Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 08:45 am BST

PDB ID	:	2A7S
Title	:	Crystal Structure of the Acyl-CoA Carboxylase, AccD5, from Mycobacterium tuberculosis
Authors	:	Lin, T.; Melgar, M.; Purdon, J.; Tseng, T.; Tsai, S.C.
Deposited on	:	2005-07-06
Resolution	:	2.90 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 following versions of software and data (see references ⓘ) were used in the production of this report:

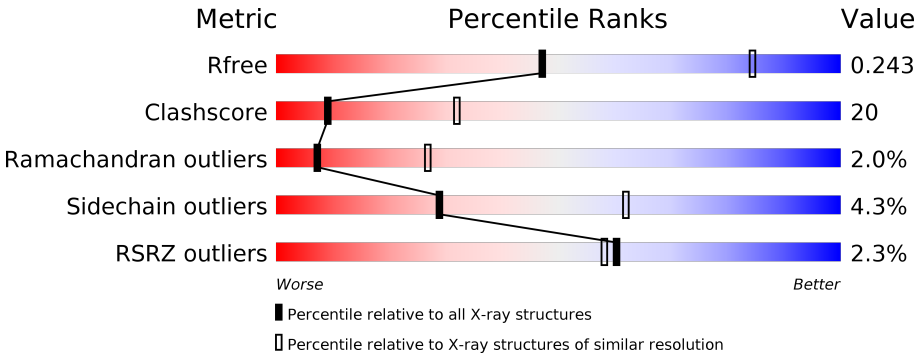
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria 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	548	2% 62% 31%
1	B	548	2% 64% 30%
1	C	548	3% 65% 29%
1	D	548	2% 64% 30%
1	E	548	2% 57% 36%
1	F	548	2% 67% 26%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 25316 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 Probable propionyl-CoA carboxylase beta chain 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	529	Total	C	N	O	S	0	0	0
			4030	2539	698	777	16			
1	B	529	Total	C	N	O	S	0	0	0
			4030	2539	698	777	16			
1	C	529	Total	C	N	O	S	0	0	0
			4030	2539	698	777	16			
1	D	529	Total	C	N	O	S	0	0	0
			4030	2539	698	777	16			
1	E	529	Total	C	N	O	S	0	0	0
			4030	2539	698	777	16			
1	F	529	Total	C	N	O	S	0	0	0
			4030	2539	698	777	16			

- Molecule 2 is water.

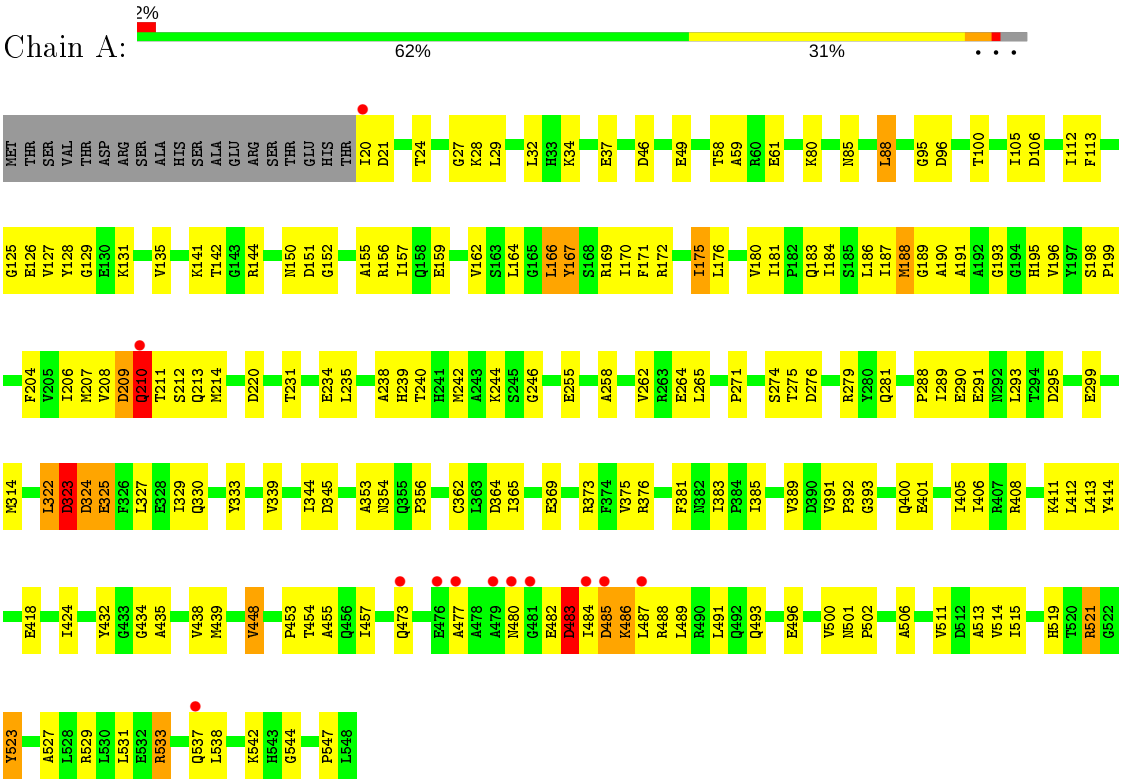
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	203	Total	O	0	0
			203	203		
2	B	220	Total	O	0	0
			220	220		
2	C	176	Total	O	0	0
			176	176		
2	D	175	Total	O	0	0
			175	175		
2	E	187	Total	O	0	0
			187	187		
2	F	175	Total	O	0	0
			175	175		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

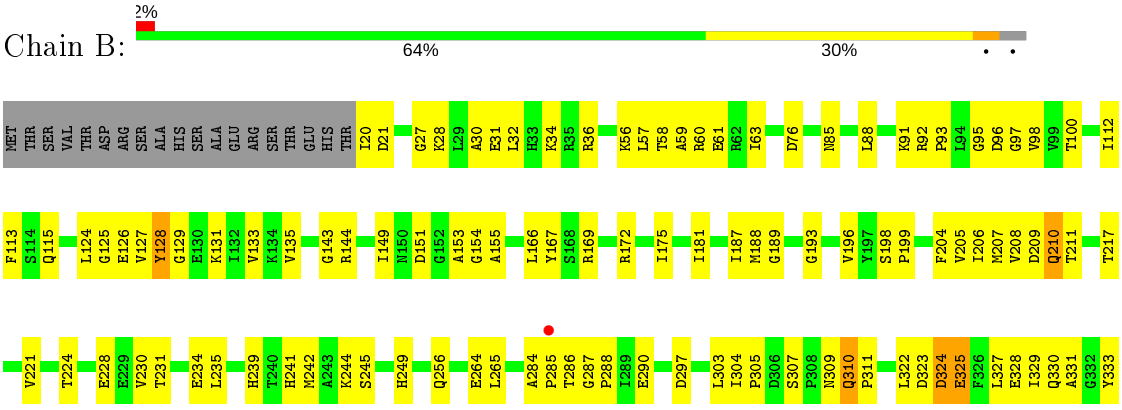
- Molecule 1: Probable propionyl-CoA carboxylase beta chain 5

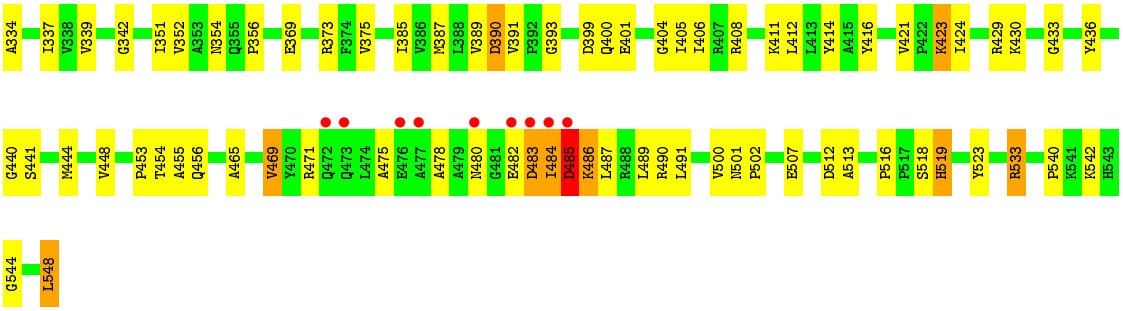
Chain A:

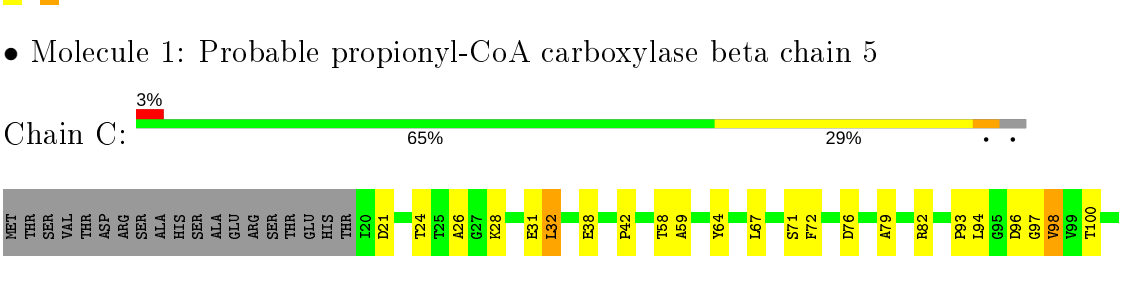


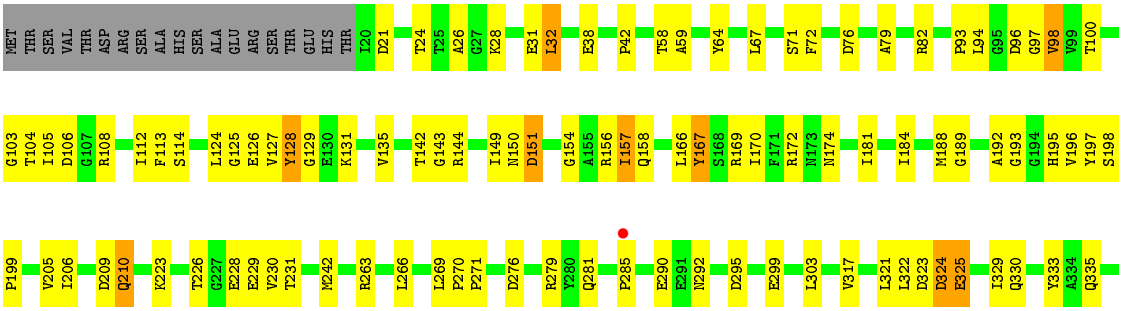
- Molecule 1: Probable propionyl-CoA carboxylase beta chain 5

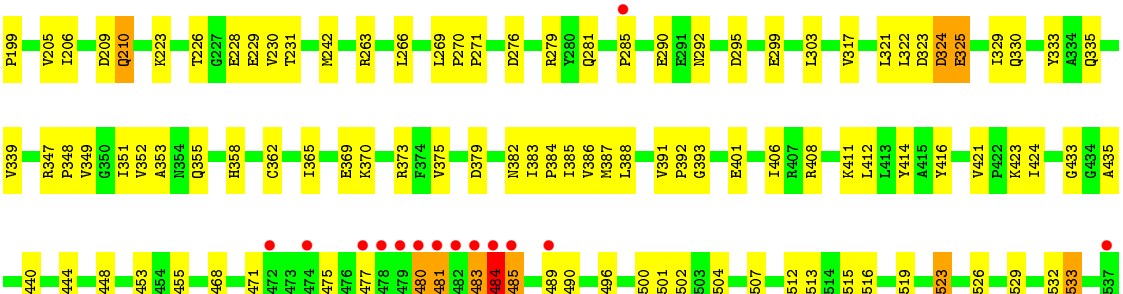
Chain B:









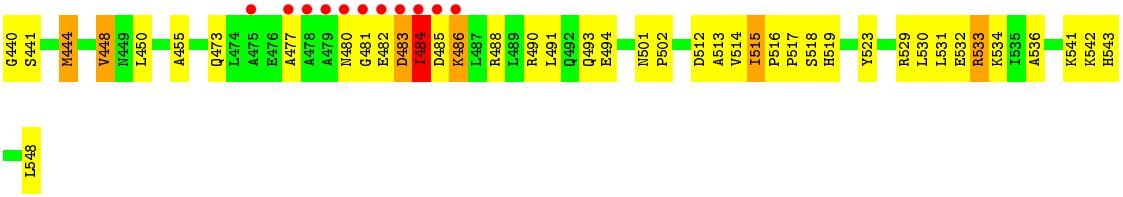


• Molecule 1: Probable propionyl-CoA carboxylase beta chain 5

Chain C:

