WORLDWIDE PDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 08:37 pm BST

PDB ID	:	1MNF
Title	:	Domain motions in GroEL upon binding of an oligopeptide
Authors	:	Wang, J.; Chen, L.
Deposited on	:	2002-09-05
Resolution	:	3.00 Å(reported)

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

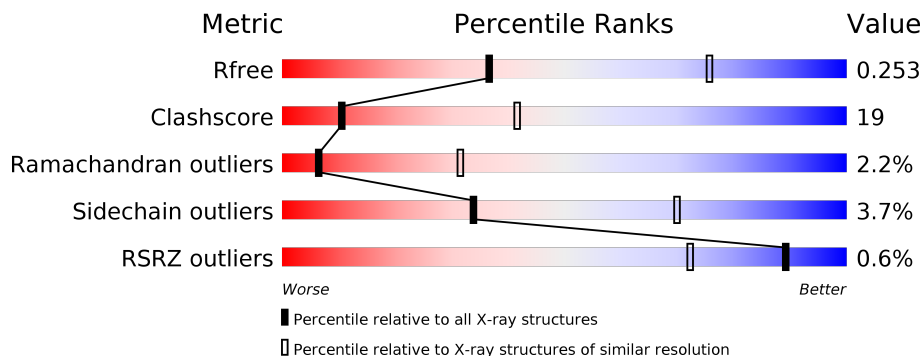|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 3.00 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	Percentile Ranks	Value
Rfree		0.253
Clashscore		19
Ramachandran outliers		2.2%
Sidechain outliers		3.7%
RSRZ outliers		0.6%

Worse　　　　　　　　　　　　　　*Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
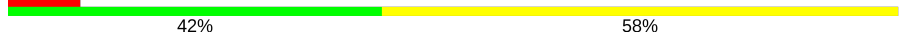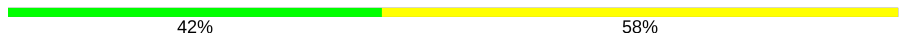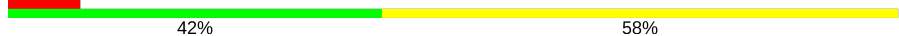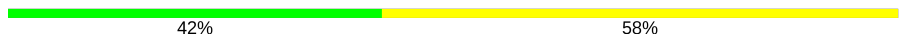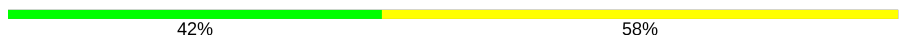
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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	547	65% 28% · ·
1	B	547	65% 28% · ·
1	C	547	% 63% 30% · ·
1	D	547	61% 32% · ·
1	E	547	% 65% 28% · ·
1	F	547	% 64% 29% · ·

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Mol	Chain	Length	Quality of chain
1	G	547	65% 29%
1	H	547	% 64% 29%
1	I	547	% 62% 31%
1	J	547	% 61% 32%
1	K	547	62% 31%
1	L	547	65% 28%
1	M	547	% 65% 29%
1	N	547	% 64% 29%
2	1	12	8% 42% 58%
2	2	12	42% 58%
2	O	12	8% 42% 58%
2	P	12	42% 58%
2	Q	12	42% 58%
2	R	12	42% 58%
2	S	12	8% 42% 58%
2	T	12	42% 58%
2	U	12	42% 58%
2	V	12	42% 58%
2	W	12	42% 58%
2	X	12	42% 58%
2	Y	12	42% 58%
2	Z	12	75% 25%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 55765 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 groEL protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	525	Total	C	N	O	S	0	0	0
			3864	2403	667	774	20			
1	B	525	Total	C	N	O	S	0	0	0
			3864	2403	667	774	20			
1	C	525	Total	C	N	O	S	0	0	0
			3864	2403	667	774	20			
1	D	525	Total	C	N	O	S	0	0	0
			3864	2403	667	774	20			
1	E	525	Total	C	N	O	S	0	0	0
			3864	2403	667	774	20			
1	F	525	Total	C	N	O	S	0	0	0
			3864	2403	667	774	20			
1	G	525	Total	C	N	O	S	0	0	0
			3864	2403	667	774	20			
1	H	525	Total	C	N	O	S	0	0	0
			3864	2403	667	774	20			
1	I	525	Total	C	N	O	S	0	0	0
			3864	2403	667	774	20			
1	J	525	Total	C	N	O	S	0	0	0
			3864	2403	667	774	20			
1	K	525	Total	C	N	O	S	0	0	0
			3864	2403	667	774	20			
1	L	525	Total	C	N	O	S	0	0	0
			3864	2403	667	774	20			
1	M	525	Total	C	N	O	S	0	0	0
			3864	2403	667	774	20			
1	N	525	Total	C	N	O	S	0	0	0
			3864	2403	667	774	20			

- Molecule 2 is a protein called 12-residue peptide substrate.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	O	12	Total 104	C 71	N 16	O 16	S 1	0	0	0
2	P	12	Total 104	C 71	N 16	O 16	S 1	0	0	0
2	Q	12	Total 104	C 71	N 16	O 16	S 1	0	0	0
2	R	12	Total 104	C 71	N 16	O 16	S 1	0	0	0
2	S	12	Total 104	C 71	N 16	O 16	S 1	0	0	0
2	T	12	Total 104	C 71	N 16	O 16	S 1	0	0	0
2	U	12	Total 104	C 71	N 16	O 16	S 1	0	0	0
2	V	12	Total 104	C 71	N 16	O 16	S 1	0	0	0
2	W	12	Total 104	C 71	N 16	O 16	S 1	0	0	0
2	X	12	Total 104	C 71	N 16	O 16	S 1	0	0	0
2	Y	12	Total 104	C 71	N 16	O 16	S 1	0	0	0
2	Z	12	Total 104	C 71	N 16	O 16	S 1	0	0	0
2	1	12	Total 104	C 71	N 16	O 16	S 1	0	0	0
2	2	12	Total 104	C 71	N 16	O 16	S 1	0	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	20	Total 20	O 20	0	0
3	B	29	Total 29	O 29	0	0
3	C	12	Total 12	O 12	0	0
3	D	22	Total 22	O 22	0	0
3	E	19	Total 19	O 19	0	0
3	F	15	Total 15	O 15	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	11	Total 11	O 11	0	0
3	H	13	Total 13	O 13	0	0
3	I	23	Total 23	O 23	0	0
3	J	10	Total 10	O 10	0	0
3	K	8	Total 8	O 8	0	0
3	L	10	Total 10	O 10	0	0
3	M	6	Total 6	O 6	0	0
3	N	15	Total 15	O 15	0	0

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: groEL protein
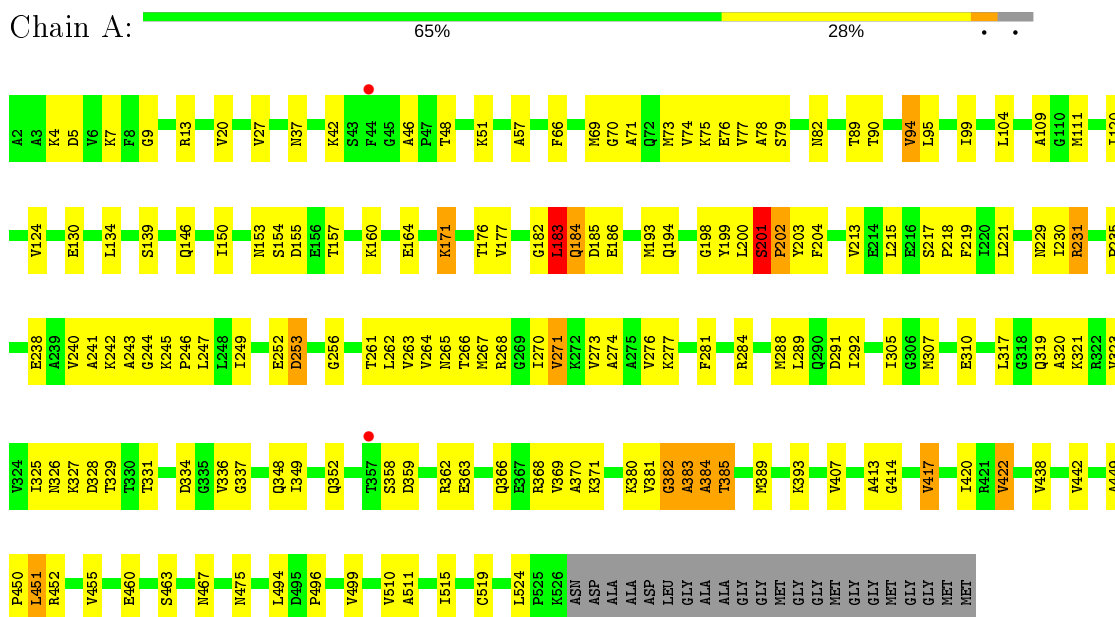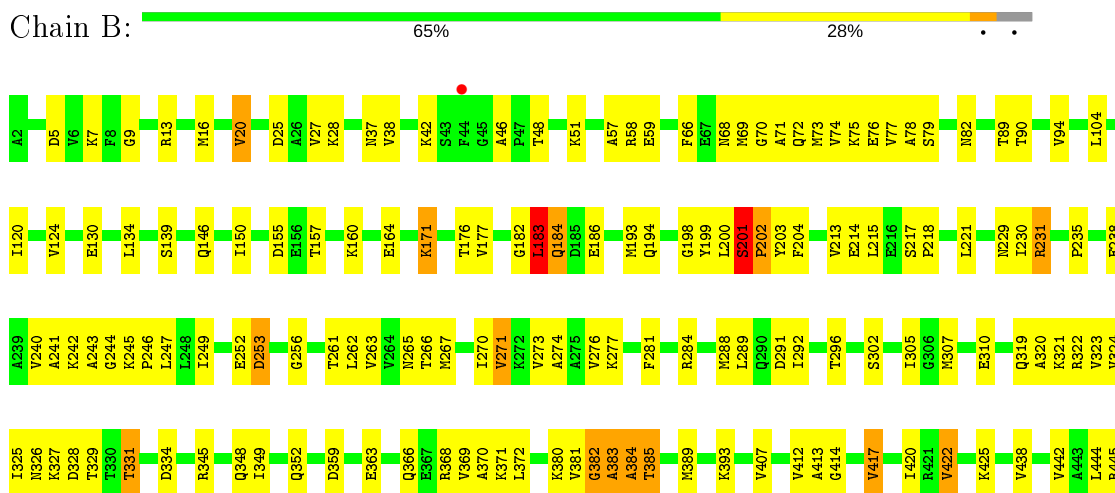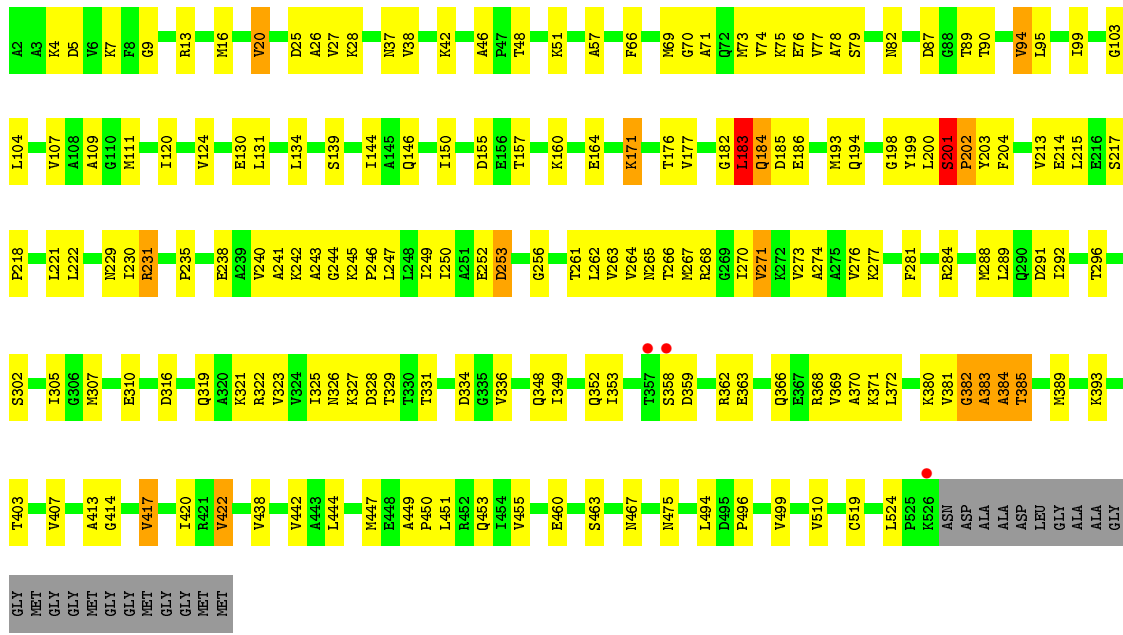
- Molecule 1: groEL protein

