:ALA:CB	1:B:310:VAL:HG12	2.51	0.40
1:B:306:ASN:C	1:B:308:ASN:H	2.25	0.40
1:C:19:ALA:O	1:C:23:LEU:HG	2.22	0.40
1:C:159:LEU:HD13	1:C:245:VAL:CG1	2.49	0.40
1:C:177:MET:HG2	1:C:178:THR:N	2.35	0.40
1:O:63:ILE:HD12	1:O:63:ILE:N	2.23	0.40
1:O:86:GLU:O	1:O:87:ILE:C	2.60	0.40
1:A:52:VAL:HG13	1:A:53:HIS:CD2	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:ILE:O	1:A:294:SER:N	2.47	0.40
1:B:293:ARG:NH2	1:B:293:ARG:HG2	2.35	0.40
1:O:207:ASN:HB3	1:C:285:SER:HB3	2.02	0.40
1:A:56:TRP:CD1	1:A:56:TRP:O	2.74	0.40
1:A:84:PRO:HG3	1:A:104:PHE:CE2	2.57	0.40
1:A:173:ILE:CD1	1:A:251:ILE:C	2.90	0.40
1:B:99:GLU:HB3	1:B:123:ILE:HD13	2.03	0.40
1:B:104:PHE:HA	1:B:109:LYS:HD3	2.03	0.40
1:B:194:SER:O	1:B:195:SER:C	2.59	0.40
1:C:114:LEU:HA	1:C:118:ALA:HB3	2.04	0.40
1:C:143:THR:O	1:C:144:SER:C	2.59	0.40
1:O:14:ILE:HG12	1:O:322:TYR:HD2	1.86	0.40
1:O:174:GLU:HB2	1:C:305:LEU:CD2	2.50	0.40
1:O:216:ALA:C	1:O:218:ALA:N	2.71	0.40
1:O:245:VAL:CG1	1:O:246:ASP:H	2.33	0.40
1:B:244:VAL:CG2	1:B:245:VAL:N	2.83	0.40
1:B:271:LYS:HD2	1:B:271:LYS:N	2.37	0.40
1:B:293:ARG:HG2	1:B:293:ARG:HH21	1.85	0.40
1:O:9:ASN:HD22	1:O:113:HIS:HE1	1.69	0.40
1:O:311:LYS:HB2	1:C:176:LEU:HD12	2.03	0.40
1:A:9:ASN:ND2	1:A:87:ILE:CD1	2.85	0.40
1:A:38:ILE:HG21	1:A:46:MET:SD	2.61	0.40
1:B:26:GLU:OE1	1:B:26:GLU:N	2.52	0.40
1:B:153:SER:HA	1:B:322:TYR:HE1	1.87	0.40
1:B:183:ILE:O	1:B:184:THR:HG23	2.22	0.40
1:B:202:ARG:O	1:B:203:ALA:C	2.59	0.40
1:C:95:GLU:HB3	1:C:96:TYR:CD1	2.57	0.40

All (29) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:6940:HOH:O	3:C:6947:HOH:O[2_644]	0.07	2.13
3:B:6960:HOH:O	3:C:6948:HOH:O[1_455]	0.13	2.07
3:O:6950:HOH:O	3:A:6928:HOH:O[1_455]	0.14	2.06
3:O:6940:HOH:O	3:A:6939:HOH:O[1_455]	0.20	2.00
3:O:6933:HOH:O	3:A:6933:HOH:O[1_556]	0.21	1.99
3:A:6939:HOH:O	3:C:6937:HOH:O[2_645]	0.30	1.90
3:A:6932:HOH:O	3:C:6941:HOH:O[2_645]	0.33	1.87
3:A:6946:HOH:O	3:C:6946:HOH:O[2_644]	0.33	1.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:6944:HOH:O	3:C:6951:HOH:O[1_454]	0.35	1.85
3:O:6951:HOH:O	3:A:6945:HOH:O[1_656]	0.36	1.84
3:A:6936:HOH:O	3:B:6963:HOH:O[2_544]	0.36	1.84
3:A:6937:HOH:O	3:C:6952:HOH:O[2_645]	0.36	1.84
3:A:6938:HOH:O	3:C:6930:HOH:O[2_645]	0.36	1.84
3:O:6948:HOH:O	3:B:6959:HOH:O[2_545]	0.38	1.82
3:O:6948:HOH:O	3:B:6962:HOH:O[2_544]	0.38	1.82
3:B:6959:HOH:O	3:B:6962:HOH:O[1_556]	0.40	1.80
3:A:6941:HOH:O	3:C:6939:HOH:O[2_544]	0.45	1.75
3:B:6961:HOH:O	3:C:6949:HOH:O[1_454]	0.45	1.75
3:A:6934:HOH:O	3:C:6934:HOH:O[2_645]	0.46	1.74
3:O:6940:HOH:O	3:C:6937:HOH:O[2_545]	0.50	1.70
3:A:6937:HOH:O	3:B:6957:HOH:O[2_544]	0.51	1.69
3:A:6945:HOH:O	3:C:6944:HOH:O[2_544]	0.53	1.67
3:A:6944:HOH:O	3:C:6930:HOH:O[2_544]	0.60	1.60
3:A:6938:HOH:O	3:A:6944:HOH:O[1_656]	0.61	1.59
3:A:6943:HOH:O	3:C:6953:HOH:O[1_554]	0.61	1.59
3:B:6957:HOH:O	3:C:6952:HOH:O[1_454]	0.62	1.58
3:O:6951:HOH:O	3:C:6944:HOH:O[2_645]	0.71	1.49
3:B:6953:HOH:O	3:C:6950:HOH:O[1_454]	1.17	1.03
3:O:6942:HOH:O	3:A:6924:HOH:O[1_556]	1.33	0.87