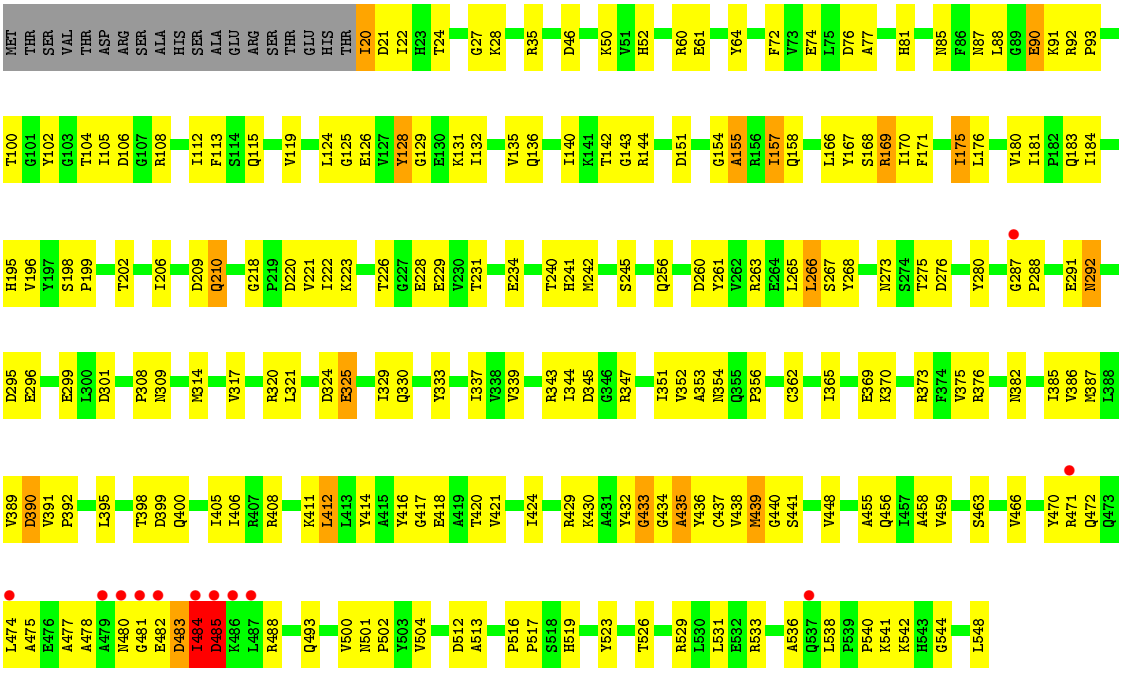
• Molecule 1: Probable propionyl-CoA carboxylase beta chain 5

Chain D:



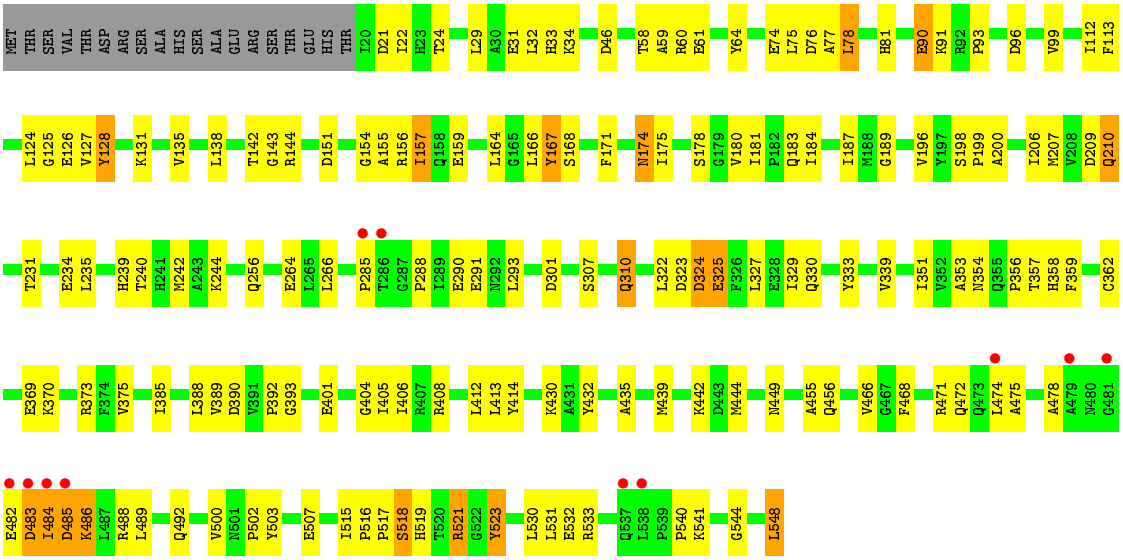
• Molecule 1: Probable propionyl-CoA carboxylase beta chain 5

Chain E:



• Molecule 1: Probable propionyl-CoA carboxylase beta chain 5

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	175.25Å 175.25Å 343.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.88 – 2.90 47.88 – 2.90	Depositor EDS
% Data completeness (in resolution range)	91.5 (47.88-2.90) 91.6 (47.88-2.90)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	2.56 (at 2.91Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.193 , 0.245 0.192 , 0.243	Depositor DCC
R_{free} test set	10829 reflections (9.41%)	wwPDB-VP
Wilson B-factor (Å^2)	39.3	Xtriage
Anisotropy	0.038	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 44.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	25316	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.15% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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	0.38	0/4107	0.63	0/5576
1	B	0.39	0/4107	0.62	0/5576
1	C	0.41	0/4107	0.66	0/5576
1	D	0.40	0/4107	0.63	0/5576
1	E	0.39	0/4107	0.63	0/5576
1	F	0.38	0/4107	0.63	0/5576
All	All	0.39	0/24642	0.63	0/33456

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	C	0	1
1	D	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	128	TYR	Sidechain
1	D	128	TYR	Sidechain

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	A	4030	0	3997	174	0
1	B	4030	0	3997	158	0
1	C	4030	0	3997	158	0
1	D	4030	0	3997	157	0
1	E	4030	0	3997	197	0
1	F	4030	0	3997	153	0
2	A	203	0	0	19	0
2	B	220	0	0	23	0
2	C	176	0	0	14	0
2	D	175	0	0	9	0
2	E	187	0	0	31	0
2	F	175	0	0	26	0
All	All	25316	0	23982	964	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 20.