• Molecule 1: groEL protein

• Molecule 1: groEL protein

• Molecule 1: groEL protein

Chain E:

• Molecule 1: groEL protein

Chain F:

• Molecule 1: groEL protein

Chain G:

• Molecule 1: groEL protein

Chain H:

• Molecule 1: groEL protein

Chain I:

• Molecule 1: groEL protein

Chain J:

• Molecule 1: groEL protein

Chain K:

- Molecule 1: groEL protein

Chain L:

- Molecule 1: groEL protein

Chain M:
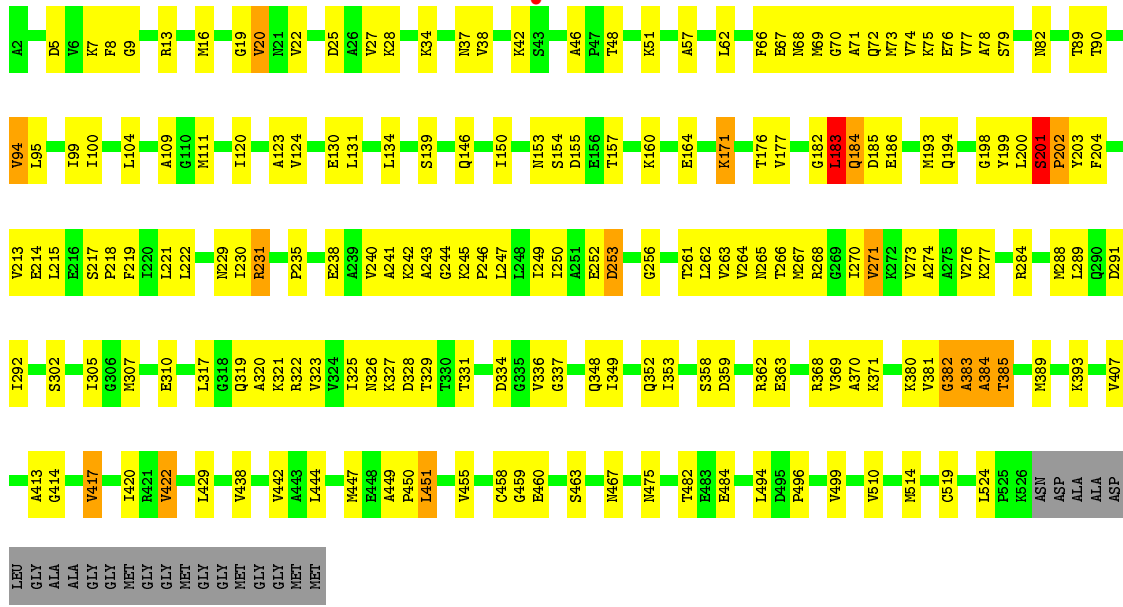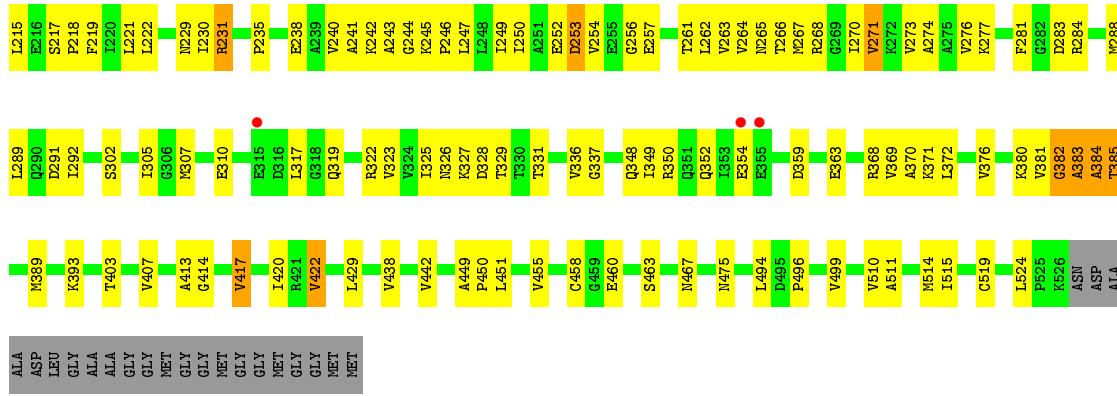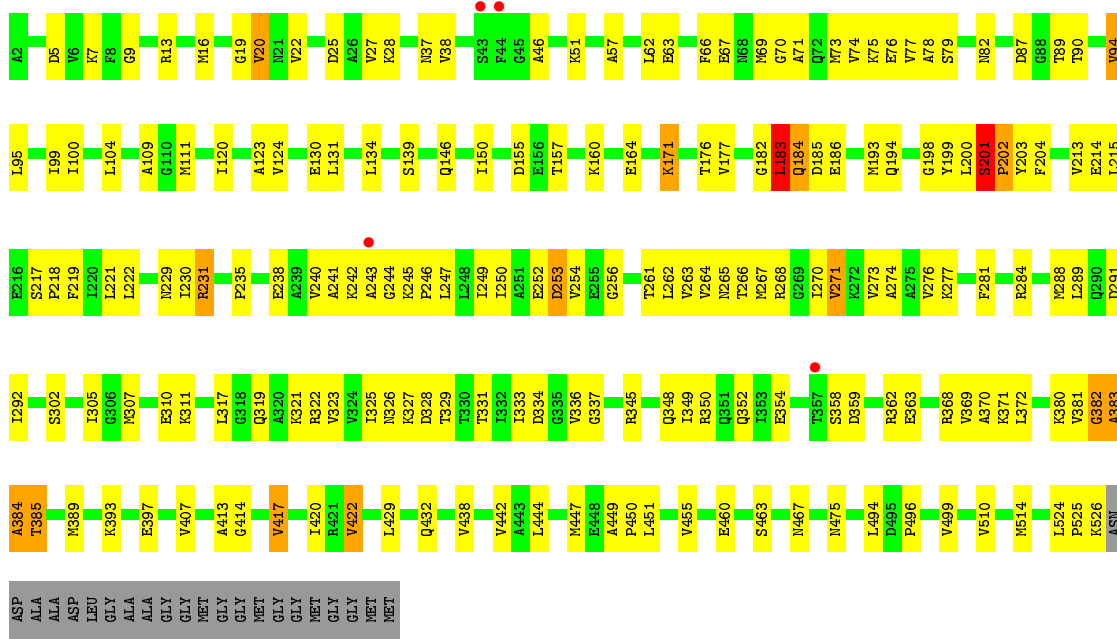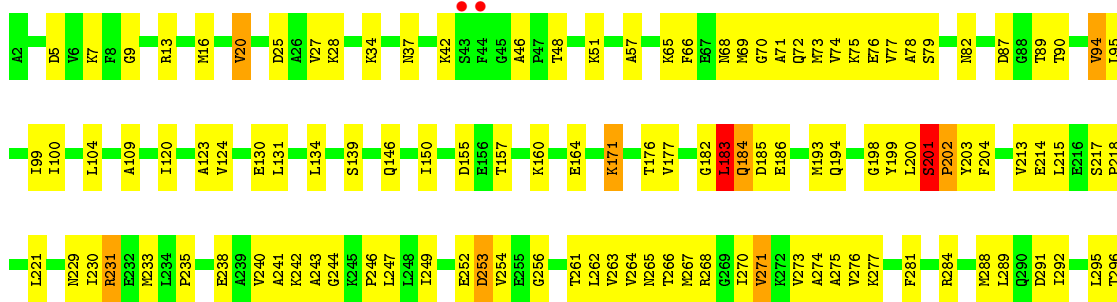
MET
MET

• Molecule 1: groEL protein

Chain N:

• Molecule 2: 12-residue peptide substrate
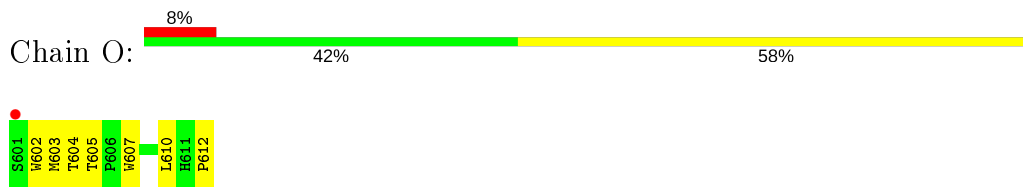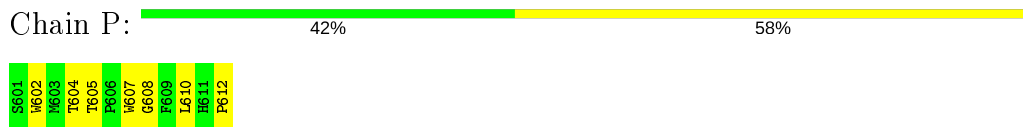
Chain O:

• Molecule 2: 12-residue peptide substrate

Chain P:

• Molecule 2: 12-residue peptide substrate

Chain Q:

• Molecule 2: 12-residue peptide substrate

Chain R:

S601 W602 M603 T604 T605 P606 W607 G608 F609 L610 H611 P612

• Molecule 2: 12-residue peptide substrate

Chain S:

S601 W602 M603 T604 T605 P606 W607 G608 F609 L610 H611 P612

• Molecule 2: 12-residue peptide substrate

Chain T:

S601 W602 M603 T604 T605 P606 W607 G608 F609 L610 H611 P612

• Molecule 2: 12-residue peptide substrate

Chain U:

S601 W602 M603 T604 T605 P606 W607 G608 F609 L610 H611 P612

• Molecule 2: 12-residue peptide substrate

Chain V:

S601 W602 M603 T604 T605 P606 W607 G608 F609 L610 H611 P612

• Molecule 2: 12-residue peptide substrate

Chain W:

S601 W602 M603 T604 T605 P606 W607 G608 F609 L610 H611 P612

• Molecule 2: 12-residue peptide substrate

Chain X:

S601 W602 M603 T604 T605 P606 W607 G608 F609 L610 H611 P612

• Molecule 2: 12-residue peptide substrate

Chain Y:

S601 W602 M603 T604 T605 P606 W607 G608 F609 L610 H611 P612
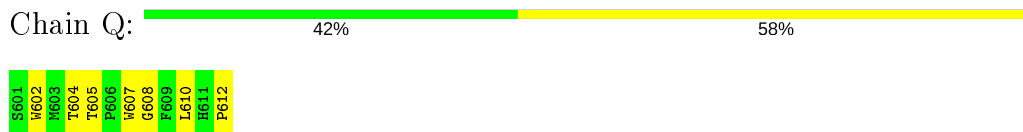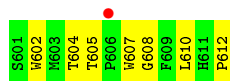
- Molecule 2: 12-residue peptide substrate

Chain Z:

- Molecule 2: 12-residue peptide substrate

Chain 1:

- Molecule 2: 12-residue peptide substrate

Chain 2:

4   Data and refinement statistics   (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	135.41Å 260.69Å 148.69Å 90.00° 100.94° 90.00°	Depositor
Resolution (Å)	20.01 – 3.00 20.01 – 3.00	Depositor EDS
% Data completeness (in resolution range)	83.4 (20.01-3.00) 83.5 (20.01-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.84 (at 2.98Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.236 , 0.259 0.232 , 0.253	Depositor DCC
R_{free} test set	16677 reflections (9.95%)	wwPDB-VP
Wilson B-factor (Å^2)	40.9	Xtriage
Anisotropy	0.815	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 38.4	EDS
L-test for twinning[2]	$< |L| > = 0.45, < L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	55765	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 12.79% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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)

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	0.37	0/3892	0.60	0/5254
1	B	0.39	0/3892	0.84	4/5254 (0.1%)
1	C	0.36	0/3892	0.60	0/5254
1	D	0.38	0/3892	0.60	0/5254
1	E	0.38	0/3892	0.60	0/5254
1	F	0.37	0/3892	0.59	0/5254
1	G	0.38	0/3892	0.59	0/5254
1	H	0.36	0/3892	0.60	0/5254
1	I	0.37	0/3892	0.60	0/5254
1	J	0.36	0/3892	0.59	0/5254
1	K	0.37	0/3892	0.60	0/5254
1	L	0.38	0/3892	0.59	0/5254
1	M	0.36	0/3892	0.66	3/5254 (0.1%)
1	N	0.37	0/3892	0.67	3/5254 (0.1%)
2	1	0.35	0/111	0.57	0/152
2	2	0.42	0/111	0.57	0/152
2	O	0.36	0/111	0.55	0/152
2	P	0.43	0/111	0.58	0/152
2	Q	0.43	0/111	0.56	0/152
2	R	0.37	0/111	0.55	0/152
2	S	0.38	0/111	0.57	0/152
2	T	0.34	0/111	0.57	0/152
2	U	0.42	0/111	0.56	0/152
2	V	0.37	0/111	0.58	0/152
2	W	0.38	0/111	0.55	0/152
2	X	0.40	0/111	0.55	0/152
2	Y	0.40	0/111	0.56	0/152
2	Z	0.33	0/111	0.57	0/152
All	All	0.37	0/56042	0.62	10/75684 (0.0%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	58	ARG	NE-CZ-NH1	-28.48	106.06	120.30
1	B	58	ARG	NE-CZ-NH2	26.84	133.72	120.30
1	N	368	ARG	NE-CZ-NH1	-15.03	112.78	120.30
1	B	58	ARG	CD-NE-CZ	14.68	144.15	123.60
1	N	368	ARG	NE-CZ-NH2	14.15	127.37	120.30
1	M	284	ARG	NE-CZ-NH2	13.47	127.03	120.30
1	M	284	ARG	NE-CZ-NH1	-12.82	113.89	120.30
1	B	58	ARG	CG-CD-NE	-7.40	96.26	111.80
1	N	368	ARG	CD-NE-CZ	5.90	131.86	123.60
1	M	284	ARG	CD-NE-CZ	5.03	130.65	123.60

There are no chirality outliers.

There are no planarity outliers.

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	3864	0	3989	149	0
1	B	3864	0	3989	145	0
1	C	3864	0	3989	151	1
1	D	3864	0	3989	168	0
1	E	3864	0	3989	151	0
1	F	3864	0	3989	151	0
1	G	3864	0	3989	149	1
1	H	3864	0	3989	158	1
1	I	3864	0	3989	159	0
1	J	3864	0	3989	162	2
1	K	3864	0	3989	161	0
1	L	3864	0	3989	151	1
1	M	3864	0	3989	149	0
1	N	3864	0	3989	155	0
2	1	104	0	91	8	0
2	2	104	0	91	8	0
2	O	104	0	91	8	0
2	P	104	0	91	9	0
2	Q	104	0	91	10	0
2	R	104	0	91	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	S	104	0	91	9	0
2	T	104	0	91	9	0
2	U	104	0	91	9	0
2	V	104	0	91	9	0
2	W	104	0	91	9	0
2	X	104	0	91	8	0
2	Y	104	0	91	10	0
2	Z	104	0	91	6	0
3	A	20	0	0	2	0
3	B	29	0	0	4	0
3	C	12	0	0	0	0
3	D	22	0	0	0	0
3	E	19	0	0	0	0
3	F	15	0	0	0	0
3	G	11	0	0	0	0
3	H	13	0	0	2	0
3	I	23	0	0	1	0
3	J	10	0	0	3	0
3	K	8	0	0	0	0
3	L	10	0	0	1	0
3	M	6	0	0	0	0
3	N	15	0	0	3	0
All	All	55765	0	57120	2085	3

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 19.