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	A	332/336 (99%)	255 (77%)	51 (15%)	26 (8%)	1 14
1	B	333/336 (99%)	233 (70%)	70 (21%)	30 (9%)	1 11
1	C	333/336 (99%)	236 (71%)	67 (20%)	30 (9%)	1 11
1	O	333/336 (99%)	246 (74%)	64 (19%)	23 (7%)	1 17
All	All	1331/1344 (99%)	970 (73%)	252 (19%)	109 (8%)	1 12

All (109) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	O	24	GLN
1	O	56	TRP
1	O	67	LYS
1	O	69	LEU
1	O	145	ASP
1	O	156	THR
1	O	242	VAL
1	O	285	SER
1	A	44	THR
1	A	191	ASP
1	A	202	ARG
1	A	231	THR
1	A	292	SER
1	A	309	PHE
1	B	152	ALA
1	B	242	VAL
1	B	282	ASP
1	C	53	HIS
1	C	69	LEU
1	C	70	LEU
1	C	144	SER
1	C	285	SER
1	C	307	ASP
1	O	3	LYS
1	O	59	SER
1	O	70	LEU
1	O	72	GLY
1	O	107	LYS
1	O	155	THR
1	O	171	GLY
1	O	282	ASP
1	A	48	LYS
1	A	67	LYS
1	A	85	ASP
1	A	171	GLY
1	A	194	SER
1	A	242	VAL
1	A	299	ALA
1	A	306	ASN
1	B	4	ILE
1	B	47	PHE
1	B	66	SER

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Mol	Chain	Res	Type
1	B	70	LEU
1	B	84	PRO
1	B	85	ASP
1	B	104	PHE
1	B	113	HIS
1	B	135	CYS
1	B	137	VAL
1	B	216	ALA
1	B	229	LYS
1	B	231	THR
1	C	54	GLY
1	C	59	SER
1	C	61	ILE
1	C	115	LYS
1	C	158	CYS
1	C	171	GLY
1	C	191	ASP
1	C	195	SER
1	C	203	ALA
1	C	242	VAL
1	C	271	LYS
1	C	323	SER
1	C	335	LYS
1	O	66	SER
1	A	65	ASP
1	A	195	SER
1	A	228	GLY
1	A	307	ASP
1	B	118	ALA
1	B	154	CYS
1	B	195	SER
1	B	270	GLY
1	B	319	GLU
1	C	58	HIS
1	C	146	ILE
1	C	318	ASN
1	O	23	LEU
1	O	231	THR
1	O	316	TYR
1	A	291	ASP
1	B	54	GLY
1	B	69	LEU

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Mol	Chain	Res	Type
1	B	112	ALA
1	B	114	LEU
1	B	238	PRO
1	C	226	LEU
1	C	319	GLU
1	A	185	ALA
1	A	318	ASN
1	B	3	LYS
1	B	40	THR
1	C	26	GLU
1	C	36	PRO
1	C	163	ALA
1	O	238	PRO
1	A	66	SER
1	A	200	GLY
1	A	224	PRO
1	B	215	ALA
1	B	327	ILE
1	C	125	ALA
1	C	183	ILE
1	A	270	GLY
1	C	52	VAL
1	O	88	PRO
1	O	224	PRO
1	A	10	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	274/276 (99%)	252 (92%)	22 (8%)	12	42
1	B	275/276 (100%)	260 (94%)	15 (6%)	21	53
1	C	275/276 (100%)	255 (93%)	20 (7%)	14	45
1	O	275/276 (100%)	252 (92%)	23 (8%)	11	40
All	All	1099/1104 (100%)	1019 (93%)	80 (7%)	14	45