All (964) 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:C:484:ILE:O	1:C:485:ASP:HB2	1.46	1.11
1:A:209:ASP:O	1:A:210:GLN:HB2	1.31	1.09
1:C:483:ASP:O	1:C:484:ILE:O	1.69	1.09
1:F:485:ASP:CB	1:F:488:ARG:HB2	1.83	1.08
1:D:209:ASP:O	1:D:210:GLN:HB2	1.38	1.08
1:E:157:ILE:HD12	1:E:157:ILE:H	1.18	1.06
1:D:157:ILE:HD12	1:D:157:ILE:H	1.18	1.06
1:F:157:ILE:HD12	1:F:157:ILE:H	1.18	1.04
1:D:483:ASP:O	1:D:484:ILE:O	1.74	1.04
1:B:482:GLU:CG	1:B:483:ASP:H	1.71	1.03
1:B:209:ASP:O	1:B:210:GLN:HB2	1.56	1.02
1:B:482:GLU:HG3	1:B:483:ASP:H	0.88	1.01
1:B:482:GLU:HG3	1:B:483:ASP:N	1.65	1.00
1:C:209:ASP:O	1:C:210:GLN:HB2	1.60	0.99
1:A:157:ILE:H	1:A:157:ILE:HD12	1.25	0.99
1:A:483:ASP:OD1	1:A:486:LYS:HB3	1.64	0.97
1:F:485:ASP:CA	1:F:488:ARG:HB2	1.94	0.97
1:F:301:ASP:HA	1:F:517:PRO:HG2	1.47	0.96
1:A:190:ALA:HB3	2:A:731:HOH:O	1.66	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:485:ASP:HB2	1:F:488:ARG:CB	1.98	0.94
1:F:485:ASP:CB	1:F:488:ARG:CB	2.44	0.94
1:C:105:ILE:O	1:C:106:ASP:HB2	1.68	0.93
1:E:209:ASP:O	1:E:210:GLN:HB2	1.66	0.92
1:B:471:ARG:HG2	2:B:606:HOH:O	1.69	0.92
1:E:105:ILE:O	1:E:106:ASP:HB2	1.69	0.90
1:F:324:ASP:O	1:F:325:GLU:HB2	1.71	0.89
1:A:483:ASP:CG	1:A:483:ASP:O	2.11	0.88
1:E:240:THR:HG23	2:E:598:HOH:O	1.73	0.88
1:B:288:PRO:HG2	1:B:290:GLU:HG2	1.55	0.87
1:F:353:ALA:CB	1:F:388:LEU:HB2	2.04	0.87
1:A:58:THR:HB	1:A:61:GLU:HG3	1.54	0.87
1:B:324:ASP:O	1:B:325:GLU:HB2	1.74	0.87
1:A:484:ILE:O	1:A:485:ASP:HB2	1.74	0.86
1:E:369:GLU:OE1	1:E:408:ARG:HD2	1.74	0.86
1:F:483:ASP:OD1	1:F:486:LYS:HD2	1.75	0.86
1:F:198:SER:HB3	1:F:199:PRO:HD3	1.57	0.86
1:C:477:ALA:HB1	1:C:484:ILE:HG23	1.58	0.86
1:F:353:ALA:HB2	1:F:388:LEU:HB2	1.56	0.85
1:C:329:ILE:HG22	1:C:330:GLN:HG3	1.59	0.85
1:A:484:ILE:O	1:A:485:ASP:CB	2.23	0.85
1:F:485:ASP:HB2	1:F:488:ARG:HB2	1.55	0.85
1:F:166:LEU:HB3	2:F:602:HOH:O	1.77	0.84
1:D:484:ILE:O	1:D:485:ASP:HB3	1.76	0.84
1:D:76:ASP:HB2	1:D:131:LYS:HD2	1.58	0.84
1:B:239:HIS:HB3	2:B:678:HOH:O	1.78	0.83
1:A:105:ILE:O	1:A:106:ASP:HB2	1.79	0.83
1:F:209:ASP:O	1:F:210:GLN:HB2	1.75	0.82
1:A:209:ASP:HA	1:A:238:ALA:HB3	1.61	0.82
1:E:234:GLU:O	1:E:240:THR:HG21	1.78	0.82
1:A:324:ASP:O	1:A:325:GLU:HB3	1.80	0.82
1:E:347:ARG:HH21	1:E:529:ARG:HG2	1.43	0.81
1:A:240:THR:HG23	2:A:569:HOH:O	1.80	0.81
1:A:324:ASP:O	1:A:325:GLU:CB	2.29	0.81
1:A:209:ASP:O	1:A:210:GLN:CB	2.21	0.81
1:C:455:ALA:HB3	1:C:502:PRO:HG3	1.61	0.81
1:A:211:THR:HG21	2:A:658:HOH:O	1.80	0.80
1:C:126:GLU:HA	1:C:166:LEU:CD1	2.11	0.80
1:B:485:ASP:O	1:B:489:LEU:HD13	1.81	0.80
1:B:484:ILE:N	1:B:484:ILE:HD13	1.98	0.79
1:B:96:ASP:OD1	1:B:127:VAL:HB	1.83	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:353:ALA:CB	1:D:388:LEU:HB2	2.13	0.79
1:B:209:ASP:O	1:B:210:GLN:CB	2.32	0.78
1:A:96:ASP:OD1	1:A:127:VAL:HB	1.83	0.77
1:A:239:HIS:HB3	2:A:549:HOH:O	1.83	0.77
1:B:329:ILE:HG22	1:B:330:GLN:HG3	1.65	0.77
1:A:126:GLU:HA	1:A:166:LEU:CD1	2.15	0.77
1:A:29:LEU:HD11	1:C:516:PRO:HB3	1.66	0.77
1:E:424:ILE:HG12	1:E:448:VAL:CG1	2.14	0.77
1:F:485:ASP:HB2	1:F:488:ARG:HB3	1.65	0.76
1:C:198:SER:HB3	1:C:199:PRO:HD3	1.66	0.75
1:E:209:ASP:O	1:E:210:GLN:CB	2.34	0.75
1:D:157:ILE:CD1	1:D:157:ILE:H	1.97	0.75
1:F:78:LEU:HD22	2:F:674:HOH:O	1.86	0.75
1:C:483:ASP:O	1:C:484:ILE:C	2.24	0.75
1:A:482:GLU:O	1:A:483:ASP:CB	2.35	0.75
1:A:198:SER:HB3	1:A:199:PRO:HD3	1.67	0.74
1:E:157:ILE:CD1	1:E:157:ILE:H	1.94	0.74
1:F:157:ILE:CD1	1:F:157:ILE:H	1.95	0.74
1:C:151:ASP:OD1	1:C:189:GLY:HA3	1.88	0.74
1:C:369:GLU:OE1	1:C:408:ARG:HD2	1.87	0.74
1:E:115:GLN:NE2	1:E:151:ASP:H	1.86	0.74
1:D:162:VAL:HG23	2:D:556:HOH:O	1.86	0.73
1:A:186:LEU:HD11	1:A:262:VAL:HG21	1.71	0.73
1:D:420:THR:HB	1:D:536:ALA:HB3	1.70	0.73
1:C:424:ILE:HG12	1:C:448:VAL:CG1	2.18	0.73
1:E:196:VAL:O	1:E:199:PRO:HD2	1.88	0.73
1:F:483:ASP:OD2	1:F:486:LYS:HB2	1.89	0.73
1:D:353:ALA:HB2	1:D:388:LEU:HB2	1.71	0.73
1:E:455:ALA:HB3	1:E:502:PRO:HB3	1.69	0.73
1:B:484:ILE:O	1:B:486:LYS:N	2.21	0.72
1:A:142:THR:OG1	1:A:144:ARG:HG2	1.89	0.72
1:B:484:ILE:C	1:B:486:LYS:H	1.91	0.72
1:F:76:ASP:HB2	1:F:131:LYS:HE3	1.69	0.72
1:A:208:VAL:CG1	1:A:211:THR:OG1	2.37	0.72
1:C:76:ASP:HB2	1:C:131:LYS:HE3	1.71	0.72
1:B:175:ILE:HD11	1:E:417:GLY:HA3	1.70	0.72
1:F:483:ASP:OD2	1:F:486:LYS:CB	2.37	0.72
1:E:198:SER:HB3	1:E:199:PRO:HD3	1.72	0.72
1:A:323:ASP:O	1:A:324:ASP:HB2	1.90	0.72
1:A:482:GLU:O	1:A:483:ASP:HB3	1.88	0.72
1:A:455:ALA:HB3	1:A:502:PRO:HB3	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:471:ARG:HH12	1:E:475:ALA:HB2	1.55	0.71
1:F:484:ILE:HG22	1:F:488:ARG:HG3	1.70	0.71
1:B:483:ASP:CG	1:B:483:ASP:O	2.29	0.71
1:A:501:ASN:HB2	1:A:502:PRO:HD2	1.71	0.71
1:C:322:LEU:C	1:C:324:ASP:H	1.94	0.71
1:E:52:HIS:HD2	2:E:645:HOH:O	1.72	0.71
1:E:434:GLY:O	1:E:437:CYS:N	2.23	0.71
1:A:155:ALA:HB2	1:A:167:TYR:HE2	1.56	0.71
1:C:97:GLY:O	1:C:98:VAL:HB	1.91	0.71
1:D:231:THR:OG1	1:D:234:GLU:HG3	1.90	0.71
1:E:488:ARG:HH11	1:E:488:ARG:HB3	1.56	0.70
1:F:90:GLU:HG2	2:F:637:HOH:O	1.92	0.70
1:C:209:ASP:O	1:C:210:GLN:CB	2.38	0.70
1:E:347:ARG:NH2	1:E:529:ARG:HG2	2.06	0.70
1:D:416:TYR:CZ	1:D:440:GLY:HA2	2.27	0.70
1:E:424:ILE:HG23	1:E:448:VAL:HG13	1.74	0.70
1:F:484:ILE:HG22	1:F:488:ARG:CG	2.21	0.70
1:A:144:ARG:HD3	1:C:533:ARG:HH21	1.55	0.70
1:B:369:GLU:OE1	1:B:408:ARG:HD2	1.91	0.69
1:E:143:GLY:HA2	1:E:181:ILE:HD11	1.74	0.69
1:C:484:ILE:O	1:C:485:ASP:CB	2.30	0.69
1:B:36:ARG:HD2	2:B:612:HOH:O	1.93	0.69
1:C:475:ALA:HA	2:C:631:HOH:O	1.92	0.69
1:E:536:ALA:HA	2:E:601:HOH:O	1.92	0.69
1:E:504:VAL:HB	2:E:561:HOH:O	1.93	0.69
1:A:295:ASP:O	1:A:299:GLU:HG3	1.92	0.68
1:A:157:ILE:CD1	1:A:157:ILE:H	2.03	0.68
1:B:486:LYS:C	1:B:486:LYS:HD2	2.14	0.68
1:D:483:ASP:O	1:D:484:ILE:C	2.31	0.68
1:F:242:MET:O	1:F:333:TYR:HB2	1.94	0.68
1:F:329:ILE:HG22	1:F:330:GLN:HG3	1.74	0.68
1:D:209:ASP:O	1:D:210:GLN:CB	2.26	0.67
1:D:375:VAL:HG13	1:D:385:ILE:HD13	1.74	0.67
1:C:353:ALA:CB	1:C:388:LEU:HB2	2.24	0.67
1:B:401:GLU:HA	1:B:405:ILE:HG22	1.77	0.67
1:B:453:PRO:HG3	1:C:32:LEU:HD12	1.76	0.67
1:B:533:ARG:HD3	1:B:533:ARG:H	1.59	0.67
1:D:131:LYS:O	1:D:135:VAL:HG23	1.94	0.67
1:D:198:SER:HB3	1:D:199:PRO:HD3	1.76	0.67
1:D:91:LYS:HG2	1:D:93:PRO:HD3	1.76	0.66
1:A:424:ILE:HG12	1:A:448:VAL:CG1	2.25	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:391:VAL:HG22	1:D:393:GLY:H	1.60	0.66
1:F:46:ASP:HB2	2:F:663:HOH:O	1.95	0.66
1:A:242:MET:O	1:A:333:TYR:HB2	1.96	0.66
1:C:269:LEU:HD23	1:C:383:ILE:HD11	1.78	0.66
1:E:408:ARG:HA	1:E:411:LYS:HE3	1.76	0.66
1:D:455:ALA:HB3	1:D:502:PRO:HB3	1.76	0.66
1:B:100:THR:HG22	1:B:113:PHE:HB2	1.77	0.65
1:C:324:ASP:O	1:C:325:GLU:HB2	1.96	0.65
1:E:100:THR:HB	1:E:135:VAL:HG21	1.79	0.65
1:B:322:LEU:C	1:B:324:ASP:H	2.00	0.65
1:D:416:TYR:CE1	1:D:440:GLY:HA2	2.31	0.65
1:E:50:LYS:HB3	1:E:50:LYS:NZ	2.12	0.65
1:A:381:PHE:O	1:A:383:ILE:HG13	1.96	0.65
1:B:124:LEU:HD13	1:B:167:TYR:CE1	2.31	0.65
1:B:516:PRO:HG2	1:B:519:HIS:CE1	2.31	0.65
1:C:353:ALA:HB1	1:C:388:LEU:HB2	1.79	0.65
1:E:268:TYR:N	2:E:670:HOH:O	2.29	0.65
1:E:375:VAL:HG13	1:E:385:ILE:HD13	1.79	0.65
1:C:170:ILE:HG22	2:C:641:HOH:O	1.96	0.65
1:B:406:ILE:HB	2:B:564:HOH:O	1.97	0.64
1:D:171:PHE:O	1:D:175:ILE:HG23	1.97	0.64
1:D:254:GLY:N	2:D:589:HOH:O	2.31	0.64
1:E:221:VAL:HG23	2:E:696:HOH:O	1.97	0.64
1:E:85:ASN:O	1:E:88:LEU:HB2	1.96	0.64
1:E:435:ALA:O	1:E:439:MET:HB2	1.96	0.64
1:E:488:ARG:NH1	1:E:488:ARG:HB3	2.12	0.64
1:D:329:ILE:HG22	1:D:330:GLN:HG3	1.80	0.64
1:C:411:LYS:HD3	1:F:548:LEU:HG	1.80	0.64
1:A:220:ASP:HB2	2:A:641:HOH:O	1.98	0.63
1:B:58:THR:HG21	2:B:737:HOH:O	1.97	0.63
1:B:76:ASP:HB2	1:B:131:LYS:HE3	1.79	0.63
1:B:548:LEU:HG	2:E:602:HOH:O	1.99	0.63
1:E:414:TYR:OH	1:E:544:GLY:HA3	1.98	0.63
1:A:206:ILE:N	1:A:206:ILE:HD12	2.13	0.63
1:C:533:ARG:H	1:C:533:ARG:HD3	1.64	0.63
1:A:208:VAL:HG11	1:A:211:THR:OG1	1.98	0.63
1:B:373:ARG:HG2	1:B:373:ARG:HH11	1.64	0.62
1:F:485:ASP:HA	1:F:488:ARG:HB2	1.79	0.62
1:D:157:ILE:HD12	1:D:157:ILE:N	2.02	0.62
1:F:325:GLU:HA	1:F:325:GLU:OE2	1.99	0.62
1:F:78:LEU:CD2	2:F:674:HOH:O	2.43	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:MET:HE1	1:A:255:GLU:HG2	1.82	0.62
1:A:473:GLN:HE21	1:A:487:LEU:HD11	1.64	0.62
1:B:352:VAL:O	1:B:387:MET:HB2	1.98	0.62
1:B:264:GLU:HG2	1:B:327:LEU:HD13	1.81	0.62
1:A:424:ILE:HG12	1:A:448:VAL:HG13	1.81	0.62
1:B:414:TYR:OH	1:B:544:GLY:HA3	2.00	0.62
1:C:96:ASP:OD1	1:C:127:VAL:HB	1.99	0.62
1:D:412:LEU:HD13	1:D:438:VAL:HG22	1.81	0.62
1:B:309:ASN:O	1:B:311:PRO:HD3	1.98	0.61
1:A:521:ARG:HG3	1:A:521:ARG:HH11	1.63	0.61
1:F:503:TYR:O	1:F:507:GLU:HG3	1.99	0.61
1:B:328:GLU:HG2	1:B:331:ALA:HB2	1.82	0.61
1:B:486:LYS:HD2	1:B:486:LYS:O	2.01	0.61
1:D:301:ASP:HA	1:D:517:PRO:HG2	1.82	0.61
1:F:322:LEU:C	1:F:324:ASP:H	2.03	0.61
1:D:100:THR:HB	1:D:135:VAL:HG21	1.80	0.61
1:A:189:GLY:O	1:A:212:SER:HA	2.01	0.61
1:A:527:ALA:O	1:A:531:LEU:HD23	2.01	0.61
1:C:433:GLY:HA2	1:F:164:LEU:HD21	1.81	0.61
1:D:166:LEU:O	1:D:170:ILE:HG13	2.00	0.61
1:E:501:ASN:HB2	1:E:502:PRO:HD2	1.80	0.61
1:B:455:ALA:HB3	1:B:502:PRO:HB3	1.83	0.61
1:A:533:ARG:HD3	1:A:533:ARG:H	1.66	0.61
1:B:155:ALA:HB2	1:B:167:TYR:HE2	1.65	0.61
1:F:307:SER:HB3	1:F:310:GLN:HB2	1.83	0.61
1:F:135:VAL:HG22	2:F:688:HOH:O	2.00	0.61
1:B:198:SER:HB3	1:B:199:PRO:HD3	1.82	0.60
1:D:175:ILE:HG13	1:D:176:LEU:N	2.14	0.60
1:E:301:ASP:HA	1:E:517:PRO:HG2	1.83	0.60
1:F:58:THR:HB	1:F:61:GLU:HG3	1.83	0.60
1:A:126:GLU:HA	1:A:166:LEU:HD13	1.82	0.60
1:A:235:LEU:HD11	1:D:401:GLU:HG3	1.82	0.60
1:E:483:ASP:O	1:E:485:ASP:N	2.34	0.60
1:F:373:ARG:HG2	1:F:373:ARG:HH11	1.65	0.60
1:D:473:GLN:HE22	1:D:491:LEU:HD21	1.67	0.60
1:D:477:ALA:HB1	1:D:484:ILE:HG23	1.84	0.60
1:E:180:VAL:HA	1:E:273:ASN:ND2	2.17	0.60
1:E:288:PRO:HD2	1:E:291:GLU:OE2	2.01	0.60
1:E:365:ILE:HG13	1:E:400:GLN:OE1	2.02	0.60
1:E:129:GLY:HA3	1:E:166:LEU:HD13	1.82	0.60
1:B:228:GLU:OE2	1:E:398:THR:HG23	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:516:PRO:HG2	1:E:519:HIS:CE1	2.36	0.60
1:C:156:ARG:O	1:C:157:ILE:C	2.40	0.60
1:E:478:ALA:HA	1:E:484:ILE:HD11	1.84	0.60
1:A:413:LEU:HD21	1:A:438:VAL:HG12	1.82	0.59
1:C:365:ILE:HG21	1:C:408:ARG:NH2	2.17	0.59
1:C:401:GLU:HG3	1:F:235:LEU:HD11	1.84	0.59
1:C:126:GLU:HA	1:C:166:LEU:HD12	1.82	0.59
1:A:484:ILE:O	1:A:485:ASP:CG	2.39	0.59
1:C:375:VAL:HG13	1:C:385:ILE:CD1	2.32	0.59
1:A:354:ASN:O	1:A:356:PRO:HD3	2.03	0.59
1:B:58:THR:HB	1:B:61:GLU:HG3	1.84	0.59
1:D:441:SER:OG	1:D:444:MET:HB2	2.01	0.59
1:B:115:GLN:HG3	1:B:149:ILE:O	2.02	0.59
1:D:477:ALA:CB	1:D:484:ILE:HG23	2.33	0.59
1:B:484:ILE:HG22	1:B:485:ASP:H	1.67	0.59
1:C:149:ILE:HG23	1:C:188:MET:HG3	1.85	0.59
1:D:60:ARG:HG2	1:D:64:TYR:CE2	2.37	0.59