All (2085) 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:L:183:LEU:H	1:L:383:ALA:HB3	1.08	1.18
1:B:183:LEU:H	1:B:383:ALA:HB3	1.06	1.16
1:K:183:LEU:H	1:K:383:ALA:HB3	1.08	1.16
1:J:183:LEU:H	1:J:383:ALA:HB3	1.09	1.15
1:C:183:LEU:H	1:C:383:ALA:HB3	1.09	1.14
1:I:183:LEU:H	1:I:383:ALA:HB3	1.08	1.13
1:M:183:LEU:H	1:M:383:ALA:HB3	1.11	1.13
1:H:183:LEU:H	1:H:383:ALA:HB3	1.07	1.12
1:N:183:LEU:H	1:N:383:ALA:HB3	1.11	1.12
1:F:183:LEU:H	1:F:383:ALA:HB3	1.12	1.10
1:E:183:LEU:H	1:E:383:ALA:HB3	1.05	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:183:LEU:H	1:D:383:ALA:HB3	1.02	1.10
1:A:183:LEU:H	1:A:383:ALA:HB3	1.11	1.09
1:G:183:LEU:H	1:G:383:ALA:HB3	1.10	1.05
1:D:383:ALA:HB1	1:E:281:PHE:HZ	1.23	1.01
1:C:46:ALA:HB2	1:D:76:GLU:HG3	1.45	0.97
1:F:46:ALA:HB2	1:G:76:GLU:HG3	1.44	0.97
1:K:265:ASN:HD21	2:Y:610:LEU:H	1.16	0.94
1:C:265:ASN:HD21	2:Q:610:LEU:H	1.17	0.93
1:I:46:ALA:HB2	1:J:76:GLU:HG3	1.52	0.92
1:F:46:ALA:CB	1:G:76:GLU:HG3	1.99	0.91
1:B:383:ALA:HB1	1:C:281:PHE:HZ	1.35	0.91
1:D:183:LEU:N	1:D:383:ALA:HB3	1.86	0.90
1:H:383:ALA:HB1	1:I:281:PHE:HZ	1.37	0.90
1:A:281:PHE:HZ	1:G:383:ALA:HB1	1.37	0.89
1:A:46:ALA:HB2	1:B:76:GLU:HG3	1.54	0.89
1:I:46:ALA:CB	1:J:76:GLU:HG3	2.03	0.89
1:I:229:ASN:OD1	1:I:231:ARG:HB2	1.74	0.88
1:E:183:LEU:N	1:E:383:ALA:HB3	1.89	0.88
1:D:383:ALA:HB1	1:E:281:PHE:CZ	2.09	0.87
1:M:229:ASN:OD1	1:M:231:ARG:HB2	1.74	0.87
1:B:183:LEU:N	1:B:383:ALA:HB3	1.90	0.86
1:H:229:ASN:OD1	1:H:231:ARG:HB2	1.75	0.86
1:K:183:LEU:N	1:K:383:ALA:HB3	1.91	0.85
1:C:46:ALA:CB	1:D:76:GLU:HG3	2.05	0.85
1:D:265:ASN:HD21	2:R:610:LEU:H	1.23	0.85
1:L:183:LEU:N	1:L:383:ALA:HB3	1.92	0.85
1:L:265:ASN:HD21	2:Z:610:LEU:H	1.21	0.84
1:J:183:LEU:N	1:J:383:ALA:HB3	1.92	0.84
1:F:265:ASN:HD21	2:T:610:LEU:H	1.26	0.83
1:B:412:VAL:HG21	3:B:1206:HOH:O	1.79	0.83
1:C:183:LEU:N	1:C:383:ALA:HB3	1.94	0.83
1:J:526:LYS:HG3	3:J:1175:HOH:O	1.77	0.83
1:L:229:ASN:OD1	1:L:231:ARG:HB2	1.79	0.83
1:I:183:LEU:N	1:I:383:ALA:HB3	1.92	0.82
1:J:46:ALA:CB	1:K:76:GLU:HG3	2.08	0.82
1:A:46:ALA:CB	1:B:76:GLU:HG3	2.07	0.82
1:H:183:LEU:N	1:H:383:ALA:HB3	1.91	0.82
1:M:183:LEU:N	1:M:383:ALA:HB3	1.95	0.82
1:B:383:ALA:HB1	1:C:281:PHE:CZ	2.15	0.81
1:J:229:ASN:OD1	1:J:231:ARG:HB2	1.80	0.81
1:A:183:LEU:N	1:A:383:ALA:HB3	1.95	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:183:LEU:N	1:G:383:ALA:HB3	1.94	0.80
1:M:46:ALA:HB2	1:N:76:GLU:HG3	1.62	0.80
1:K:82:ASN:HB2	1:K:89:THR:HG23	1.64	0.80
1:A:229:ASN:OD1	1:A:231:ARG:HB2	1.81	0.79
1:M:46:ALA:CB	1:N:76:GLU:HG3	2.11	0.79
1:I:183:LEU:HD23	1:I:384:ALA:HB2	1.65	0.79
1:B:265:ASN:HD21	2:P:610:LEU:H	1.30	0.79
1:F:229:ASN:OD1	1:F:231:ARG:HB2	1.84	0.78
1:E:229:ASN:OD1	1:E:231:ARG:HB2	1.83	0.78
1:G:229:ASN:OD1	1:G:231:ARG:HB2	1.83	0.78
1:B:82:ASN:HB2	1:B:89:THR:HG23	1.66	0.78
1:H:76:GLU:HG3	1:N:46:ALA:CB	2.12	0.78
1:B:229:ASN:OD1	1:B:231:ARG:HB2	1.84	0.78
1:J:46:ALA:HB2	1:K:76:GLU:HG3	1.66	0.78
1:A:82:ASN:HB2	1:A:89:THR:HG23	1.66	0.78
1:H:183:LEU:HD23	1:H:384:ALA:HB2	1.66	0.78
1:A:183:LEU:HD23	1:A:384:ALA:HB2	1.65	0.78
1:J:383:ALA:HB1	1:K:281:PHE:HZ	1.47	0.78
1:M:265:ASN:HD21	2:1:610:LEU:H	1.32	0.77
1:E:46:ALA:CB	1:F:76:GLU:HG3	2.13	0.77
1:J:193:MET:HE1	1:J:292:ILE:HG12	1.66	0.77
1:D:229:ASN:OD1	1:D:231:ARG:HB2	1.83	0.77
1:L:82:ASN:HB2	1:L:89:THR:HG23	1.66	0.77
1:F:82:ASN:HB2	1:F:89:THR:HG23	1.64	0.77
1:M:82:ASN:HB2	1:M:89:THR:HG23	1.66	0.77
1:H:82:ASN:HB2	1:H:89:THR:HG23	1.66	0.77
1:K:381:VAL:HG21	1:K:393:LYS:HA	1.67	0.77
1:E:183:LEU:HD23	1:E:384:ALA:HB2	1.66	0.77
1:N:229:ASN:OD1	1:N:231:ARG:HB2	1.85	0.77
1:N:82:ASN:HB2	1:N:89:THR:HG23	1.66	0.77
1:G:183:LEU:HD23	1:G:384:ALA:HB2	1.67	0.77
1:J:82:ASN:HB2	1:J:89:THR:HG23	1.67	0.77
1:N:183:LEU:HD23	1:N:384:ALA:HB2	1.67	0.77
1:E:183:LEU:H	1:E:383:ALA:CB	1.94	0.76
1:F:183:LEU:N	1:F:383:ALA:HB3	1.96	0.76
1:G:82:ASN:HB2	1:G:89:THR:HG23	1.67	0.76
1:H:265:ASN:HD21	2:V:610:LEU:H	1.28	0.76
1:K:496:PRO:O	1:K:499:VAL:HG12	1.84	0.76
1:B:46:ALA:CB	1:C:76:GLU:HG3	2.16	0.76
1:I:82:ASN:HB2	1:I:89:THR:HG23	1.67	0.76
1:M:183:LEU:HD23	1:M:384:ALA:HB2	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:183:LEU:N	1:N:383:ALA:HB3	1.95	0.76
1:F:193:MET:HE1	1:F:292:ILE:HG12	1.68	0.76
1:N:496:PRO:O	1:N:499:VAL:HG12	1.85	0.76
1:C:82:ASN:HB2	1:C:89:THR:HG23	1.68	0.76
1:B:183:LEU:HD23	1:B:384:ALA:HB2	1.66	0.76
1:D:82:ASN:HB2	1:D:89:THR:HG23	1.67	0.76
1:K:183:LEU:HD23	1:K:384:ALA:HB2	1.66	0.76
1:A:281:PHE:CZ	1:G:383:ALA:HB1	2.21	0.75
1:F:381:VAL:HG21	1:F:393:LYS:HA	1.68	0.75
1:L:262:LEU:O	1:L:266:THR:HG23	1.87	0.75
1:E:265:ASN:HD21	2:S:610:LEU:H	1.31	0.75
1:H:76:GLU:HG3	1:N:46:ALA:HB2	1.69	0.75
1:F:183:LEU:HD23	1:F:384:ALA:HB2	1.69	0.75
1:A:265:ASN:HD21	2:O:610:LEU:H	1.34	0.75
1:H:383:ALA:HB1	1:I:281:PHE:CZ	2.21	0.75
1:J:183:LEU:HD23	1:J:384:ALA:HB2	1.68	0.75
1:L:381:VAL:HG21	1:L:393:LYS:HA	1.69	0.75
1:C:229:ASN:OD1	1:C:231:ARG:HB2	1.87	0.74
1:H:381:VAL:HG21	1:H:393:LYS:HA	1.70	0.74
1:D:183:LEU:H	1:D:383:ALA:CB	1.91	0.74
1:L:183:LEU:HD23	1:L:384:ALA:HB2	1.68	0.74
1:C:183:LEU:HD23	1:C:384:ALA:HB2	1.68	0.74
1:K:262:LEU:O	1:K:266:THR:HG23	1.87	0.74
1:C:381:VAL:HG21	1:C:393:LYS:HA	1.69	0.74
1:I:381:VAL:HG21	1:I:393:LYS:HA	1.70	0.74
1:K:46:ALA:CB	1:L:76:GLU:HG3	2.17	0.74
1:D:262:LEU:O	1:D:266:THR:HG23	1.88	0.74
1:C:193:MET:CE	1:C:292:ILE:HG12	2.18	0.74
1:M:171:LYS:HB2	1:M:407:VAL:HG11	1.70	0.74
1:G:381:VAL:HG21	1:G:393:LYS:HA	1.70	0.73
1:E:82:ASN:HB2	1:E:89:THR:HG23	1.69	0.73
1:G:265:ASN:HD21	2:U:610:LEU:H	1.35	0.73
1:J:496:PRO:O	1:J:499:VAL:HG12	1.88	0.73
1:M:496:PRO:O	1:M:499:VAL:HG12	1.87	0.73
1:C:262:LEU:O	1:C:266:THR:HG23	1.89	0.73
1:E:46:ALA:HB2	1:F:76:GLU:HG3	1.69	0.73
1:F:193:MET:CE	1:F:292:ILE:HG12	2.17	0.73
1:N:265:ASN:HD21	2:2:610:LEU:H	1.34	0.73
1:D:183:LEU:HD23	1:D:384:ALA:HB2	1.69	0.73
1:G:57:ALA:O	1:G:75:LYS:HE3	1.88	0.73
1:N:381:VAL:HG21	1:N:393:LYS:HA	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:381:VAL:HG21	1:E:393:LYS:HA	1.71	0.73
1:E:171:LYS:HB2	1:E:407:VAL:HG11	1.70	0.73
1:J:193:MET:CE	1:J:292:ILE:HG12	2.18	0.73