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	6	ILE
1	O	11	PHE
1	O	13	ARG
1	O	16	ARG
1	O	23	LEU
1	O	27	ASP
1	O	39	THR
1	O	46	MET
1	O	57	LYS
1	O	61	ILE
1	O	71	LEU
1	O	82	ARG
1	O	101	THR
1	O	128	LYS
1	O	183	ILE
1	O	199	ARG
1	O	225	ASP
1	O	240	VAL
1	O	260	ILE
1	O	286	THR
1	O	291	ASP
1	O	293	ARG
1	O	328	ASP
1	A	8	ILE
1	A	18	VAL
1	A	27	ASP
1	A	82	ARG
1	A	83	ASN
1	A	100	SER
1	A	105	THR
1	A	106	ASP
1	A	145	ASP
1	A	158	CYS
1	A	173	ILE
1	A	179	THR
1	A	189	THR
1	A	191	ASP
1	A	251	ILE
1	A	258	ASP
1	A	280	GLU
1	A	293	ARG
1	A	307	ASP

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Mol	Chain	Res	Type
1	A	308	ASN
1	A	313	VAL
1	A	324	ASN
1	B	6	ILE
1	B	11	PHE
1	B	26	GLU
1	B	27	ASP
1	B	38	ILE
1	B	41	ASP
1	B	139	GLU
1	B	178	THR
1	B	191	ASP
1	B	222	VAL
1	B	258	ASP
1	B	293	ARG
1	B	322	TYR
1	B	324	ASN
1	B	328	ASP
1	C	11	PHE
1	C	14	ILE
1	C	39	THR
1	C	41	ASP
1	C	62	LYS
1	C	65	ASP
1	C	68	THR
1	C	73	GLU
1	C	83	ASN
1	C	85	ASP
1	C	108	GLU
1	C	140	ASP
1	C	158	CYS
1	C	177	MET
1	C	183	ILE
1	C	250	ARG
1	C	251	ILE
1	C	293	ARG
1	C	307	ASP
1	C	312	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	O	9	ASN
1	O	83	ASN
1	O	187	GLN
1	O	227	ASN
1	O	324	ASN
1	A	9	ASN
1	A	24	GLN
1	A	34	ASN
1	A	53	HIS
1	A	58	HIS
1	A	83	ASN
1	A	187	GLN
1	A	308	ASN
1	A	318	ASN
1	B	9	ASN
1	B	24	GLN
1	B	53	HIS
1	B	157	ASN
1	B	207	ASN
1	B	324	ASN
1	C	24	GLN
1	C	55	GLN
1	C	83	ASN
1	C	157	ASN
1	C	181	HIS
1	C	207	ASN
1	C	324	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

8 ligands are modelled in this entry.

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	$\#\|Z\| > 2$
2	SO4	B	6924	-	4,4,4	0.36	0	6,6,6	0.13	0
2	SO4	A	6923	-	4,4,4	0.40	0	6,6,6	0.11	0
2	SO4	C	6927	-	4,4,4	0.39	0	6,6,6	0.07	0
2	SO4	O	6921	-	4,4,4	0.38	0	6,6,6	0.08	0
2	SO4	O	6920	-	4,4,4	0.36	0	6,6,6	0.11	0
2	SO4	B	6925	-	4,4,4	0.33	0	6,6,6	0.09	0
2	SO4	C	6926	-	4,4,4	0.39	0	6,6,6	0.23	0
2	SO4	A	6922	-	4,4,4	0.34	0	6,6,6	0.08	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	6924	SO4	1	0
2	A	6923	SO4	3	0
2	O	6921	SO4	1	0
2	C	6926	SO4	11	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 (i)

6.1 Protein, DNA and RNA chains (i)

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	A	334/336 (99%)	-0.31	2 (0%)	89	88	0, 0, 0, 0	2 (0%)
1	B	335/336 (99%)	-0.32	2 (0%)	89	88	0, 0, 0, 0	2 (0%)
1	C	335/336 (99%)	-0.29	2 (0%)	89	88	0, 0, 0, 0	2 (0%)
1	O	335/336 (99%)	-0.31	2 (0%)	89	88	0, 0, 0, 0	2 (0%)
All	All	1339/1344 (99%)	-0.31	8 (0%)	89	88	0, 0, 0, 0	8 (0%)

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	154	CYS	3.4
1	O	195	SER	3.3
1	C	195	SER	3.0
1	B	154	CYS	2.9
1	A	252	GLU	2.7
1	C	154	CYS	2.5
1	B	196	LYS	2.3
1	O	85	ASP	2.3

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SO4	C	6926	5/5	0.76	0.50	0,0,0,0	0
2	SO4	A	6923	5/5	0.87	0.29	0,0,0,0	0
2	SO4	B	6924	5/5	0.89	0.31	0,0,0,0	0
2	SO4	C	6927	5/5	0.90	0.36	0,0,0,0	0
2	SO4	O	6921	5/5	0.93	0.22	0,0,0,0	0
2	SO4	B	6925	5/5	0.96	0.19	0,0,0,0	0
2	SO4	O	6920	5/5	0.96	0.27	0,0,0,0	0
2	SO4	A	6922	5/5	0.96	0.19	0,0,0,0	0

6.5 Other polymers (i)

There are no such residues in this entry.