1:B:151:ASP:OD2	1:B:189:GLY:HA3	2.03	0.59
1:E:399:ASP:HB2	2:E:681:HOH:O	2.03	0.59
1:F:264:GLU:HG2	1:F:327:LEU:HD13	1.84	0.59
1:C:108:ARG:HH21	1:C:271:PRO:HD3	1.68	0.59
1:E:432:TYR:O	1:E:433:GLY:O	2.21	0.59
1:C:196:VAL:O	1:C:199:PRO:HD2	2.03	0.58
1:C:263:ARG:HD3	2:C:675:HOH:O	2.03	0.58
1:C:24:THR:O	1:C:28:LYS:HG3	2.02	0.58
1:F:389:VAL:HG22	1:F:439:MET:HB3	1.85	0.58
1:E:88:LEU:HD13	1:E:158:GLN:HG2	1.84	0.58
1:E:477:ALA:O	1:E:482:GLU:HA	2.04	0.58
1:F:471:ARG:CG	2:F:586:HOH:O	2.51	0.58
1:A:20:ILE:HA	2:A:677:HOH:O	2.02	0.58
1:A:209:ASP:HA	1:A:238:ALA:CB	2.32	0.58
1:B:424:ILE:HG12	1:B:448:VAL:CG1	2.34	0.58
1:D:155:ALA:HB2	1:D:167:TYR:HE2	1.69	0.58
1:D:242:MET:O	1:D:333:TYR:HB2	2.03	0.58
1:A:542:LYS:HE2	2:D:614:HOH:O	2.03	0.58
1:B:482:GLU:CG	1:B:483:ASP:N	2.42	0.58
1:A:125:GLY:H	1:A:128:TYR:HB3	1.69	0.58
1:B:484:ILE:C	1:B:486:LYS:N	2.57	0.58
1:D:58:THR:HG22	1:D:60:ARG:H	1.69	0.58
1:A:188:MET:CE	1:A:255:GLU:HG2	2.34	0.57
1:A:131:LYS:O	1:A:135:VAL:HG23	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:143:GLY:O	1:D:144:ARG:HD2	2.04	0.57
1:D:353:ALA:HB1	1:D:388:LEU:HB2	1.85	0.57
1:E:470:TYR:O	1:E:474:LEU:HB2	2.05	0.57
1:A:369:GLU:OE2	1:A:408:ARG:HD2	2.04	0.57
1:A:473:GLN:NE2	1:A:487:LEU:HD11	2.20	0.57
1:B:187:ILE:HB	1:B:207:MET:HG2	1.86	0.57
1:E:226:THR:OG1	1:E:228:GLU:HG3	2.05	0.57
1:D:22:ILE:HG13	1:D:22:ILE:O	2.05	0.57
1:E:471:ARG:NH1	1:E:475:ALA:HB2	2.20	0.57
1:F:339:VAL:HA	1:F:351:ILE:O	2.05	0.57
1:F:516:PRO:HG2	1:F:519:HIS:CE1	2.40	0.57
1:C:416:TYR:CE1	1:C:440:GLY:HA2	2.39	0.57
1:E:292:ASN:HD22	1:E:292:ASN:N	2.03	0.57
1:F:485:ASP:HB3	1:F:488:ARG:CB	2.33	0.57
1:C:373:ARG:HG2	2:C:639:HOH:O	2.05	0.57
1:D:288:PRO:HG2	1:D:290:GLU:HG2	1.86	0.57
1:D:330:GLN:HB2	1:D:370:LYS:HE3	1.86	0.57
1:F:126:GLU:HA	1:F:166:LEU:CD1	2.35	0.57
1:A:375:VAL:HG13	1:A:385:ILE:CD1	2.35	0.57
1:C:172:ARG:HG2	1:C:172:ARG:HH11	1.70	0.57
1:B:175:ILE:HG21	1:E:414:TYR:HA	1.87	0.56
1:A:162:VAL:HG23	2:A:637:HOH:O	2.05	0.56
1:D:96:ASP:OD1	1:D:127:VAL:HB	2.05	0.56
1:F:414:TYR:OH	1:F:544:GLY:HA3	2.05	0.56
1:A:418:GLU:HG2	1:A:538:LEU:HD11	1.88	0.56
1:C:477:ALA:CB	1:C:484:ILE:HG23	2.34	0.56
1:C:192:ALA:O	1:C:195:HIS:HB2	2.06	0.56
1:D:48:VAL:HG23	1:D:49:GLU:N	2.19	0.56
1:C:290:GLU:H	1:C:290:GLU:CD	2.09	0.56
1:B:175:ILE:CD1	1:E:417:GLY:HA3	2.36	0.56
1:A:344:ILE:O	1:A:345:ASP:HB3	2.05	0.56
1:A:21:ASP:HB3	1:A:24:THR:HG23	1.87	0.56
1:C:151:ASP:CG	1:C:189:GLY:HA3	2.26	0.56
1:D:126:GLU:HA	1:D:166:LEU:HD13	1.88	0.56
1:E:21:ASP:O	1:E:27:GLY:HA3	2.05	0.56
1:C:483:ASP:C	1:C:484:ILE:O	2.40	0.56
1:D:351:ILE:HD13	1:D:386:VAL:HB	1.87	0.56
1:D:501:ASN:HB2	1:D:502:PRO:HD2	1.88	0.56
1:E:229:GLU:HA	2:E:622:HOH:O	2.05	0.56
1:C:477:ALA:O	1:C:484:ILE:HD13	2.05	0.56
1:D:206:ILE:HD12	1:D:206:ILE:N	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:136:GLN:O	1:E:140:ILE:HG13	2.06	0.56
1:A:211:THR:CG2	2:A:658:HOH:O	2.48	0.56
1:E:100:THR:HB	1:E:135:VAL:CG2	2.36	0.56
1:F:466:VAL:HG11	1:F:492:GLN:HA	1.88	0.56
1:A:408:ARG:HA	1:A:411:LYS:HE3	1.86	0.55
1:D:175:ILE:HG22	1:D:201:LEU:HD13	1.87	0.55
1:D:288:PRO:HD2	1:D:291:GLU:OE2	2.06	0.55
1:E:295:ASP:O	1:E:299:GLU:HG3	2.05	0.55
1:F:449:ASN:HB3	2:F:621:HOH:O	2.06	0.55
1:D:322:LEU:HD22	1:D:342:GLY:HA3	1.88	0.55
1:D:485:ASP:OD2	1:D:485:ASP:O	2.24	0.55
1:D:516:PRO:HG2	1:D:519:HIS:ND1	2.20	0.55
1:F:155:ALA:HB2	1:F:167:TYR:HE2	1.72	0.55
1:F:91:LYS:HG2	1:F:93:PRO:HD3	1.89	0.55
1:A:279:ARG:HD2	2:A:706:HOH:O	2.06	0.55
1:D:100:THR:HB	1:D:135:VAL:CG2	2.36	0.55
1:D:45:GLU:HG3	2:D:605:HOH:O	2.06	0.55
1:E:339:VAL:HA	1:E:351:ILE:O	2.06	0.55
1:F:181:ILE:O	1:F:183:GLN:HG3	2.07	0.55
1:B:30:ALA:O	1:B:34:LYS:HG3	2.07	0.55
1:C:424:ILE:HG23	1:C:448:VAL:HG13	1.89	0.55
1:D:136:GLN:O	1:D:140:ILE:HG13	2.07	0.55
1:D:448:VAL:HA	1:D:512:ASP:OD2	2.06	0.55
1:D:529:ARG:O	1:D:532:GLU:HB2	2.06	0.55
1:A:157:ILE:N	1:A:157:ILE:HD12	2.08	0.55
1:A:193:GLY:O	1:A:196:VAL:HG22	2.07	0.55
1:D:58:THR:HB	1:D:61:GLU:HG3	1.87	0.55
1:A:190:ALA:O	1:A:213:GLN:O	2.25	0.55
1:B:208:VAL:HB	1:B:211:THR:OG1	2.06	0.55
1:C:242:MET:O	1:C:333:TYR:HB2	2.07	0.55
1:A:80:LYS:H	1:C:507:GLU:HG2	1.72	0.55
1:A:533:ARG:HE	1:B:144:ARG:HD3	1.71	0.55
1:B:354:ASN:O	1:B:356:PRO:HD3	2.06	0.55
1:B:424:ILE:HG23	1:B:448:VAL:HG13	1.88	0.55
1:C:379:ASP:OD1	1:C:421:VAL:HG13	2.06	0.55
1:D:401:GLU:HA	1:D:405:ILE:HG22	1.89	0.55
1:E:434:GLY:O	1:E:435:ALA:C	2.45	0.55
1:A:100:THR:HB	1:A:135:VAL:HG21	1.89	0.54
1:E:87:ASN:O	1:E:90:GLU:HB2	2.08	0.54
1:F:126:GLU:HA	1:F:166:LEU:HD12	1.89	0.54
1:A:514:VAL:O	1:B:32:LEU:HD21	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:193:GLY:O	1:D:196:VAL:HG22	2.07	0.54
1:B:206:ILE:N	1:B:206:ILE:HD12	2.23	0.54
1:B:540:PRO:HA	2:B:752:HOH:O	2.07	0.54
1:D:125:GLY:H	1:D:128:TYR:HB3	1.73	0.54
1:E:474:LEU:HG	1:E:484:ILE:CG2	2.37	0.54
1:E:85:ASN:N	1:E:85:ASN:HD22	2.04	0.54
1:A:487:LEU:O	1:A:487:LEU:HG	2.07	0.54
1:E:354:ASN:O	1:E:356:PRO:HD3	2.07	0.54
1:F:285:PRO:HA	2:F:658:HOH:O	2.06	0.54
1:F:375:VAL:HG13	1:F:385:ILE:HD13	1.90	0.54
1:B:286:THR:HG22	1:B:287:GLY:H	1.73	0.54
1:D:324:ASP:O	1:D:325:GLU:CB	2.55	0.54
1:D:339:VAL:HG22	1:D:370:LYS:HE2	1.89	0.54
1:E:184:ILE:N	1:E:184:ILE:HD12	2.23	0.54
1:F:455:ALA:HB3	1:F:502:PRO:HG3	1.89	0.54
1:D:483:ASP:C	1:D:484:ILE:O	2.44	0.54
1:E:362:CYS:SG	1:E:392:PRO:HG2	2.48	0.54
1:E:434:GLY:O	1:E:436:TYR:N	2.41	0.54
1:E:471:ARG:HH22	1:E:475:ALA:HB2	1.72	0.54
1:C:223:LYS:HD3	1:C:229:GLU:HG3	1.90	0.54
1:B:256:GLN:HG3	2:B:561:HOH:O	2.06	0.54
1:D:54:LYS:HA	1:D:54:LYS:HE3	1.89	0.54
1:F:151:ASP:OD1	1:F:189:GLY:HA3	2.07	0.54
1:C:490:ARG:HD2	1:C:490:ARG:O	2.09	0.53
1:E:76:ASP:HB2	1:E:131:LYS:HE3	1.90	0.53
1:F:206:ILE:HD12	1:F:206:ILE:N	2.22	0.53
1:D:58:THR:HG22	1:D:60:ARG:N	2.24	0.53
1:F:58:THR:HG23	2:F:592:HOH:O	2.07	0.53
1:E:231:THR:OG1	1:E:234:GLU:HG3	2.08	0.53
1:F:353:ALA:HB1	1:F:388:LEU:HB2	1.86	0.53
1:F:75:LEU:HD12	2:F:688:HOH:O	2.07	0.53
1:A:533:ARG:HG3	2:B:563:HOH:O	2.07	0.53
1:C:375:VAL:HG13	1:C:385:ILE:HD13	1.88	0.53
1:D:100:THR:HG22	1:D:113:PHE:HB2	1.89	0.53
1:D:516:PRO:HG2	1:D:519:HIS:CG	2.43	0.53
1:D:301:ASP:OD1	1:D:517:PRO:HD2	2.07	0.53
1:E:329:ILE:HG22	1:E:330:GLN:HG3	1.90	0.53
1:E:432:TYR:O	1:E:433:GLY:C	2.45	0.53
1:E:142:THR:OG1	1:E:144:ARG:HG2	2.08	0.53
1:A:175:ILE:O	1:A:175:ILE:HD12	2.09	0.53
1:A:152:GLY:O	1:A:191:ALA:HA	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:515:ILE:HG21	1:A:523:TYR:CE2	2.43	0.53
1:C:206:ILE:N	1:C:206:ILE:HD12	2.24	0.53
1:E:20:ILE:N	1:E:20:ILE:HD13	2.23	0.53
1:F:401:GLU:HA	1:F:405:ILE:HG22	1.91	0.53
1:F:60:ARG:HG2	1:F:64:TYR:CE2	2.43	0.53
1:B:533:ARG:HD2	2:B:750:HOH:O	2.08	0.53
1:F:521:ARG:HG3	1:F:521:ARG:HH11	1.73	0.53
1:B:444:MET:HG2	1:E:168:SER:HB3	1.89	0.53
1:C:104:THR:HA	1:C:108:ARG:O	2.09	0.53
1:C:408:ARG:HA	1:C:411:LYS:HE3	1.91	0.52
1:A:375:VAL:HG13	1:A:385:ILE:HD13	1.90	0.52
1:B:231:THR:OG1	1:B:234:GLU:HG3	2.09	0.52
1:C:330:GLN:HB2	1:C:370:LYS:HE3	1.91	0.52
1:C:477:ALA:O	1:C:484:ILE:CD1	2.57	0.52
1:D:477:ALA:O	1:D:484:ILE:HD13	2.08	0.52
1:D:85:ASN:O	1:D:88:LEU:HB2	2.09	0.52
1:E:484:ILE:O	1:E:485:ASP:CB	2.56	0.52
1:E:540:PRO:HA	2:E:722:HOH:O	2.08	0.52
1:A:129:GLY:HA3	1:A:166:LEU:HD22	1.91	0.52
1:A:501:ASN:HB2	1:A:502:PRO:CD	2.39	0.52
1:C:471:ARG:HA	1:C:471:ARG:CZ	2.39	0.52
1:F:484:ILE:HG22	1:F:485:ASP:HA	1.89	0.52
1:F:483:ASP:OD2	1:F:486:LYS:HB3	2.09	0.52
1:A:344:ILE:O	1:A:345:ASP:CB	2.56	0.52
1:E:105:ILE:O	1:E:106:ASP:CB	2.46	0.52
1:E:291:GLU:C	1:E:292:ASN:HD22	2.13	0.52
1:B:230:VAL:HG21	1:B:235:LEU:HD13	1.90	0.52
1:D:171:PHE:CE1	1:D:197:TYR:HB2	2.44	0.52
1:C:295:ASP:O	1:C:299:GLU:HG3	2.10	0.52
1:C:424:ILE:HG12	1:C:448:VAL:HG13	1.92	0.52
1:A:151:ASP:OD1	1:A:189:GLY:HA3	2.09	0.52
1:D:512:ASP:O	1:D:513:ALA:HB2	2.09	0.52
1:E:196:VAL:C	1:E:199:PRO:HD2	2.29	0.52
1:D:389:VAL:HB	1:D:427:ILE:HA	1.91	0.52
1:D:514:VAL:O	1:F:32:LEU:HD11	2.09	0.52
1:E:93:PRO:HG3	1:E:119:VAL:HG13	1.90	0.52
1:A:376:ARG:HD3	1:D:548:LEU:HD11	1.91	0.51
1:A:521:ARG:HG3	1:A:521:ARG:NH1	2.26	0.51
1:D:213:GLN:HG2	1:D:232:MET:HB3	1.92	0.51
1:D:516:PRO:HG2	1:D:519:HIS:CE1	2.46	0.51
1:A:391:VAL:HG22	1:A:393:GLY:N	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:391:VAL:HG22	1:B:393:GLY:H	1.75	0.51
1:D:322:LEU:C	1:D:324:ASP:H	2.13	0.51
1:C:391:VAL:HG22	1:C:393:GLY:H	1.75	0.51
1:D:275:THR:HG23	2:D:557:HOH:O	2.09	0.51
1:E:242:MET:O	1:E:333:TYR:HB2	2.10	0.51
1:E:411:LYS:HG2	2:E:602:HOH:O	2.09	0.51
1:E:74:GLU:HG2	1:E:77:ALA:HB2	1.91	0.51
1:A:432:TYR:O	1:A:435:ALA:HB3	2.09	0.51
1:A:424:ILE:HG23	1:A:448:VAL:HG13	1.92	0.51
1:C:97:GLY:N	2:C:599:HOH:O	2.36	0.51
1:A:187:ILE:HG13	1:A:214:MET:HE1	1.93	0.51
1:B:204:PHE:CD1	1:B:265:LEU:HD21	2.45	0.51
1:D:300:LEU:HD23	1:D:303:LEU:HD12	1.92	0.51
1:D:313:ASP:OD1	1:D:315:HIS:HB2	2.11	0.51
1:E:483:ASP:O	1:E:484:ILE:C	2.49	0.51
1:A:529:ARG:NH1	2:A:648:HOH:O	2.44	0.51
1:B:91:LYS:HG2	1:B:93:PRO:HD3	1.93	0.51
1:E:329:ILE:HB	1:E:339:VAL:HG23	1.91	0.51
1:F:339:VAL:HG22	1:F:370:LYS:HE2	1.93	0.51
1:F:406:ILE:HB	2:F:555:HOH:O	2.09	0.51
1:F:515:ILE:HG21	1:F:523:TYR:CE2	2.45	0.51
1:E:418:GLU:HG3	1:E:538:LEU:HD21	1.93	0.51
1:F:369:GLU:OE1	1:F:408:ARG:HD2	2.11	0.51
1:A:515:ILE:HA	1:B:36:ARG:HH22	1.76	0.51
1:A:24:THR:O	1:A:28:LYS:HG3	2.10	0.51
1:C:71:SER:O	1:C:103:GLY:HA2	2.11	0.51
1:E:344:ILE:O	1:E:345:ASP:CB	2.57	0.51
1:A:100:THR:HG22	1:A:113:PHE:HB2	1.93	0.50
1:B:512:ASP:O	1:B:513:ALA:HB2	2.11	0.50
1:D:424:ILE:HG12	1:D:448:VAL:CG1	2.40	0.50
1:D:530:LEU:HD21	1:F:138:LEU:HD21	1.91	0.50
1:F:515:ILE:O	1:F:515:ILE:HD12	2.11	0.50
1:A:85:ASN:HA	2:A:614:HOH:O	2.10	0.50
1:B:58:THR:HA	2:B:627:HOH:O	2.10	0.50
1:D:22:ILE:HG23	1:D:23:HIS:HD2	1.77	0.50
1:E:433:GLY:O	1:E:434:GLY:C	2.49	0.50
1:E:463:SER:O	1:E:466:VAL:HG22	2.11	0.50
1:E:512:ASP:O	1:E:513:ALA:HB2	2.11	0.50
1:A:373:ARG:HG2	1:A:373:ARG:HH11	1.75	0.50
1:D:208:VAL:O	1:D:212:SER:OG	2.21	0.50
1:E:344:ILE:O	1:E:345:ASP:HB3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:125:GLY:H	1:C:128:TYR:HB3	1.76	0.50
1:F:532:GLU:HB3	1:F:533:ARG:HD2	1.94	0.50
2:B:729:HOH:O	1:C:26:ALA:HA	2.12	0.50
1:E:167:TYR:CE1	1:E:195:HIS:HB2	2.47	0.50
1:E:472:GLN:NE2	2:E:634:HOH:O	2.40	0.50
1:E:52:HIS:HE1	1:E:61:GLU:OE1	1.94	0.50
1:E:91:LYS:NZ	2:E:668:HOH:O	2.45	0.50
1:F:198:SER:HB3	1:F:199:PRO:CD	2.37	0.50
1:F:74:GLU:HG2	1:F:77:ALA:HB2	1.94	0.50
1:A:329:ILE:HG22	1:A:330:GLN:HG3	1.94	0.50
1:A:477:ALA:O	1:A:482:GLU:HA	2.12	0.50
1:A:46:ASP:HA	1:A:49:GLU:OE1	2.12	0.50
1:B:126:GLU:HA	1:B:166:LEU:CD1	2.41	0.50
1:B:421:VAL:O	1:B:423:LYS:HD3	2.11	0.50