1:J:381:VAL:HG21	1:J:393:LYS:HA	1.71	0.73
1:B:381:VAL:HG21	1:B:393:LYS:HA	1.71	0.72
1:D:381:VAL:HG21	1:D:393:LYS:HA	1.71	0.72
1:F:496:PRO:O	1:F:499:VAL:HG12	1.88	0.72
1:B:171:LYS:HB2	1:B:407:VAL:HG11	1.72	0.72
1:H:281:PHE:HZ	1:N:383:ALA:HB1	1.55	0.72
1:A:262:LEU:O	1:A:266:THR:HG23	1.89	0.72
1:F:171:LYS:HB2	1:F:407:VAL:HG11	1.70	0.72
1:K:229:ASN:OD1	1:K:231:ARG:HB2	1.88	0.72
1:N:171:LYS:HB2	1:N:407:VAL:HG11	1.70	0.72
1:K:171:LYS:HB2	1:K:407:VAL:HG11	1.72	0.72
1:I:265:ASN:HD21	2:W:610:LEU:H	1.35	0.72
1:I:183:LEU:H	1:I:383:ALA:CB	1.97	0.72
1:C:171:LYS:HB2	1:C:407:VAL:HG11	1.70	0.72
1:L:171:LYS:HB2	1:L:407:VAL:HG11	1.72	0.72
1:H:496:PRO:O	1:H:499:VAL:HG12	1.89	0.72
1:A:381:VAL:HG21	1:A:393:LYS:HA	1.72	0.72
1:K:183:LEU:H	1:K:383:ALA:CB	1.96	0.72
1:B:262:LEU:O	1:B:266:THR:HG23	1.90	0.71
1:L:383:ALA:HB1	1:M:281:PHE:HZ	1.55	0.71
1:M:381:VAL:HG21	1:M:393:LYS:HA	1.72	0.71
1:D:171:LYS:HB2	1:D:407:VAL:HG11	1.72	0.71
1:B:183:LEU:H	1:B:383:ALA:CB	1.96	0.71
1:H:171:LYS:HB2	1:H:407:VAL:HG11	1.72	0.71
1:L:183:LEU:H	1:L:383:ALA:CB	1.97	0.71
1:A:171:LYS:HB2	1:A:407:VAL:HG11	1.73	0.71
1:I:262:LEU:O	1:I:266:THR:HG23	1.90	0.71
1:L:265:ASN:ND2	2:Z:610:LEU:H	1.88	0.71
1:G:171:LYS:HB2	1:G:407:VAL:HG11	1.72	0.71
1:A:77:VAL:HG21	1:A:510:VAL:HB	1.72	0.70
1:H:183:LEU:H	1:H:383:ALA:CB	1.96	0.70
1:A:78:ALA:O	1:A:89:THR:HG22	1.91	0.70
1:E:383:ALA:HB1	1:F:281:PHE:HZ	1.54	0.70
1:H:78:ALA:O	1:H:89:THR:HG22	1.90	0.70
1:J:183:LEU:H	1:J:383:ALA:CB	1.97	0.70
1:J:171:LYS:HB2	1:J:407:VAL:HG11	1.73	0.70
1:N:262:LEU:O	1:N:266:THR:HG23	1.91	0.70
1:A:496:PRO:O	1:A:499:VAL:HG12	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:496:PRO:O	1:C:499:VAL:HG12	1.92	0.70
1:B:77:VAL:HG21	1:B:510:VAL:HB	1.74	0.70
1:C:77:VAL:HG21	1:C:510:VAL:HB	1.74	0.69
1:L:496:PRO:O	1:L:499:VAL:HG12	1.91	0.69
1:M:262:LEU:O	1:M:266:THR:HG23	1.92	0.69
1:K:46:ALA:HB2	1:L:76:GLU:HG3	1.73	0.69
1:D:78:ALA:O	1:D:89:THR:HG22	1.91	0.69
1:F:262:LEU:O	1:F:266:THR:HG23	1.92	0.69
1:N:183:LEU:H	1:N:383:ALA:CB	1.99	0.69
1:D:496:PRO:O	1:D:499:VAL:HG12	1.92	0.69
1:L:46:ALA:CB	1:M:76:GLU:HG3	2.23	0.69
1:I:171:LYS:HB2	1:I:407:VAL:HG11	1.73	0.69
1:J:265:ASN:HD21	2:X:610:LEU:H	1.39	0.69
1:M:78:ALA:O	1:M:89:THR:HG22	1.92	0.69
1:E:496:PRO:O	1:E:499:VAL:HG12	1.93	0.69
1:K:265:ASN:ND2	2:Y:610:LEU:H	1.88	0.69
1:B:496:PRO:O	1:B:499:VAL:HG12	1.92	0.68
1:A:76:GLU:HG3	1:G:46:ALA:CB	2.23	0.68
1:F:77:VAL:HG21	1:F:510:VAL:HB	1.74	0.68
1:J:77:VAL:HG21	1:J:510:VAL:HB	1.75	0.68
1:I:496:PRO:O	1:I:499:VAL:HG12	1.92	0.68
1:L:77:VAL:HG21	1:L:510:VAL:HB	1.76	0.68
1:G:262:LEU:O	1:G:266:THR:HG23	1.94	0.68
1:A:13:ARG:HD3	3:A:1143:HOH:O	1.94	0.68
1:E:193:MET:CE	1:E:292:ILE:HG12	2.23	0.68
1:E:77:VAL:HG21	1:E:510:VAL:HB	1.75	0.68
1:M:193:MET:CE	1:M:292:ILE:HG12	2.23	0.68
1:D:46:ALA:CB	1:E:76:GLU:HG3	2.23	0.68
1:I:193:MET:HE1	1:I:292:ILE:HG12	1.76	0.68
1:D:193:MET:CE	1:D:292:ILE:HG12	2.22	0.68
1:E:193:MET:HE1	1:E:292:ILE:HG12	1.76	0.68
1:B:221:LEU:HD23	1:B:249:ILE:HD12	1.75	0.68
1:G:78:ALA:O	1:G:89:THR:HG22	1.94	0.68
1:I:77:VAL:HG21	1:I:510:VAL:HB	1.75	0.68
1:J:262:LEU:O	1:J:266:THR:HG23	1.94	0.68
1:C:78:ALA:O	1:C:89:THR:HG22	1.94	0.67
1:H:262:LEU:O	1:H:266:THR:HG23	1.94	0.67
1:C:265:ASN:ND2	2:Q:610:LEU:H	1.89	0.67
1:N:359:ASP:O	1:N:363:GLU:HG2	1.95	0.67
1:K:449:ALA:HB3	1:K:450:PRO:HD3	1.76	0.67
1:H:46:ALA:CB	1:I:76:GLU:HG3	2.24	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:78:ALA:O	1:J:89:THR:HG22	1.94	0.67
1:C:221:LEU:HD23	1:C:249:ILE:HD12	1.77	0.67
1:G:496:PRO:O	1:G:499:VAL:HG12	1.94	0.67
1:H:359:ASP:O	1:H:363:GLU:HG2	1.95	0.67
1:M:183:LEU:H	1:M:383:ALA:CB	2.00	0.67
1:B:193:MET:CE	1:B:292:ILE:HG12	2.24	0.67
1:A:229:ASN:ND2	1:G:270:ILE:HA	2.10	0.67
1:B:46:ALA:HB2	1:C:76:GLU:HG3	1.75	0.67
1:B:78:ALA:O	1:B:89:THR:HG22	1.95	0.67
1:C:183:LEU:H	1:C:383:ALA:CB	1.99	0.67
1:I:383:ALA:HB1	1:J:281:PHE:HZ	1.60	0.67
1:E:183:LEU:O	1:E:184:GLN:HB2	1.96	0.66
1:I:231:ARG:NH1	2:W:612:PRO:O	2.29	0.66
1:N:57:ALA:O	1:N:75:LYS:HE3	1.94	0.66
1:B:359:ASP:O	1:B:363:GLU:HG2	1.95	0.66
1:J:359:ASP:O	1:J:363:GLU:HG2	1.95	0.66
1:N:77:VAL:HG21	1:N:510:VAL:HB	1.77	0.66
1:B:270:ILE:HA	1:C:229:ASN:ND2	2.11	0.66
1:F:46:ALA:HB2	1:G:76:GLU:CG	2.21	0.66
1:D:221:LEU:HD23	1:D:249:ILE:HD12	1.76	0.66
1:G:193:MET:CE	1:G:292:ILE:HG12	2.25	0.66
1:I:193:MET:CE	1:I:292:ILE:HG12	2.25	0.66
1:N:193:MET:CE	1:N:292:ILE:HG12	2.25	0.66
1:H:193:MET:CE	1:H:292:ILE:HG12	2.26	0.66
1:H:77:VAL:HG21	1:H:510:VAL:HB	1.76	0.66
1:C:449:ALA:HB3	1:C:450:PRO:HD3	1.78	0.66
1:N:78:ALA:O	1:N:89:THR:HG22	1.94	0.66
1:C:193:MET:HE1	1:C:292:ILE:HG12	1.76	0.66
1:G:77:VAL:HG21	1:G:510:VAL:HB	1.77	0.66
1:H:348:GLN:O	1:H:352:GLN:HG2	1.96	0.66
1:N:183:LEU:O	1:N:184:GLN:HB2	1.95	0.66
1:A:183:LEU:H	1:A:383:ALA:CB	2.00	0.65
1:A:221:LEU:HD23	1:A:249:ILE:HD12	1.78	0.65
1:L:193:MET:CE	1:L:292:ILE:HG12	2.26	0.65
1:F:183:LEU:H	1:F:383:ALA:CB	2.02	0.65
1:K:193:MET:CE	1:K:292:ILE:HG12	2.26	0.65
1:K:78:ALA:O	1:K:89:THR:HG22	1.96	0.65
1:K:383:ALA:HB1	1:L:281:PHE:HZ	1.61	0.65
1:B:183:LEU:O	1:B:184:GLN:HB2	1.97	0.65
1:E:78:ALA:O	1:E:89:THR:HG22	1.95	0.65
1:D:77:VAL:HG21	1:D:510:VAL:HB	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:77:VAL:HG21	1:M:510:VAL:HB	1.79	0.65
1:D:359:ASP:O	1:D:363:GLU:HG2	1.96	0.65
1:I:348:GLN:O	1:I:352:GLN:HG2	1.97	0.65
1:I:57:ALA:O	1:I:75:LYS:HE3	1.95	0.65
1:L:449:ALA:HB3	1:L:450:PRO:HD3	1.78	0.65
1:H:221:LEU:HD23	1:H:249:ILE:HD12	1.79	0.65
1:K:183:LEU:O	1:K:184:GLN:HB2	1.97	0.65
1:E:262:LEU:O	1:E:266:THR:HG23	1.97	0.64
1:F:70:GLY:HA2	1:F:73:MET:HE2	1.78	0.64
1:K:221:LEU:HD23	1:K:249:ILE:HD12	1.80	0.64
1:E:266:THR:HG21	1:E:273:VAL:H	1.62	0.64
1:H:46:ALA:HB2	1:I:76:GLU:HG3	1.79	0.64
1:I:359:ASP:O	1:I:363:GLU:HG2	1.98	0.64
1:J:69:MET:O	1:J:73:MET:HG3	1.97	0.64
1:G:183:LEU:H	1:G:383:ALA:CB	1.99	0.64
1:I:183:LEU:O	1:I:184:GLN:HB2	1.97	0.64
1:K:359:ASP:O	1:K:363:GLU:HG2	1.97	0.64
1:C:109:ALA:HB2	1:K:109:ALA:HB2	1.79	0.64
1:C:183:LEU:O	1:C:184:GLN:HB2	1.98	0.64
1:D:183:LEU:O	1:D:184:GLN:HB2	1.98	0.64