1:C:150:ASN:ND2	2:C:627:HOH:O	2.45	0.50
1:D:234:GLU:O	1:D:240:THR:HG21	2.12	0.50
1:E:22:ILE:O	1:E:22:ILE:HG13	2.12	0.50
1:B:387:MET:O	1:B:387:MET:HG3	2.10	0.50
1:C:355:GLN:OE1	1:C:355:GLN:HA	2.11	0.50
1:C:269:LEU:HD23	1:C:383:ILE:CD1	2.41	0.50
1:D:81:HIS:HA	1:D:127:VAL:HG21	1.92	0.50
1:E:395:LEU:HD21	2:E:715:HOH:O	2.11	0.50
1:F:324:ASP:O	1:F:325:GLU:CB	2.51	0.50
1:A:434:GLY:O	1:A:438:VAL:HG13	2.12	0.49
1:A:58:THR:HG22	1:A:59:ALA:N	2.27	0.49
1:C:157:ILE:HD12	1:F:468:PHE:HB2	1.94	0.49
1:D:404:GLY:O	1:D:408:ARG:HG3	2.12	0.49
1:B:242:MET:O	1:B:333:TYR:HB2	2.12	0.49
1:D:339:VAL:HA	1:D:351:ILE:O	2.12	0.49
1:A:208:VAL:HG11	1:A:211:THR:HG1	1.77	0.49
1:D:420:THR:HB	1:D:536:ALA:CB	2.39	0.49
1:B:100:THR:HG22	1:B:113:PHE:CB	2.43	0.49
1:C:98:VAL:HG13	1:C:98:VAL:O	2.12	0.49
1:E:265:LEU:C	2:E:670:HOH:O	2.51	0.49
1:F:485:ASP:CB	1:F:488:ARG:HB3	2.31	0.49
1:A:322:LEU:O	1:A:324:ASP:N	2.46	0.49
1:C:480:ASN:ND2	1:C:481:GLY:H	2.11	0.49
1:C:533:ARG:HD3	1:C:533:ARG:N	2.26	0.49
1:D:477:ALA:O	1:D:484:ILE:CD1	2.60	0.49
1:D:488:ARG:HG2	1:D:488:ARG:HH11	1.76	0.49
1:F:209:ASP:O	1:F:210:GLN:CB	2.52	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:THR:HB	1:A:135:VAL:CG2	2.43	0.49
1:B:58:THR:HG22	1:B:60:ARG:H	1.76	0.49
1:C:352:VAL:O	1:C:387:MET:HB2	2.13	0.49
1:D:312:TYR:OH	1:D:390:ASP:OD2	2.27	0.49
1:D:477:ALA:HA	1:D:481:GLY:O	2.13	0.49
1:E:529:ARG:HB3	2:E:699:HOH:O	2.13	0.49
1:F:143:GLY:C	1:F:144:ARG:HD2	2.33	0.49
1:B:339:VAL:HA	1:B:351:ILE:O	2.13	0.49
1:C:197:TYR:HE2	2:F:593:HOH:O	1.95	0.49
1:E:154:GLY:O	1:E:155:ALA:HB3	2.13	0.49
2:B:580:HOH:O	1:E:542:LYS:HE2	2.13	0.49
1:F:256:GLN:HB2	2:F:589:HOH:O	2.12	0.49
1:E:102:TYR:CE2	1:F:530:LEU:HD22	2.48	0.49
1:F:58:THR:HG22	2:F:613:HOH:O	2.13	0.49
1:C:205:VAL:C	1:C:206:ILE:HD12	2.34	0.49
1:C:387:MET:HG2	2:C:549:HOH:O	2.11	0.49
1:F:471:ARG:HG3	2:F:586:HOH:O	2.12	0.49
1:A:393:GLY:HA2	1:A:435:ALA:HB2	1.94	0.48
1:B:209:ASP:OD1	1:B:210:GLN:HG2	2.13	0.48
1:C:329:ILE:HB	1:C:339:VAL:HG23	1.94	0.48
1:A:141:LYS:HE3	2:A:705:HOH:O	2.12	0.48
1:B:284:ALA:C	2:B:588:HOH:O	2.50	0.48
1:B:390:ASP:OD1	1:B:429:ARG:HB3	2.13	0.48
1:B:471:ARG:HA	1:B:471:ARG:CZ	2.43	0.48
1:D:352:VAL:O	1:D:387:MET:HA	2.12	0.48
1:D:515:ILE:HD13	1:D:515:ILE:H	1.76	0.48
1:E:206:ILE:HD12	1:E:206:ILE:N	2.28	0.48
1:A:150:ASN:HB2	1:A:187:ILE:HD13	1.93	0.48
1:B:129:GLY:HA3	1:B:166:LEU:HD13	1.95	0.48
1:E:392:PRO:O	1:E:432:TYR:HB2	2.13	0.48
1:F:516:PRO:HG2	1:F:519:HIS:ND1	2.28	0.48
1:A:537:GLN:HG3	2:A:670:HOH:O	2.13	0.48
1:A:414:TYR:OH	1:A:544:GLY:HA3	2.12	0.48
1:B:224:THR:HG21	2:B:723:HOH:O	2.14	0.48
1:C:290:GLU:OE2	1:C:290:GLU:N	2.43	0.48
1:C:353:ALA:HB2	1:C:388:LEU:HB2	1.95	0.48
1:F:471:ARG:HG2	2:F:586:HOH:O	2.12	0.48
1:F:485:ASP:C	1:F:488:ARG:HB2	2.32	0.48
1:C:67:LEU:HD13	1:C:103:GLY:HA3	1.95	0.48
1:F:330:GLN:NE2	2:F:618:HOH:O	2.46	0.48
1:A:484:ILE:HG23	1:A:488:ARG:HD2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:28:LYS:O	1:B:31:GLU:HB3	2.14	0.48
1:E:456:GLN:HB3	1:E:500:VAL:CG1	2.43	0.48
1:A:208:VAL:HB	1:A:211:THR:OG1	2.13	0.48
1:E:484:ILE:O	1:E:485:ASP:HB3	2.13	0.48
1:F:413:LEU:HA	2:F:689:HOH:O	2.13	0.48
1:F:456:GLN:HB3	1:F:500:VAL:CG1	2.43	0.48
1:C:193:GLY:O	1:C:196:VAL:HG22	2.14	0.48
1:C:347:ARG:HH12	1:C:532:GLU:HG3	1.78	0.48
1:C:541:LYS:HD3	1:F:180:VAL:HG23	1.95	0.48
1:D:477:ALA:O	1:D:482:GLU:HA	2.13	0.48
1:D:72:PHE:CE2	1:D:74:GLU:HG3	2.49	0.48
1:E:296:GLU:HG2	1:E:320:ARG:HG2	1.96	0.48
1:E:420:THR:HG23	2:E:576:HOH:O	2.13	0.48
1:F:29:LEU:HD11	1:F:33:HIS:HE1	1.79	0.48
1:F:430:LYS:HD3	1:F:432:TYR:HE2	1.77	0.48
1:A:362:CYS:SG	1:A:392:PRO:HG2	2.53	0.47
1:A:389:VAL:HG22	1:A:439:MET:HB3	1.96	0.47
1:B:375:VAL:HG13	1:B:385:ILE:HD13	1.96	0.47
1:D:124:LEU:C	1:D:124:LEU:HD23	2.35	0.47
1:A:457:ILE:HD13	1:A:502:PRO:HA	1.95	0.47
1:A:32:LEU:HD22	1:C:453:PRO:HG3	1.96	0.47
1:F:96:ASP:OD1	1:F:127:VAL:HB	2.14	0.47
1:F:171:PHE:O	1:F:174:ASN:HB2	2.13	0.47
1:B:143:GLY:HA2	1:B:181:ILE:HD11	1.97	0.47
1:D:325:GLU:OE2	1:D:325:GLU:HA	2.14	0.47
1:D:276:ASP:OD2	1:D:533:ARG:NH2	2.47	0.47
1:F:231:THR:OG1	1:F:234:GLU:HG3	2.14	0.47
1:F:329:ILE:HB	1:F:339:VAL:HG23	1.96	0.47
1:E:330:GLN:NE2	1:E:370:LYS:HG3	2.30	0.47
1:E:501:ASN:HB2	1:E:502:PRO:CD	2.44	0.47
1:F:142:THR:OG1	1:F:144:ARG:HG2	2.14	0.47
1:B:501:ASN:HB2	1:B:502:PRO:HD2	1.96	0.47
1:E:352:VAL:O	1:E:387:MET:HB2	2.13	0.47
1:A:240:THR:O	1:A:244:LYS:HB2	2.13	0.47
1:C:143:GLY:HA2	1:C:181:ILE:HD11	1.97	0.47
1:D:76:ASP:CB	1:D:131:LYS:HD2	2.36	0.47
1:D:533:ARG:HA	1:D:533:ARG:HD2	1.67	0.47
1:E:437:CYS:HA	1:E:441:SER:HB3	1.96	0.47
1:F:240:THR:HG23	1:F:244:LYS:HD2	1.97	0.47
1:C:349:VAL:HG12	1:C:384:PRO:HB2	1.95	0.47
1:E:337:ILE:HG23	1:E:370:LYS:HD3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:67:LEU:HD12	1:C:72:PHE:HB2	1.97	0.47
1:E:112:ILE:HG12	1:E:113:PHE:N	2.30	0.47
1:A:85:ASN:O	1:A:88:LEU:HB2	2.15	0.47
1:C:496:GLU:HA	1:C:500:VAL:HG23	1.97	0.47
1:B:193:GLY:O	1:B:196:VAL:HG22	2.14	0.47
1:B:57:LEU:HD12	1:B:57:LEU:N	2.30	0.47
1:A:486:LYS:HG2	1:A:486:LYS:O	2.13	0.47
1:C:142:THR:OG1	1:C:144:ARG:HG2	2.15	0.47
1:D:58:THR:HG22	1:D:61:GLU:H	1.80	0.47
1:A:196:VAL:O	1:A:199:PRO:HD2	2.15	0.46
1:B:310:GLN:O	1:B:429:ARG:NH2	2.46	0.46
1:C:285:PRO:HB2	1:C:292:ASN:ND2	2.29	0.46
1:C:303:LEU:HD23	1:C:303:LEU:C	2.36	0.46
1:C:324:ASP:O	1:C:325:GLU:CB	2.62	0.46
1:E:390:ASP:OD1	1:E:430:LYS:HB2	2.15	0.46
1:F:515:ILE:C	1:F:515:ILE:HD12	2.36	0.46
1:E:337:ILE:CG2	1:E:370:LYS:HD3	2.45	0.46
1:F:239:HIS:HB3	2:F:562:HOH:O	2.15	0.46
1:F:483:ASP:CG	1:F:486:LYS:HB3	2.35	0.46
1:A:231:THR:OG1	1:A:234:GLU:HG3	2.14	0.46
1:D:376:ARG:HG2	2:D:586:HOH:O	2.15	0.46
1:E:128:TYR:CD1	1:E:128:TYR:C	2.89	0.46
1:F:78:LEU:CD2	2:F:711:HOH:O	2.64	0.46
1:A:246:GLY:HA2	2:A:586:HOH:O	2.15	0.46
1:C:58:THR:O	1:C:59:ALA:C	2.54	0.46
1:E:104:THR:HA	1:E:108:ARG:O	2.16	0.46
1:F:540:PRO:O	1:F:541:LYS:HB3	2.14	0.46
1:A:166:LEU:O	1:A:170:ILE:HG13	2.16	0.46
1:A:188:MET:HB3	1:A:188:MET:HE2	1.67	0.46
1:B:334:ALA:O	1:B:337:ILE:HG22	2.15	0.46
1:A:483:ASP:OD1	1:A:483:ASP:O	2.33	0.46
1:A:95:GLY:O	1:A:96:ASP:CB	2.63	0.46
1:B:56:LYS:HG2	2:B:767:HOH:O	2.15	0.46
1:C:42:PRO:HB2	1:C:93:PRO:HB2	1.98	0.46
1:D:171:PHE:O	1:D:174:ASN:HB2	2.16	0.46
1:E:488:ARG:HH11	1:E:488:ARG:CB	2.26	0.46
1:F:81:HIS:HA	1:F:127:VAL:HG21	1.98	0.46
1:A:126:GLU:HA	1:A:166:LEU:HD12	1.94	0.46
1:C:270:PRO:HB3	1:C:276:ASP:O	2.16	0.46
1:D:112:ILE:HG13	1:D:147:ILE:O	2.16	0.46
1:D:174:ASN:HA	1:D:174:ASN:HD22	1.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:204:PHE:CD1	1:D:265:LEU:HD21	2.51	0.46
1:E:241:HIS:HA	1:E:245:SER:OG	2.16	0.46
1:F:485:ASP:O	1:F:489:LEU:N	2.40	0.46
1:B:112:ILE:HG12	1:B:113:PHE:N	2.30	0.46
1:B:533:ARG:HD3	1:B:533:ARG:N	2.29	0.46
1:C:393:GLY:HA2	1:C:435:ALA:HB2	1.98	0.46
1:E:288:PRO:HD2	1:E:291:GLU:CD	2.36	0.46
1:A:290:GLU:N	2:A:676:HOH:O	2.31	0.46
1:A:323:ASP:OD2	1:A:323:ASP:N	2.44	0.46
1:B:20:ILE:CA	2:B:579:HOH:O	2.64	0.46
1:B:303:LEU:HD23	1:B:303:LEU:C	2.36	0.46
1:B:404:GLY:O	1:B:408:ARG:HG3	2.16	0.46
1:E:157:ILE:HD12	1:E:157:ILE:N	2.04	0.46
1:E:240:THR:C	1:E:242:MET:H	2.19	0.46
1:E:324:ASP:O	1:E:325:GLU:HB2	2.16	0.46
1:A:187:ILE:HG13	1:A:214:MET:CE	2.46	0.46
1:C:197:TYR:CE2	2:F:593:HOH:O	2.56	0.46
1:C:529:ARG:CZ	1:C:529:ARG:HB2	2.45	0.46
1:D:98:VAL:HG13	1:D:131:LYS:HE2	1.97	0.46
1:D:183:GLN:O	1:D:202:THR:HB	2.16	0.46
1:E:88:LEU:HD22	1:E:158:GLN:HB3	1.98	0.46
1:B:305:PRO:CB	1:B:310:GLN:HB3	2.47	0.45
1:C:98:VAL:CG1	1:C:98:VAL:O	2.63	0.45
1:E:412:LEU:HD13	1:E:438:VAL:HG22	1.96	0.45
1:D:301:ASP:OD2	1:D:518:SER:HB3	2.16	0.45
1:D:369:GLU:OE1	1:D:408:ARG:HD2	2.16	0.45
1:F:143:GLY:C	1:F:181:ILE:HD11	2.36	0.45
1:F:288:PRO:HD2	1:F:291:GLU:OE2	2.15	0.45
1:A:181:ILE:O	1:A:183:GLN:HG3	2.16	0.45
1:A:515:ILE:HD12	1:A:515:ILE:O	2.17	0.45
1:C:154:GLY:H	1:C:195:HIS:HD2	1.64	0.45
1:E:280:TYR:HB3	2:E:662:HOH:O	2.16	0.45
1:F:187:ILE:HB	1:F:207:MET:HG2	1.98	0.45
1:F:392:PRO:HA	1:F:432:TYR:HD2	1.79	0.45
1:A:314:MET:HG2	1:A:353:ALA:HB1	1.98	0.45
1:E:132:ILE:HG21	1:E:170:ILE:HD13	1.99	0.45
1:F:404:GLY:HA2	2:F:555:HOH:O	2.16	0.45
1:A:34:LYS:O	1:A:37:GLU:HB3	2.15	0.45
1:B:97:GLY:N	2:B:595:HOH:O	2.41	0.45
1:E:124:LEU:HD13	1:E:167:TYR:CE1	2.52	0.45
1:E:389:VAL:HG13	1:E:439:MET:HG3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:ALA:HB2	1:A:167:TYR:CE2	2.45	0.45
1:B:471:ARG:HA	1:B:471:ARG:NE	2.32	0.45
1:C:362:CYS:SG	1:C:392:PRO:HG2	2.56	0.45
1:E:541:LYS:NZ	2:E:657:HOH:O	2.41	0.45
1:F:483:ASP:O	1:F:486:LYS:HB3	2.17	0.45
1:A:196:VAL:C	1:A:199:PRO:HD2	2.37	0.45
1:A:208:VAL:CB	1:A:211:THR:OG1	2.65	0.45
1:B:124:LEU:C	1:B:124:LEU:HD23	2.36	0.45
1:B:487:LEU:O	1:B:491:LEU:HG	2.17	0.45
1:D:223:LYS:HD2	2:D:670:HOH:O	2.16	0.45
1:E:478:ALA:HA	1:E:484:ILE:CD1	2.46	0.45
1:F:174:ASN:HA	1:F:174:ASN:HD22	1.61	0.45
1:C:317:VAL:O	1:C:321:LEU:HG	2.17	0.45
1:C:496:GLU:HA	1:C:500:VAL:CG2	2.47	0.45
1:A:180:VAL:CG2	1:D:541:LYS:HD3	2.47	0.45
1:A:234:GLU:O	1:A:240:THR:HG21	2.17	0.45
1:A:275:THR:HG22	1:A:276:ASP:N	2.32	0.45
1:A:322:LEU:C	1:A:324:ASP:H	2.19	0.45
1:D:426:VAL:HG22	1:D:450:LEU:HB2	1.98	0.45
1:D:72:PHE:HE2	1:D:74:GLU:HG3	1.81	0.45
1:E:405:ILE:HG23	1:E:406:ILE:N	2.31	0.45
1:E:448:VAL:HA	1:E:512:ASP:OD2	2.16	0.45
1:E:85:ASN:N	1:E:85:ASN:ND2	2.65	0.45
1:B:507:GLU:HA	1:C:79:ALA:HA	2.00	0.45
1:C:526:THR:HB	2:C:620:HOH:O	2.16	0.45
1:A:365:ILE:HG13	1:A:400:GLN:OE1	2.17	0.44
1:B:209:ASP:OD2	1:B:239:HIS:NE2	2.50	0.44
1:B:416:TYR:CZ	1:B:440:GLY:HA2	2.52	0.44
1:D:534:LYS:HE2	1:D:536:ALA:HB2	1.99	0.44
1:A:184:ILE:HD12	1:A:265:LEU:HD23	1.99	0.44
1:B:100:THR:HB	1:B:135:VAL:HG11	1.99	0.44
1:D:253:SER:HB2	2:D:589:HOH:O	2.18	0.44
1:E:171:PHE:O	1:E:175:ILE:HG23	2.17	0.44
1:E:352:VAL:HB	1:E:387:MET:HB3	1.98	0.44
1:F:293:LEU:HD22	1:F:518:SER:HB2	1.99	0.44
1:A:453:PRO:HG3	1:B:32:LEU:HD22	1.99	0.44
1:B:249:HIS:HA	1:B:330:GLN:HG2	1.98	0.44
1:D:424:ILE:HG12	1:D:448:VAL:HG13	2.00	0.44
1:F:128:TYR:C	1:F:128:TYR:CD1	2.89	0.44
1:F:157:ILE:HD12	1:F:157:ILE:N	2.03	0.44
1:E:175:ILE:HG13	1:E:176:LEU:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:143:GLY:CA	1:E:181:ILE:HD11	2.45	0.44
1:E:183:GLN:O	1:E:202:THR:HB	2.17	0.44
1:F:474:LEU:HD22	1:F:488:ARG:HG2	2.00	0.44
1:A:206:ILE:N	1:A:206:ILE:CD1	2.81	0.44
1:E:352:VAL:O	1:E:387:MET:CB	2.65	0.44
1:E:81:HIS:HB2	2:E:583:HOH:O	2.17	0.44
1:B:401:GLU:HA	1:B:405:ILE:CG2	2.46	0.44
1:D:78:LEU:N	1:D:78:LEU:HD12	2.33	0.44
1:E:382:ASN:HA	1:E:421:VAL:CG1	2.47	0.44
1:E:471:ARG:NH2	1:E:475:ALA:HB2	2.32	0.44
1:B:153:ALA:HB3	2:B:636:HOH:O	2.17	0.44
1:B:322:LEU:HD13	1:B:342:GLY:HA3	2.00	0.44