1:E:70:GLY:HA2	1:E:73:MET:HE2	1.79	0.64
1:N:221:LEU:HD23	1:N:249:ILE:HD12	1.79	0.64
1:D:284:ARG:O	1:D:288:MET:HG3	1.97	0.64
1:G:183:LEU:O	1:G:184:GLN:HB2	1.96	0.64
1:J:183:LEU:O	1:J:184:GLN:HB2	1.98	0.63
1:N:348:GLN:O	1:N:352:GLN:HG2	1.98	0.63
1:H:193:MET:HE1	1:H:292:ILE:HG12	1.81	0.63
1:H:284:ARG:O	1:H:288:MET:HG3	1.96	0.63
1:J:348:GLN:O	1:J:352:GLN:HG2	1.98	0.63
1:K:69:MET:O	1:K:73:MET:HG3	1.99	0.63
1:L:46:ALA:HB2	1:M:76:GLU:HG3	1.79	0.63
1:M:359:ASP:O	1:M:363:GLU:HG2	1.98	0.63
1:A:218:PRO:HB3	1:A:246:PRO:HG2	1.81	0.63
1:B:348:GLN:O	1:B:352:GLN:HG2	1.99	0.63
1:M:348:GLN:O	1:M:352:GLN:HG2	1.99	0.63
1:B:82:ASN:HB2	1:B:89:THR:CG2	2.29	0.63
1:C:57:ALA:O	1:C:75:LYS:HE3	1.99	0.63
1:F:57:ALA:O	1:F:75:LYS:HE3	1.97	0.63
1:K:230:ILE:HD13	1:K:261:THR:CG2	2.28	0.63
1:K:284:ARG:O	1:K:288:MET:HG3	1.98	0.63
1:K:77:VAL:HG21	1:K:510:VAL:HB	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:449:ALA:HB3	1:D:450:PRO:HD3	1.80	0.63
1:E:221:LEU:HD23	1:E:249:ILE:HD12	1.79	0.63
1:G:449:ALA:HB3	1:G:450:PRO:HD3	1.80	0.63
1:G:266:THR:HG21	1:G:273:VAL:H	1.64	0.63
1:A:348:GLN:O	1:A:352:GLN:HG2	1.99	0.63
1:H:229:ASN:ND2	1:N:270:ILE:HA	2.14	0.63
1:K:130:GLU:HB3	1:K:422:VAL:HG22	1.80	0.63
1:A:71:ALA:O	1:A:75:LYS:HB2	1.99	0.62
1:H:57:ALA:O	1:H:75:LYS:HE3	1.99	0.62
1:C:230:ILE:HD13	1:C:261:THR:CG2	2.28	0.62
1:D:348:GLN:O	1:D:352:GLN:HG2	1.98	0.62
1:J:383:ALA:HB1	1:K:281:PHE:CZ	2.32	0.62
1:C:359:ASP:O	1:C:363:GLU:HG2	1.99	0.62
1:D:202:PRO:O	1:D:203:TYR:HB2	1.99	0.62
1:A:183:LEU:O	1:A:184:GLN:HB2	1.99	0.62
1:B:57:ALA:O	1:B:75:LYS:HE3	1.99	0.62
1:F:82:ASN:HB2	1:F:89:THR:CG2	2.29	0.62
1:G:230:ILE:HD13	1:G:261:THR:CG2	2.29	0.62
1:G:359:ASP:O	1:G:363:GLU:HG2	1.99	0.62
1:H:183:LEU:O	1:H:184:GLN:HB2	1.99	0.62
1:M:266:THR:HG21	1:M:273:VAL:H	1.64	0.62
1:B:284:ARG:O	1:B:288:MET:HG3	1.99	0.62
1:A:359:ASP:O	1:A:363:GLU:HG2	2.00	0.62
1:M:193:MET:HE1	1:M:292:ILE:HG12	1.80	0.62
1:M:218:PRO:HB3	1:M:246:PRO:HG2	1.81	0.62
1:L:183:LEU:O	1:L:184:GLN:HB2	2.00	0.62
1:A:193:MET:CE	1:A:292:ILE:HG12	2.29	0.62
1:A:109:ALA:HB2	1:M:109:ALA:HB2	1.82	0.61
1:C:130:GLU:HB3	1:C:422:VAL:HG22	1.82	0.61
1:D:266:THR:HG21	1:D:273:VAL:H	1.65	0.61
1:H:270:ILE:HD13	2:V:608:GLY:HA3	1.82	0.61
1:L:348:GLN:O	1:L:352:GLN:HG2	1.99	0.61
1:M:183:LEU:O	1:M:184:GLN:HB2	1.99	0.61
1:M:221:LEU:HD23	1:M:249:ILE:HD12	1.80	0.61
1:E:284:ARG:O	1:E:288:MET:HG3	1.99	0.61
1:C:194:GLN:O	1:C:371:LYS:HE3	2.00	0.61
1:I:202:PRO:O	1:I:203:TYR:HB2	2.00	0.61
1:M:417:VAL:HA	1:M:420:ILE:HG22	1.82	0.61
1:B:449:ALA:HB3	1:B:450:PRO:HD3	1.83	0.61
1:J:70:GLY:HA2	1:J:73:MET:HE2	1.82	0.61
1:A:82:ASN:HB2	1:A:89:THR:CG2	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:417:VAL:HA	1:C:420:ILE:HG22	1.82	0.61
1:L:271:VAL:HG12	1:L:273:VAL:HG23	1.83	0.61
1:M:82:ASN:HB2	1:M:89:THR:CG2	2.30	0.61
1:N:194:GLN:O	1:N:371:LYS:HE3	2.00	0.61
1:A:194:GLN:O	1:A:371:LYS:HE3	2.00	0.61
1:A:417:VAL:HA	1:A:420:ILE:HG22	1.82	0.61
1:C:348:GLN:O	1:C:352:GLN:HG2	2.00	0.61
1:F:183:LEU:O	1:F:184:GLN:HB2	2.01	0.61
1:K:266:THR:HG21	1:K:273:VAL:H	1.65	0.61
1:N:82:ASN:HB2	1:N:89:THR:CG2	2.31	0.61
1:C:82:ASN:HB2	1:C:89:THR:CG2	2.30	0.61
1:G:70:GLY:HA2	1:G:73:MET:HE2	1.83	0.61
1:C:242:LYS:O	1:C:243:ALA:HB3	2.01	0.61
1:D:57:ALA:O	1:D:75:LYS:HE3	2.00	0.61
1:J:266:THR:HG21	1:J:273:VAL:H	1.64	0.61
1:K:82:ASN:HB2	1:K:89:THR:CG2	2.31	0.61
1:M:230:ILE:HD13	1:M:261:THR:CG2	2.30	0.61
1:F:348:GLN:O	1:F:352:GLN:HG2	2.01	0.60
1:I:230:ILE:HD13	1:I:261:THR:CG2	2.31	0.60
1:I:449:ALA:HB3	1:I:450:PRO:HD3	1.83	0.60
1:F:215:LEU:HB2	1:F:323:VAL:HG22	1.83	0.60
1:E:270:ILE:HA	1:F:229:ASN:ND2	2.15	0.60
1:K:348:GLN:O	1:K:352:GLN:HG2	2.01	0.60
1:F:78:ALA:O	1:F:89:THR:HG22	2.01	0.60
1:G:348:GLN:O	1:G:352:GLN:HG2	2.01	0.60
1:A:76:GLU:HG3	1:G:46:ALA:HB2	1.83	0.60
1:I:160:LYS:O	1:I:164:GLU:HG3	2.01	0.60
1:I:215:LEU:HB2	1:I:323:VAL:HG22	1.83	0.60
1:L:82:ASN:HB2	1:L:89:THR:CG2	2.32	0.60
1:C:202:PRO:O	1:C:203:TYR:HB2	2.01	0.60
1:G:7:LYS:HG3	1:G:66:PHE:CZ	2.37	0.60
1:H:82:ASN:HB2	1:H:89:THR:CG2	2.32	0.60
1:K:194:GLN:O	1:K:371:LYS:HE3	2.00	0.60
1:L:417:VAL:HA	1:L:420:ILE:HG22	1.83	0.60
1:L:271:VAL:HG21	2:Z:607:TRP:HZ3	1.66	0.60
1:J:57:ALA:O	1:J:75:LYS:HE3	2.02	0.60
1:K:202:PRO:O	1:K:203:TYR:HB2	2.00	0.60
1:M:270:ILE:HA	1:N:229:ASN:ND2	2.16	0.60
1:D:271:VAL:HG21	2:R:607:TRP:HZ3	1.66	0.60
1:G:221:LEU:HD23	1:G:249:ILE:HD12	1.83	0.60
1:N:417:VAL:HA	1:N:420:ILE:HG22	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:265:ASN:ND2	2:R:610:LEU:H	1.94	0.60
1:E:202:PRO:O	1:E:203:TYR:HB2	2.01	0.60
1:F:265:ASN:ND2	2:T:610:LEU:H	1.95	0.60
1:H:10:ASN:HB2	3:H:1030:HOH:O	2.00	0.60
1:H:215:LEU:HB2	1:H:323:VAL:HG22	1.83	0.60
1:L:230:ILE:HD13	1:L:261:THR:CG2	2.32	0.60
1:E:417:VAL:HA	1:E:420:ILE:HG22	1.83	0.60
1:F:221:LEU:HD23	1:F:249:ILE:HD12	1.83	0.60
1:M:284:ARG:O	1:M:288:MET:HG3	2.01	0.60
1:B:266:THR:HG21	1:B:273:VAL:H	1.66	0.60
1:B:215:LEU:HB2	1:B:323:VAL:HG22	1.82	0.60
1:B:27:VAL:HG12	1:B:90:THR:HG23	1.84	0.60
1:D:218:PRO:HB3	1:D:246:PRO:HG2	1.84	0.60
1:E:359:ASP:O	1:E:363:GLU:HG2	2.02	0.60
1:I:46:ALA:HB2	1:J:76:GLU:CG	2.27	0.60
1:J:271:VAL:HG12	1:J:273:VAL:HG23	1.83	0.60
1:L:27:VAL:HG12	1:L:90:THR:HG23	1.84	0.60
1:C:284:ARG:O	1:C:288:MET:HG3	2.02	0.59
1:D:242:LYS:O	1:D:243:ALA:HB3	2.02	0.59
1:D:230:ILE:HD13	1:D:261:THR:CG2	2.32	0.59
1:F:359:ASP:O	1:F:363:GLU:HG2	2.02	0.59
1:I:78:ALA:O	1:I:89:THR:HG22	2.01	0.59
1:J:130:GLU:HB3	1:J:422:VAL:HG22	1.84	0.59
1:D:194:GLN:O	1:D:371:LYS:HE3	2.02	0.59
1:A:69:MET:O	1:A:73:MET:HG3	2.02	0.59
1:A:27:VAL:HG12	1:A:90:THR:HG23	1.84	0.59
1:E:348:GLN:O	1:E:352:GLN:HG2	2.02	0.59
1:J:284:ARG:O	1:J:288:MET:HG3	2.01	0.59
1:L:69:MET:O	1:L:73:MET:HG3	2.02	0.59
1:D:160:LYS:O	1:D:164:GLU:HG3	2.01	0.59
1:G:383:ALA:O	1:G:384:ALA:HB3	2.03	0.59
1:G:417:VAL:HA	1:G:420:ILE:HG22	1.83	0.59
1:H:27:VAL:HG12	1:H:90:THR:HG23	1.85	0.59
1:I:69:MET:O	1:I:73:MET:HG3	2.02	0.59
1:I:82:ASN:HB2	1:I:89:THR:CG2	2.32	0.59
1:N:27:VAL:HG12	1:N:90:THR:HG23	1.85	0.59
1:L:266:THR:HG21	1:L:273:VAL:H	1.66	0.59