1:B:389:VAL:O	1:B:390:ASP:HB2	2.17	0.44
1:B:400:GLN:O	1:B:405:ILE:HB	2.17	0.44
1:B:416:TYR:CE1	1:B:440:GLY:HA2	2.53	0.44
1:B:475:ALA:O	1:B:478:ALA:HB3	2.17	0.44
1:B:516:PRO:HG2	1:B:519:HIS:ND1	2.32	0.44
1:C:174:ASN:OD1	2:C:641:HOH:O	2.21	0.44
1:C:196:VAL:C	1:C:199:PRO:HD2	2.38	0.44
1:C:501:ASN:HB2	1:C:502:PRO:HD2	2.00	0.44
1:D:52:HIS:HE1	1:D:61:GLU:OE2	2.01	0.44
1:E:24:THR:O	1:E:28:LYS:HG3	2.18	0.44
1:A:401:GLU:HA	1:A:405:ILE:HG22	1.99	0.44
1:A:411:LYS:HE2	1:A:547:PRO:O	2.18	0.44
1:B:244:LYS:HE3	2:B:706:HOH:O	2.18	0.44
1:B:391:VAL:HG22	1:B:393:GLY:N	2.33	0.44
1:C:100:THR:HB	1:C:135:VAL:CG2	2.48	0.44
1:D:324:ASP:O	1:D:325:GLU:HB2	2.18	0.44
1:E:126:GLU:HA	1:E:166:LEU:HD12	1.99	0.44
1:E:309:ASN:ND2	1:E:430:LYS:NZ	2.65	0.44
1:A:187:ILE:HB	1:A:207:MET:HG2	2.00	0.44
1:A:513:ALA:HB2	2:A:558:HOH:O	2.18	0.44
1:D:80:LYS:HE2	1:D:92:ARG:NH1	2.33	0.44
1:E:144:ARG:O	1:E:181:ILE:CG2	2.66	0.44
1:E:314:MET:HG2	1:E:353:ALA:HB1	1.99	0.44
1:F:354:ASN:O	1:F:356:PRO:HD3	2.18	0.44
1:C:108:ARG:HH22	1:C:270:PRO:HA	1.82	0.43
1:C:279:ARG:HD2	2:C:657:HOH:O	2.17	0.43
1:C:322:LEU:C	1:C:324:ASP:N	2.65	0.43
1:F:184:ILE:N	1:F:184:ILE:HD12	2.32	0.43
1:F:288:PRO:HG2	1:F:290:GLU:HG2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:433:GLY:O	1:B:436:TYR:HB3	2.18	0.43
1:E:275:THR:HG22	1:E:276:ASP:N	2.33	0.43
1:E:391:VAL:HG11	1:E:439:MET:HG2	1.99	0.43
1:E:60:ARG:HG2	1:E:64:TYR:CE2	2.53	0.43
1:C:38:GLU:HG2	1:C:94:LEU:HD12	2.00	0.43
1:F:178:SER:HA	2:F:600:HOH:O	2.17	0.43
1:F:517:PRO:O	1:F:518:SER:C	2.57	0.43
1:D:416:TYR:CE1	1:D:423:LYS:HE3	2.53	0.43
1:E:126:GLU:HA	1:E:166:LEU:CD1	2.48	0.43
1:E:144:ARG:O	1:E:181:ILE:HG23	2.18	0.43
1:F:21:ASP:HB3	1:F:24:THR:HG23	2.01	0.43
1:A:171:PHE:O	1:A:175:ILE:HG23	2.18	0.43
1:C:108:ARG:NH2	1:C:270:PRO:HA	2.33	0.43
1:C:444:MET:HG2	1:F:168:SER:HB3	2.00	0.43
1:C:172:ARG:HG2	1:C:172:ARG:NH1	2.30	0.43
1:E:81:HIS:NE2	1:E:92:ARG:HG2	2.34	0.43
1:F:131:LYS:O	1:F:135:VAL:HG23	2.18	0.43
1:F:483:ASP:OD2	1:F:483:ASP:O	2.37	0.43
1:B:542:LYS:HE2	2:E:578:HOH:O	2.19	0.43
1:B:85:ASN:O	1:B:88:LEU:HB2	2.18	0.43
1:C:352:VAL:HB	1:C:387:MET:HB3	2.00	0.43
1:C:512:ASP:O	1:C:513:ALA:HB2	2.18	0.43
1:E:432:TYR:O	1:E:435:ALA:HB3	2.18	0.43
1:E:474:LEU:HG	1:E:484:ILE:HG22	2.00	0.43
1:E:516:PRO:HG2	1:E:519:HIS:ND1	2.34	0.43
1:F:373:ARG:HG2	1:F:373:ARG:NH1	2.31	0.43
1:B:21:ASP:O	1:B:27:GLY:HA3	2.18	0.43
1:C:143:GLY:C	1:C:144:ARG:HD2	2.38	0.43
1:E:416:TYR:CE1	1:E:440:GLY:HA2	2.54	0.43
1:F:196:VAL:O	1:F:199:PRO:HD2	2.18	0.43
1:A:164:LEU:O	1:A:167:TYR:HB2	2.19	0.43
1:A:190:ALA:O	1:A:191:ALA:HB3	2.19	0.43
1:C:154:GLY:H	1:C:195:HIS:CD2	2.37	0.43
1:C:157:ILE:O	1:C:158:GLN:C	2.57	0.43
1:D:438:VAL:HG22	1:D:438:VAL:O	2.18	0.43
1:D:486:LYS:HG2	1:D:486:LYS:O	2.19	0.43
1:E:166:LEU:O	1:E:170:ILE:HG13	2.19	0.43
1:F:99:VAL:O	1:F:113:PHE:HA	2.19	0.43
1:A:289:ILE:O	1:A:293:LEU:HG	2.19	0.43
1:A:485:ASP:O	1:A:489:LEU:HB2	2.19	0.43
1:B:125:GLY:H	1:B:128:TYR:HB3	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:196:VAL:O	1:B:199:PRO:HD2	2.19	0.43
1:B:20:ILE:N	2:B:579:HOH:O	2.51	0.43
1:B:211:THR:HG21	2:B:631:HOH:O	2.19	0.43
1:B:430:LYS:HE3	2:B:759:HOH:O	2.18	0.43
1:C:184:ILE:HD12	1:C:184:ILE:N	2.34	0.43
1:D:336:ASN:HB3	1:D:358:HIS:HD2	1.84	0.43
1:D:362:CYS:HA	1:D:391:VAL:HG23	2.01	0.43
1:F:156:ARG:HD2	1:F:159:GLU:OE2	2.19	0.43
1:C:406:ILE:HG22	1:F:200:ALA:HB2	2.01	0.43
1:F:393:GLY:HA2	1:F:435:ALA:HB2	2.01	0.43
1:F:472:GLN:O	1:F:475:ALA:HB3	2.18	0.43
1:E:308:PRO:C	1:E:309:ASN:HD22	2.22	0.42
1:E:433:GLY:O	1:E:436:TYR:HB3	2.19	0.42
1:B:217:THR:HG22	1:B:221:VAL:HB	2.00	0.42
1:B:352:VAL:O	1:B:387:MET:CB	2.66	0.42
1:E:128:TYR:HD1	1:E:128:TYR:C	2.22	0.42
1:E:351:ILE:HA	1:E:386:VAL:O	2.19	0.42
1:E:72:PHE:CE2	1:E:74:GLU:HB2	2.54	0.42
1:F:112:ILE:HG12	1:F:113:PHE:N	2.34	0.42
1:A:329:ILE:HB	1:A:339:VAL:HG23	2.00	0.42
1:A:496:GLU:HA	1:A:500:VAL:HG23	2.01	0.42
1:B:441:SER:OG	1:B:444:MET:HB2	2.18	0.42
1:E:125:GLY:H	1:E:128:TYR:HB3	1.85	0.42
1:E:343:ARG:HA	1:E:347:ARG:O	2.19	0.42
1:E:484:ILE:H	1:E:484:ILE:HG12	1.54	0.42
1:F:330:GLN:HB2	1:F:370:LYS:HE3	2.01	0.42
2:C:650:HOH:O	1:F:444:MET:HE1	2.19	0.42
1:A:181:ILE:HA	1:A:181:ILE:HD13	1.75	0.42
1:A:264:GLU:HG2	1:A:327:LEU:HD13	2.02	0.42
1:B:416:TYR:CZ	1:B:423:LYS:HG2	2.55	0.42
1:C:184:ILE:CD1	1:C:266:LEU:HD11	2.48	0.42
1:C:391:VAL:O	1:C:391:VAL:HG13	2.18	0.42
1:D:347:ARG:HA	1:D:348:PRO:HD3	1.92	0.42
1:D:58:THR:HB	1:D:61:GLU:CG	2.50	0.42
1:F:31:GLU:O	1:F:34:LYS:HB3	2.18	0.42
1:C:386:VAL:HG22	1:C:424:ILE:HB	2.00	0.42
1:C:501:ASN:OD1	1:C:504:VAL:HG23	2.18	0.42
1:E:169:ARG:NH1	2:E:596:HOH:O	2.51	0.42
1:E:220:ASP:O	1:E:223:LYS:HB3	2.20	0.42
1:E:459:VAL:HG23	2:E:553:HOH:O	2.19	0.42
1:F:456:GLN:HB3	1:F:500:VAL:HG12	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:98:VAL:O	1:B:98:VAL:HG13	2.18	0.42
1:D:172:ARG:O	1:D:176:LEU:HB2	2.20	0.42
1:D:78:LEU:N	1:D:78:LEU:CD1	2.83	0.42
2:D:721:HOH:O	1:E:287:GLY:HA3	2.19	0.42
1:E:50:LYS:HZ2	1:E:50:LYS:HB3	1.85	0.42
1:A:271:PRO:HD3	2:A:691:HOH:O	2.19	0.42
1:C:339:VAL:HA	1:C:351:ILE:O	2.20	0.42
1:F:322:LEU:C	1:F:324:ASP:N	2.71	0.42
1:E:35:ARG:HD2	1:F:503:TYR:CE2	2.54	0.42
1:F:81:HIS:HA	1:F:127:VAL:CG2	2.49	0.42
1:A:156:ARG:HD2	1:A:159:GLU:OE2	2.19	0.42
1:B:100:THR:HB	1:B:135:VAL:CG1	2.50	0.42
1:B:448:VAL:HA	1:B:512:ASP:OD2	2.19	0.42
1:C:421:VAL:O	1:C:423:LYS:HG3	2.20	0.42
1:D:362:CYS:SG	1:D:392:PRO:HG2	2.60	0.42
1:E:46:ASP:O	1:E:50:LYS:HG3	2.19	0.42
1:D:336:ASN:HA	1:D:358:HIS:HB3	2.00	0.42
1:E:266:LEU:HG	2:E:641:HOH:O	2.20	0.42
1:E:330:GLN:HB2	1:E:370:LYS:HE3	2.02	0.42
1:A:391:VAL:CG2	1:A:393:GLY:H	2.33	0.42
1:B:408:ARG:HA	1:B:411:LYS:HE3	2.02	0.42
1:B:465:ALA:O	1:B:469:VAL:HG23	2.20	0.42
1:C:124:LEU:HD13	1:C:167:TYR:CE1	2.55	0.42
1:C:64:TYR:CD2	1:C:64:TYR:N	2.87	0.42
1:F:22:ILE:HG22	1:F:22:ILE:O	2.18	0.42
1:B:373:ARG:HG2	1:B:373:ARG:NH1	2.34	0.41
1:C:129:GLY:HA3	1:C:166:LEU:HD22	2.02	0.41
1:A:144:ARG:CD	1:C:533:ARG:HH21	2.29	0.41
1:D:48:VAL:CG2	1:D:49:GLU:N	2.83	0.41
1:E:218:GLY:O	1:E:222:ILE:HG13	2.20	0.41
1:F:124:LEU:HD13	1:F:167:TYR:CE1	2.54	0.41
1:B:196:VAL:C	1:B:199:PRO:HD2	2.40	0.41
1:B:241:HIS:HA	1:B:245:SER:OG	2.19	0.41
1:D:485:ASP:OD2	1:D:485:ASP:C	2.59	0.41
1:E:376:ARG:NH2	2:E:565:HOH:O	2.53	0.41
1:B:455:ALA:O	1:B:502:PRO:HD3	2.20	0.41
1:D:373:ARG:HG2	1:D:373:ARG:HH11	1.84	0.41
1:E:50:LYS:HB3	1:E:50:LYS:HZ3	1.81	0.41
1:F:475:ALA:O	1:F:478:ALA:HB3	2.20	0.41
1:A:204:PHE:CG	1:A:265:LEU:HD21	2.56	0.41
1:B:205:VAL:C	1:B:206:ILE:HD12	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:58:THR:CG2	1:B:59:ALA:N	2.84	0.41
1:C:114:SER:HA	1:C:149:ILE:HB	2.03	0.41
1:C:351:ILE:HA	1:C:386:VAL:O	2.21	0.41
1:E:526:THR:HA	2:E:719:HOH:O	2.20	0.41
1:F:468:PHE:CD1	1:F:468:PHE:N	2.88	0.41
1:F:58:THR:HG22	1:F:59:ALA:N	2.35	0.41
1:A:255:GLU:O	1:A:258:ALA:HB3	2.20	0.41
1:A:288:PRO:HD2	1:A:291:GLU:OE2	2.20	0.41
1:B:307:SER:OG	1:B:310:GLN:HB2	2.19	0.41
1:B:456:GLN:HB3	1:B:500:VAL:CG1	2.50	0.41
1:B:95:GLY:C	1:B:97:GLY:H	2.24	0.41
1:C:144:ARG:NH2	1:C:271:PRO:HB3	2.35	0.41
1:C:226:THR:OG1	1:C:228:GLU:HG3	2.21	0.41
1:C:386:VAL:HA	1:C:424:ILE:O	2.20	0.41
1:D:181:ILE:HA	1:D:181:ILE:HD13	1.83	0.41
1:D:490:ARG:O	1:D:494:GLU:HG3	2.21	0.41
1:F:125:GLY:H	1:F:128:TYR:HB3	1.85	0.41
1:F:143:GLY:O	1:F:144:ARG:HD2	2.21	0.41
1:A:487:LEU:O	1:A:491:LEU:HG	2.21	0.41
1:C:339:VAL:HG22	1:C:370:LYS:HE2	2.01	0.41
1:C:485:ASP:O	1:C:489:LEU:HB2	2.20	0.41
1:E:266:LEU:HA	1:E:266:LEU:HD12	1.86	0.41
1:E:373:ARG:HG2	2:E:643:HOH:O	2.21	0.41
1:E:424:ILE:HG12	1:E:448:VAL:HG13	1.97	0.41
1:B:129:GLY:O	1:B:133:VAL:HG23	2.21	0.41
1:B:172:ARG:O	1:B:175:ILE:HG12	2.20	0.41
1:C:468:PHE:N	1:C:468:PHE:CD1	2.88	0.41
1:D:542:LYS:O	1:D:543:HIS:HB3	2.20	0.41
1:D:58:THR:CG2	1:D:60:ARG:H	2.34	0.41
1:E:432:TYR:HA	1:E:458:ALA:O	2.21	0.41
1:E:434:GLY:C	1:E:436:TYR:N	2.74	0.41
1:F:373:ARG:HG2	2:F:572:HOH:O	2.21	0.41
1:A:21:ASP:O	1:A:27:GLY:HA3	2.21	0.41
1:E:267:SER:O	1:E:343:ARG:NH2	2.53	0.41
1:E:382:ASN:HA	1:E:421:VAL:HG11	2.03	0.41
1:F:290:GLU:HG2	2:F:646:HOH:O	2.20	0.41
1:A:391:VAL:HG22	1:A:393:GLY:H	1.84	0.41
1:A:406:ILE:HD13	1:D:214:MET:HG2	2.03	0.41
1:B:128:TYR:C	1:B:128:TYR:CD1	2.94	0.41
1:B:204:PHE:CG	1:B:265:LEU:HD21	2.56	0.41
1:F:358:HIS:O	1:F:359:PHE:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:405:ILE:HG23	1:A:406:ILE:N	2.35	0.41
1:C:31:GLU:OE1	1:C:31:GLU:HA	2.21	0.41
1:C:347:ARG:HA	1:C:348:PRO:HD3	1.91	0.41
2:A:681:HOH:O	1:C:523:TYR:HE2	2.03	0.41
1:C:414:TYR:OH	1:C:544:GLY:HA3	2.21	0.41
1:D:143:GLY:HA2	1:D:181:ILE:HD11	2.02	0.41
2:A:596:HOH:O	1:D:376:ARG:HD3	2.21	0.41
1:A:180:VAL:HG23	1:D:541:LYS:HD3	2.01	0.41
1:A:506:ALA:HA	1:A:511:VAL:HB	2.02	0.41
1:B:304:ILE:HG21	1:B:454:THR:HG21	2.02	0.41
1:C:210:GLN:N	2:C:558:HOH:O	2.35	0.41
1:C:335:GLN:HB2	1:C:358:HIS:CG	2.56	0.41
1:D:204:PHE:CG	1:D:265:LEU:HD21	2.56	0.41
1:B:60:ARG:HA	1:B:63:ILE:HD12	2.03	0.40
1:C:108:ARG:HB3	2:C:609:HOH:O	2.20	0.40
1:D:100:THR:HG22	1:D:113:PHE:CB	2.51	0.40
1:D:391:VAL:HG22	1:D:393:GLY:N	2.31	0.40
1:D:45:GLU:H	1:D:45:GLU:CD	2.23	0.40
1:E:287:GLY:HA2	2:E:640:HOH:O	2.21	0.40
1:B:456:GLN:HB3	1:B:500:VAL:HG12	2.03	0.40
1:D:329:ILE:HB	1:D:339:VAL:HG23	2.03	0.40
1:E:261:TYR:OH	1:E:329:ILE:HD13	2.21	0.40
1:E:35:ARG:HH11	1:E:35:ARG:HG3	1.86	0.40
1:A:112:ILE:HG12	1:A:113:PHE:N	2.37	0.40
1:A:176:LEU:HA	1:A:176:LEU:HD23	1.92	0.40
1:B:484:ILE:H	1:B:484:ILE:CD1	2.35	0.40
1:B:297:ASP:O	1:B:518:SER:HA	2.21	0.40
1:C:353:ALA:HB2	1:C:388:LEU:HG	2.03	0.40
1:E:256:GLN:HG2	2:E:557:HOH:O	2.21	0.40
1:E:263:ARG:NH1	1:E:263:ARG:HG3	2.35	0.40
1:F:483:ASP:O	1:F:486:LYS:CB	2.69	0.40
1:B:487:LEU:HD12	1:B:490:ARG:HE	1.86	0.40
1:B:56:LYS:NZ	2:B:648:HOH:O	2.54	0.40
1:C:112:ILE:HG12	1:C:113:PHE:N	2.37	0.40
1:D:405:ILE:HG23	1:D:406:ILE:N	2.36	0.40
1:E:317:VAL:O	1:E:321:LEU:HG	2.22	0.40
1:E:538:LEU:HG	2:E:657:HOH:O	2.20	0.40
1:F:442:LYS:HE2	1:F:449:ASN:OD1	2.21	0.40
1:A:413:LEU:CD2	1:A:438:VAL:HG12	2.50	0.40
1:C:206:ILE:N	1:C:206:ILE:CD1	2.84	0.40
1:C:231:THR:HA	2:C:654:HOH:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:LEU:HD21	1:C:515:ILE:HA	2.02	0.40
1:D:76:ASP:HA	2:E:570:HOH:O	2.22	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	A	527/548 (96%)	476 (90%)	44 (8%)	7 (1%)	12 37
1	B	527/548 (96%)	482 (92%)	34 (6%)	11 (2%)	7 26
1	C	527/548 (96%)	477 (90%)	37 (7%)	13 (2%)	5 21
1	D	527/548 (96%)	474 (90%)	43 (8%)	10 (2%)	8 28
1	E	527/548 (96%)	470 (89%)	45 (8%)	12 (2%)	6 23
1	F	527/548 (96%)	484 (92%)	33 (6%)	10 (2%)	8 28
All	All	3162/3288 (96%)	2863 (90%)	236 (8%)	63 (2%)	7 27