1:N:69:MET:O	1:N:73:MET:HG3	2.02	0.59
1:G:160:LYS:O	1:G:164:GLU:HG3	2.01	0.59
1:L:160:LYS:O	1:L:164:GLU:HG3	2.02	0.59
1:N:231:ARG:NH1	2:2:612:PRO:O	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:70:GLY:HA2	1:N:73:MET:HE2	1.83	0.59
1:G:413:ALA:HB2	1:G:475:ASN:HD22	1.68	0.59
1:H:194:GLN:O	1:H:371:LYS:HE3	2.01	0.59
1:H:270:ILE:HA	1:I:229:ASN:ND2	2.18	0.59
1:I:417:VAL:HA	1:I:420:ILE:HG22	1.83	0.59
1:J:230:ILE:HD13	1:J:261:THR:CG2	2.32	0.59
1:G:82:ASN:HB2	1:G:89:THR:CG2	2.32	0.59
1:H:265:ASN:ND2	2:V:610:LEU:H	1.99	0.59
1:H:417:VAL:HA	1:H:420:ILE:HG22	1.84	0.59
1:K:183:LEU:HD13	1:K:184:GLN:HG3	1.84	0.59
1:K:215:LEU:HB2	1:K:323:VAL:HG22	1.84	0.59
1:D:82:ASN:HB2	1:D:89:THR:CG2	2.33	0.59
1:E:82:ASN:HB2	1:E:89:THR:CG2	2.33	0.59
1:F:284:ARG:O	1:F:288:MET:HG3	2.03	0.59
1:H:281:PHE:CZ	1:N:383:ALA:HB1	2.38	0.59
1:K:417:VAL:HA	1:K:420:ILE:HG22	1.85	0.59
1:A:183:LEU:HD13	1:A:184:GLN:HG3	1.85	0.59
1:A:230:ILE:HD13	1:A:261:THR:CG2	2.32	0.59
1:H:130:GLU:HB3	1:H:422:VAL:HG22	1.85	0.59
1:J:455:VAL:HG13	1:J:460:GLU:HB2	1.85	0.59
1:J:82:ASN:HB2	1:J:89:THR:CG2	2.32	0.59
1:K:218:PRO:HB3	1:K:246:PRO:HG2	1.84	0.59
1:M:70:GLY:HA2	1:M:73:MET:HE2	1.84	0.59
1:B:160:LYS:O	1:B:164:GLU:HG3	2.02	0.58
1:G:183:LEU:HD13	1:G:184:GLN:HG3	1.84	0.58
1:G:69:MET:O	1:G:73:MET:HG3	2.03	0.58
1:H:160:LYS:O	1:H:164:GLU:HG3	2.03	0.58
1:I:221:LEU:HD23	1:I:249:ILE:HD12	1.83	0.58
1:J:524:LEU:HG	3:J:1175:HOH:O	2.02	0.58
1:L:78:ALA:O	1:L:89:THR:HG22	2.02	0.58
1:H:271:VAL:HG21	2:V:607:TRP:HZ3	1.68	0.58
1:D:69:MET:O	1:D:73:MET:HG3	2.03	0.58
1:E:160:LYS:O	1:E:164:GLU:HG3	2.03	0.58
1:G:194:GLN:O	1:G:371:LYS:HE3	2.03	0.58
1:H:242:LYS:O	1:H:243:ALA:HB3	2.03	0.58
1:J:213:VAL:HB	1:J:325:ILE:HB	1.86	0.58
1:M:71:ALA:O	1:M:75:LYS:HB2	2.04	0.58
1:C:183:LEU:HD13	1:C:184:GLN:HG3	1.85	0.58
1:C:266:THR:HG21	1:C:273:VAL:H	1.67	0.58
1:D:270:ILE:HD13	2:R:608:GLY:HA3	1.85	0.58
1:E:57:ALA:O	1:E:75:LYS:HE3	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:242:LYS:O	1:M:243:ALA:HB3	2.03	0.58
1:A:46:ALA:HB2	1:B:76:GLU:CG	2.30	0.58
1:E:194:GLN:O	1:E:371:LYS:HE3	2.03	0.58
1:E:213:VAL:HB	1:E:325:ILE:HB	1.84	0.58
1:G:202:PRO:O	1:G:203:TYR:HB2	2.03	0.58
1:H:69:MET:O	1:H:73:MET:HG3	2.03	0.58
1:I:496:PRO:HD2	1:I:499:VAL:HG11	1.84	0.58
1:L:270:ILE:HA	1:M:229:ASN:ND2	2.19	0.58
1:E:183:LEU:HD13	1:E:184:GLN:HG3	1.84	0.58
1:F:449:ALA:HB3	1:F:450:PRO:HD3	1.84	0.58
1:J:183:LEU:HD13	1:J:184:GLN:HG3	1.85	0.58
1:N:215:LEU:HB2	1:N:323:VAL:HG22	1.85	0.58
1:M:266:THR:HA	1:M:271:VAL:O	2.04	0.58
1:F:120:ILE:O	1:F:124:VAL:HG23	2.03	0.58
1:A:383:ALA:O	1:A:384:ALA:HB3	2.04	0.58
1:A:57:ALA:O	1:A:75:LYS:HE3	2.04	0.58
1:D:183:LEU:HD13	1:D:184:GLN:HG3	1.84	0.58
1:I:194:GLN:O	1:I:371:LYS:HE3	2.03	0.58
1:I:7:LYS:HG3	1:I:66:PHE:CZ	2.38	0.58
1:J:221:LEU:HD23	1:J:249:ILE:HD12	1.85	0.58
1:L:57:ALA:O	1:L:75:LYS:HE3	2.04	0.58
1:N:266:THR:HG21	1:N:273:VAL:H	1.68	0.58
1:M:383:ALA:HB1	1:N:281:PHE:HZ	1.69	0.58
1:N:284:ARG:O	1:N:288:MET:HG3	2.01	0.58
1:I:270:ILE:HD13	2:W:608:GLY:HA3	1.85	0.58
1:A:70:GLY:HA2	1:A:73:MET:HE2	1.86	0.58
1:B:183:LEU:HD13	1:B:184:GLN:HG3	1.86	0.58
1:B:218:PRO:HB3	1:B:246:PRO:HG2	1.86	0.58
1:B:70:GLY:HA2	1:B:73:MET:HE2	1.86	0.58
1:G:120:ILE:O	1:G:124:VAL:HG23	2.03	0.58
1:K:242:LYS:C	1:K:244:GLY:H	2.07	0.58
1:C:218:PRO:HB3	1:C:246:PRO:HG2	1.86	0.58
1:M:449:ALA:HB3	1:M:450:PRO:HD3	1.84	0.58
1:B:194:GLN:O	1:B:371:LYS:HE3	2.03	0.57
1:D:270:ILE:HA	1:E:229:ASN:ND2	2.19	0.57
1:E:449:ALA:HB3	1:E:450:PRO:HD3	1.85	0.57
1:F:194:GLN:O	1:F:371:LYS:HE3	2.04	0.57
1:K:71:ALA:O	1:K:75:LYS:HB2	2.04	0.57
1:K:70:GLY:HA2	1:K:73:MET:HE2	1.86	0.57
1:L:183:LEU:HD13	1:L:184:GLN:HG3	1.85	0.57
1:F:417:VAL:HA	1:F:420:ILE:HG22	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:231:ARG:NH1	2:X:612:PRO:O	2.37	0.57
1:J:449:ALA:HB3	1:J:450:PRO:HD3	1.86	0.57
1:L:221:LEU:HD23	1:L:249:ILE:HD12	1.86	0.57
1:N:183:LEU:HD13	1:N:184:GLN:HG3	1.86	0.57
1:D:383:ALA:O	1:D:384:ALA:HB3	2.05	0.57
1:G:242:LYS:O	1:G:243:ALA:HB3	2.03	0.57
1:K:383:ALA:HB1	1:L:281:PHE:CZ	2.38	0.57
1:L:215:LEU:HB2	1:L:323:VAL:HG22	1.85	0.57
1:A:449:ALA:HB3	1:A:450:PRO:HD3	1.86	0.57
1:B:242:LYS:O	1:B:243:ALA:HB3	2.04	0.57
1:B:417:VAL:HA	1:B:420:ILE:HG22	1.86	0.57
1:I:242:LYS:O	1:I:243:ALA:HB3	2.04	0.57
1:I:413:ALA:HB2	1:I:475:ASN:HD22	1.70	0.57
1:M:183:LEU:HD13	1:M:184:GLN:HG3	1.85	0.57
1:E:242:LYS:O	1:E:243:ALA:HB3	2.04	0.57
1:F:266:THR:HG21	1:F:273:VAL:H	1.68	0.57
1:F:27:VAL:HG12	1:F:90:THR:HG23	1.86	0.57
1:G:193:MET:HE2	1:G:292:ILE:HG12	1.85	0.57
1:H:218:PRO:HB3	1:H:246:PRO:HG2	1.85	0.57
1:L:359:ASP:O	1:L:363:GLU:HG2	2.05	0.57
1:D:242:LYS:C	1:D:244:GLY:H	2.08	0.57
1:D:302:SER:H	1:D:307:MET:HE1	1.70	0.57
1:E:215:LEU:HB2	1:E:323:VAL:HG22	1.86	0.57
1:A:242:LYS:O	1:A:243:ALA:HB3	2.04	0.57
1:C:160:LYS:O	1:C:164:GLU:HG3	2.05	0.57
1:F:202:PRO:O	1:F:203:TYR:HB2	2.03	0.57
1:I:130:GLU:HB3	1:I:422:VAL:HG22	1.87	0.57
1:I:218:PRO:HB3	1:I:246:PRO:HG2	1.86	0.57
1:I:266:THR:HA	1:I:271:VAL:O	2.04	0.57
1:J:383:ALA:O	1:J:384:ALA:HB3	2.05	0.57
1:K:57:ALA:O	1:K:75:LYS:HE3	2.04	0.57
1:G:218:PRO:HB3	1:G:246:PRO:HG2	1.87	0.57
1:J:194:GLN:O	1:J:371:LYS:HE3	2.05	0.57
1:B:193:MET:HE3	1:B:292:ILE:HG12	1.86	0.57
1:C:69:MET:O	1:C:73:MET:HG3	2.05	0.57
1:D:70:GLY:HA2	1:D:73:MET:HE2	1.86	0.57
1:F:271:VAL:HG12	1:F:273:VAL:HG23	1.85	0.57
1:H:202:PRO:O	1:H:203:TYR:HB2	2.04	0.57
1:K:242:LYS:O	1:K:243:ALA:HB3	2.05	0.57
1:M:413:ALA:HB2	1:M:475:ASN:HD22	1.70	0.57
1:M:57:ALA:O	1:M:75:LYS:HE3	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:193:MET:HE1	1:D:292:ILE:HG12	1.87	0.57
1:J:266:THR:HA	1:J:271:VAL:O	2.05	0.57
1:J:417:VAL:HA	1:J:420:ILE:HG22	1.86	0.57
1:J:46:ALA:HB2	1:K:76:GLU:CG	2.35	0.57
1:L:383:ALA:HB1	1:M:281:PHE:CZ	2.38	0.57
1:N:242:LYS:O	1:N:243:ALA:HB3	2.05	0.57
1:N:413:ALA:HB2	1:N:475:ASN:HD22	1.70	0.57
1:B:230:ILE:HD13	1:B:261:THR:CG2	2.34	0.56
1:G:130:GLU:HB3	1:G:422:VAL:HG22	1.88	0.56
1:M:46:ALA:HB2	1:N:76:GLU:CG	2.35	0.56
1:E:265:ASN:ND2	2:S:610:LEU:H	2.00	0.56