All (63) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	210	GLN
1	A	480	ASN
1	A	483	ASP
1	B	325	GLU
1	B	480	ASN
1	B	484	ILE
1	C	98	VAL
1	C	157	ILE
1	C	325	GLU
1	C	480	ASN

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Mol	Chain	Res	Type
1	C	484	ILE
1	C	485	ASP
1	D	210	GLN
1	D	390	ASP
1	D	480	ASN
1	D	484	ILE
1	E	433	GLY
1	E	480	ASN
1	E	484	ILE
1	E	485	ASP
1	F	325	GLU
1	A	323	ASP
1	A	325	GLU
1	A	485	ASP
1	B	154	GLY
1	B	390	ASP
1	B	469	VAL
1	C	21	ASP
1	C	210	GLN
1	D	323	ASP
1	D	325	GLU
1	E	210	GLN
1	B	210	GLN
1	B	324	ASP
1	B	485	ASP
1	C	151	ASP
1	C	483	ASP
1	D	324	ASP
1	E	390	ASP
1	E	429	ARG
1	E	435	ALA
1	E	483	ASP
1	F	324	ASP
1	F	390	ASP
1	F	483	ASP
1	A	324	ASP
1	C	324	ASP
1	D	285	PRO
1	D	429	ARG
1	D	483	ASP
1	F	154	GLY
1	C	323	ASP

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Mol	Chain	Res	Type
1	E	155	ALA
1	F	210	GLN
1	F	323	ASP
1	F	357	THR
1	F	362	CYS
1	F	518	SER
1	B	323	ASP
1	C	481	GLY
1	E	325	GLU
1	E	481	GLY
1	B	285	PRO

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	423/440 (96%)	398 (94%)	25 (6%)	19 49
1	B	423/440 (96%)	408 (96%)	15 (4%)	36 70
1	C	423/440 (96%)	410 (97%)	13 (3%)	40 74
1	D	423/440 (96%)	402 (95%)	21 (5%)	24 57
1	E	423/440 (96%)	405 (96%)	18 (4%)	29 62
1	F	423/440 (96%)	405 (96%)	18 (4%)	29 62
All	All	2538/2640 (96%)	2428 (96%)	110 (4%)	29 62

All (110) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	88	LEU
1	A	166	LEU
1	A	167	TYR
1	A	169	ARG
1	A	172	ARG
1	A	175	ILE
1	A	188	MET

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Mol	Chain	Res	Type
1	A	195	HIS
1	A	209	ASP
1	A	210	GLN
1	A	274	SER
1	A	281	GLN
1	A	322	LEU
1	A	323	ASP
1	A	364	ASP
1	A	412	LEU
1	A	448	VAL
1	A	454	THR
1	A	483	ASP
1	A	486	LYS
1	A	493	GLN
1	A	519	HIS
1	A	521	ARG
1	A	523	TYR
1	A	533	ARG
1	B	92	ARG
1	B	128	TYR
1	B	169	ARG
1	B	188	MET
1	B	310	GLN
1	B	399	ASP
1	B	412	LEU
1	B	423	LYS
1	B	483	ASP
1	B	485	ASP
1	B	486	LYS
1	B	519	HIS
1	B	523	TYR
1	B	533	ARG
1	B	548	LEU
1	C	32	LEU
1	C	82	ARG
1	C	167	TYR
1	C	169	ARG
1	C	230	VAL
1	C	281	GLN
1	C	382	ASN
1	C	412	LEU
1	C	484	ILE

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Mol	Chain	Res	Type
1	C	519	HIS
1	C	523	TYR
1	C	533	ARG
1	C	548	LEU
1	D	54	LYS
1	D	58	THR
1	D	75	LEU
1	D	90	GLU
1	D	169	ARG
1	D	174	ASN
1	D	175	ILE
1	D	195	HIS
1	D	210	GLN
1	D	256	GLN
1	D	290	GLU
1	D	412	LEU
1	D	444	MET
1	D	448	VAL
1	D	484	ILE
1	D	486	LYS
1	D	493	GLN
1	D	515	ILE
1	D	523	TYR
1	D	531	LEU
1	D	533	ARG
1	E	20	ILE
1	E	90	GLU
1	E	128	TYR
1	E	157	ILE
1	E	169	ARG
1	E	175	ILE
1	E	260	ASP
1	E	266	LEU
1	E	292	ASN
1	E	412	LEU
1	E	439	MET
1	E	484	ILE
1	E	485	ASP
1	E	493	GLN
1	E	523	TYR
1	E	531	LEU
1	E	533	ARG

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Mol	Chain	Res	Type
1	E	548	LEU
1	F	78	LEU
1	F	90	GLU
1	F	128	TYR
1	F	157	ILE
1	F	167	TYR
1	F	174	ASN
1	F	175	ILE
1	F	266	LEU
1	F	310	GLN
1	F	412	LEU
1	F	482	GLU
1	F	484	ILE
1	F	485	ASP
1	F	486	LYS
1	F	521	ARG
1	F	523	TYR
1	F	531	LEU
1	F	548	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (61) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	HIS
1	A	309	ASN
1	A	366	ASN
1	A	473	GLN
1	A	492	GLN
1	B	23	HIS
1	B	174	ASN
1	B	330	GLN
1	B	335	GLN
1	B	358	HIS
1	B	366	ASN
1	B	403	ASN
1	B	492	GLN
1	C	52	HIS
1	C	87	ASN
1	C	174	ASN
1	C	195	HIS
1	C	256	GLN
1	C	292	ASN

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Mol	Chain	Res	Type
1	C	335	GLN
1	C	366	ASN
1	C	403	ASN
1	C	480	ASN
1	C	492	GLN
1	C	537	GLN
1	D	23	HIS
1	D	52	HIS
1	D	85	ASN
1	D	158	GLN
1	D	174	ASN
1	D	256	GLN
1	D	309	ASN
1	D	330	GLN
1	D	358	HIS
1	D	366	ASN
1	D	403	ASN
1	D	473	GLN
1	D	492	GLN
1	D	493	GLN
1	E	23	HIS
1	E	33	HIS
1	E	41	HIS
1	E	52	HIS
1	E	85	ASN
1	E	87	ASN
1	E	115	GLN
1	E	174	ASN
1	E	256	GLN
1	E	292	ASN
1	E	309	ASN
1	E	330	GLN
1	E	366	ASN
1	E	403	ASN
1	E	492	GLN
1	F	174	ASN
1	F	183	GLN
1	F	309	ASN
1	F	358	HIS
1	F	403	ASN
1	F	473	GLN
1	F	492	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	529/548 (96%)	-0.38	12 (2%)	60	58	19, 34, 86, 125	0
1	B	529/548 (96%)	-0.46	10 (1%)	66	65	19, 35, 82, 132	0
1	C	529/548 (96%)	-0.44	15 (2%)	53	49	18, 32, 86, 138	0
1	D	529/548 (96%)	-0.53	12 (2%)	60	58	18, 33, 84, 134	0
1	E	529/548 (96%)	-0.53	12 (2%)	60	58	18, 32, 75, 128	0
1	F	529/548 (96%)	-0.44	11 (2%)	63	61	18, 35, 82, 125	0
All	All	3174/3288 (96%)	-0.46	72 (2%)	60	58	18, 33, 84, 138	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	481	GLY	4.8
1	C	481	GLY	4.7
1	F	485	ASP	4.7
1	D	484	ILE	4.5
1	E	484	ILE	4.3
1	C	484	ILE	4.1
1	A	485	ASP	4.1
1	B	477	ALA	4.1
1	A	477	ALA	4.1
1	D	481	GLY	4.1
1	C	480	ASN	4.0
1	D	480	ASN	3.9
1	C	537	GLN	3.8
1	F	537	GLN	3.8
1	A	484	ILE	3.6
1	B	483	ASP	3.5
1	A	481	GLY	3.4
1	D	477	ALA	3.4
1	F	479	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	E	479	ALA	3.0
1	D	485	ASP	3.0
1	C	483	ASP	3.0
1	D	286	THR	2.9
1	A	537	GLN	2.9
1	F	286	THR	2.9
1	C	479	ALA	2.9
1	B	484	ILE	2.8
1	C	538	LEU	2.8
1	B	472	GLN	2.8
1	D	482	GLU	2.8
1	B	482	GLU	2.7
1	C	477	ALA	2.7
1	E	482	GLU	2.6
1	B	473	GLN	2.6
1	F	482	GLU	2.6
1	E	537	GLN	2.5
1	A	487	LEU	2.5
1	A	480	ASN	2.5
1	E	474	LEU	2.5
1	C	478	ALA	2.5
1	B	480	ASN	2.5
1	F	474	LEU	2.5
1	E	480	ASN	2.5
1	C	472	GLN	2.5
1	B	285	PRO	2.4
1	E	485	ASP	2.4
1	A	473	GLN	2.4
1	A	210	GLN	2.4
1	B	485	ASP	2.4
1	A	479	ALA	2.4
1	F	481	GLY	2.3
1	F	538	LEU	2.3
1	A	476	GLU	2.3
1	C	489	LEU	2.3
1	E	471	ARG	2.3
1	E	486	LYS	2.3
1	E	487	LEU	2.3
1	A	20	ILE	2.3
1	D	483	ASP	2.3
1	F	484	ILE	2.2
1	F	483	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	485	ASP	2.2
1	C	285	PRO	2.2
1	B	476	GLU	2.1
1	D	478	ALA	2.1
1	D	479	ALA	2.1
1	C	482	GLU	2.1
1	E	287	GLY	2.0
1	F	285	PRO	2.0
1	D	486	LYS	2.0
1	D	475	ALA	2.0
1	C	474	LEU	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.