1:B:130:GLU:HB3	1:B:422:VAL:HG22	1.87	0.56
1:D:496:PRO:HD2	1:D:499:VAL:HG11	1.87	0.56
1:F:183:LEU:HD13	1:F:184:GLN:HG3	1.86	0.56
1:H:271:VAL:HG12	1:H:273:VAL:HG23	1.86	0.56
1:J:242:LYS:O	1:J:243:ALA:HB3	2.04	0.56
1:L:242:LYS:C	1:L:244:GLY:H	2.07	0.56
1:N:120:ILE:O	1:N:124:VAL:HG23	2.06	0.56
1:N:271:VAL:HG21	2:2:607:TRP:HZ3	1.70	0.56
1:A:120:ILE:O	1:A:124:VAL:HG23	2.04	0.56
1:C:46:ALA:HB2	1:D:76:GLU:CG	2.27	0.56
1:J:202:PRO:O	1:J:203:TYR:HB2	2.05	0.56
1:L:202:PRO:O	1:L:203:TYR:HB2	2.05	0.56
1:C:455:VAL:HG13	1:C:460:GLU:HB2	1.88	0.56
1:E:242:LYS:C	1:E:244:GLY:H	2.08	0.56
1:M:7:LYS:HG3	1:M:66:PHE:CZ	2.41	0.56
1:B:271:VAL:HG12	1:B:273:VAL:HG23	1.86	0.56
1:C:302:SER:H	1:C:307:MET:HE1	1.69	0.56
1:D:417:VAL:HA	1:D:420:ILE:HG22	1.86	0.56
1:E:218:PRO:HB3	1:E:246:PRO:HG2	1.88	0.56
1:G:215:LEU:HB2	1:G:323:VAL:HG22	1.87	0.56
1:G:71:ALA:O	1:G:75:LYS:HB2	2.05	0.56
1:H:349:ILE:HA	1:H:352:GLN:HG3	1.87	0.56
1:I:70:GLY:HA2	1:I:73:MET:HE2	1.87	0.56
1:J:242:LYS:C	1:J:244:GLY:H	2.08	0.56
1:M:455:VAL:HG13	1:M:460:GLU:HB2	1.86	0.56
1:B:13:ARG:HD2	1:B:104:LEU:HD22	1.88	0.56
1:B:252:GLU:O	1:B:253:ASP:HB2	2.04	0.56
1:I:183:LEU:HD13	1:I:184:GLN:HG3	1.88	0.56
1:N:449:ALA:HB3	1:N:450:PRO:HD3	1.86	0.56
1:I:271:VAL:HG21	2:W:607:TRP:HZ3	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:202:PRO:O	1:M:203:TYR:HB2	2.05	0.56
1:N:242:LYS:C	1:N:244:GLY:H	2.09	0.56
1:B:265:ASN:ND2	2:P:610:LEU:H	2.01	0.56
1:G:5:ASP:HB2	1:G:524:LEU:HD12	1.88	0.56
1:K:455:VAL:HG13	1:K:460:GLU:HB2	1.88	0.56
1:L:496:PRO:HD2	1:L:499:VAL:HG11	1.88	0.56
1:A:202:PRO:O	1:A:203:TYR:HB2	2.05	0.56
1:A:284:ARG:O	1:A:288:MET:HG3	2.04	0.56
1:F:383:ALA:O	1:F:384:ALA:HB3	2.06	0.56
1:M:273:VAL:HG12	1:M:274:ALA:N	2.21	0.56
1:N:218:PRO:HB3	1:N:246:PRO:HG2	1.88	0.56
1:N:266:THR:HA	1:N:271:VAL:O	2.06	0.56
1:C:13:ARG:HD2	1:C:104:LEU:HD22	1.88	0.56
1:F:109:ALA:HB2	1:H:109:ALA:HB2	1.88	0.56
1:H:266:THR:HG21	1:H:273:VAL:H	1.70	0.56
1:K:383:ALA:O	1:K:384:ALA:HB3	2.06	0.56
1:C:27:VAL:HG12	1:C:90:THR:HG23	1.87	0.56
1:D:193:MET:HE3	1:D:292:ILE:HG12	1.88	0.56
1:D:266:THR:HA	1:D:271:VAL:O	2.06	0.56
1:E:230:ILE:HD13	1:E:261:THR:CG2	2.36	0.56
1:H:183:LEU:HD13	1:H:184:GLN:HG3	1.88	0.56
1:K:193:MET:HE1	1:K:292:ILE:HG12	1.87	0.56
1:M:383:ALA:O	1:M:384:ALA:HB3	2.06	0.56
1:A:130:GLU:HB3	1:A:422:VAL:HG22	1.88	0.55
1:C:71:ALA:O	1:C:75:LYS:HB2	2.06	0.55
1:F:130:GLU:HB3	1:F:422:VAL:HG22	1.88	0.55
1:H:120:ILE:O	1:H:124:VAL:HG23	2.07	0.55
1:H:273:VAL:HG12	1:H:274:ALA:N	2.21	0.55
1:L:130:GLU:HB3	1:L:422:VAL:HG22	1.88	0.55
1:M:242:LYS:C	1:M:244:GLY:H	2.10	0.55
1:N:71:ALA:O	1:N:75:LYS:HB2	2.06	0.55
1:E:120:ILE:O	1:E:124:VAL:HG23	2.06	0.55
1:G:27:VAL:HG12	1:G:90:THR:HG23	1.88	0.55
1:H:242:LYS:C	1:H:244:GLY:H	2.09	0.55
1:H:70:GLY:HA2	1:H:73:MET:HE2	1.87	0.55
1:L:120:ILE:O	1:L:124:VAL:HG23	2.06	0.55
1:M:130:GLU:HB3	1:M:422:VAL:HG22	1.88	0.55
1:L:193:MET:HE1	1:L:292:ILE:HG12	1.87	0.55
1:M:414:GLY:O	1:M:417:VAL:HG13	2.07	0.55
1:F:242:LYS:O	1:F:243:ALA:HB3	2.05	0.55
1:K:13:ARG:HD2	1:K:104:LEU:HD22	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:270:ILE:HD13	2:Q:608:GLY:HA3	1.89	0.55
1:D:46:ALA:HB2	1:E:76:GLU:HG3	1.88	0.55
1:L:70:GLY:HA2	1:L:73:MET:HE2	1.88	0.55
1:M:160:LYS:O	1:M:164:GLU:HG3	2.07	0.55
1:N:230:ILE:HD13	1:N:261:THR:CG2	2.36	0.55
1:H:383:ALA:O	1:H:384:ALA:HB3	2.07	0.55
1:M:69:MET:O	1:M:73:MET:HG3	2.07	0.55
1:B:120:ILE:O	1:B:124:VAL:HG23	2.07	0.55
1:B:69:MET:O	1:B:73:MET:HG3	2.06	0.55
1:C:70:GLY:HA2	1:C:73:MET:HE2	1.87	0.55
1:D:271:VAL:HG12	1:D:273:VAL:HG23	1.87	0.55
1:E:383:ALA:O	1:E:384:ALA:HB3	2.06	0.55
1:G:266:THR:HA	1:G:271:VAL:O	2.07	0.55
1:H:230:ILE:HD13	1:H:261:THR:CG2	2.36	0.55
1:J:160:LYS:O	1:J:164:GLU:HG3	2.06	0.55
1:J:218:PRO:HB3	1:J:246:PRO:HG2	1.88	0.55
1:L:242:LYS:O	1:L:243:ALA:HB3	2.07	0.55
1:L:266:THR:HA	1:L:271:VAL:O	2.06	0.55
1:N:160:LYS:O	1:N:164:GLU:HG3	2.06	0.55
1:L:284:ARG:O	1:L:288:MET:HG3	2.06	0.55
1:L:7:LYS:HG3	1:L:66:PHE:CZ	2.42	0.55
1:A:160:LYS:O	1:A:164:GLU:HG3	2.06	0.55
1:A:266:THR:HG21	1:A:273:VAL:H	1.71	0.55
1:A:455:VAL:HG13	1:A:460:GLU:HB2	1.89	0.55
1:C:414:GLY:O	1:C:417:VAL:HG13	2.07	0.55
1:D:27:VAL:HG12	1:D:90:THR:HG23	1.89	0.55
1:E:455:VAL:HG13	1:E:460:GLU:HB2	1.88	0.55
1:I:242:LYS:C	1:I:244:GLY:H	2.10	0.55
1:L:27:VAL:CG1	1:L:90:THR:HG23	2.37	0.55
1:N:202:PRO:O	1:N:203:TYR:HB2	2.05	0.55
1:N:383:ALA:O	1:N:384:ALA:HB3	2.07	0.55
1:A:414:GLY:O	1:A:417:VAL:HG13	2.06	0.55
1:B:71:ALA:O	1:B:75:LYS:HB2	2.07	0.55
1:C:413:ALA:HB2	1:C:475:ASN:HD22	1.71	0.55
1:E:266:THR:CG2	1:E:273:VAL:H	2.20	0.55
1:F:5:ASP:HB2	1:F:524:LEU:HD12	1.89	0.55
1:G:242:LYS:C	1:G:244:GLY:H	2.10	0.55
1:G:284:ARG:O	1:G:288:MET:HG3	2.06	0.55
1:H:13:ARG:HD2	1:H:104:LEU:HD22	1.87	0.55
1:H:200:LEU:O	1:H:201:SER:HB3	2.06	0.55
1:I:213:VAL:HB	1:I:325:ILE:HB	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:265:ASN:HD21	2:Y:610:LEU:N	1.97	0.55
1:N:496:PRO:HD2	1:N:499:VAL:HG11	1.89	0.55
1:G:265:ASN:ND2	2:U:610:LEU:H	2.02	0.55
1:A:193:MET:HE3	1:A:292:ILE:HG12	1.89	0.54
1:E:13:ARG:HD2	1:E:104:LEU:HD22	1.88	0.54
1:I:266:THR:HG21	1:I:273:VAL:H	1.72	0.54
1:K:160:LYS:O	1:K:164:GLU:HG3	2.07	0.54
1:K:271:VAL:HG12	1:K:273:VAL:HG23	1.88	0.54
1:A:413:ALA:HB2	1:A:475:ASN:HD22	1.71	0.54
1:D:71:ALA:O	1:D:75:LYS:HB2	2.08	0.54
1:E:496:PRO:HD2	1:E:499:VAL:HG11	1.89	0.54
1:F:63:GLU:OE1	1:G:524:LEU:HD21	2.07	0.54
1:I:270:ILE:HA	1:J:229:ASN:ND2	2.22	0.54
1:M:27:VAL:HG12	1:M:90:THR:HG23	1.90	0.54
1:N:414:GLY:O	1:N:417:VAL:HG13	2.07	0.54
1:A:242:LYS:C	1:A:244:GLY:H	2.10	0.54
1:D:130:GLU:HB3	1:D:422:VAL:HG22	1.90	0.54
1:J:215:LEU:HB2	1:J:323:VAL:HG22	1.88	0.54
1:N:7:LYS:HG3	1:N:66:PHE:CZ	2.42	0.54
1:B:383:ALA:O	1:B:384:ALA:HB3	2.07	0.54
1:C:266:THR:HA	1:C:271:VAL:O	2.07	0.54
1:C:383:ALA:O	1:C:384:ALA:HB3	2.07	0.54
1:D:413:ALA:HB2	1:D:475:ASN:HD22	1.72	0.54
1:E:349:ILE:HA	1:E:352:GLN:HG3	1.89	0.54
1:E:383:ALA:HB1	1:F:281:PHE:CZ	2.39	0.54
1:E:69:MET:O	1:E:73:MET:HG3	2.07	0.54
1:G:213:VAL:HB	1:G:325:ILE:HB	1.90	0.54
1:G:414:GLY:O	1:G:417:VAL:HG13	2.07	0.54
1:G:455:VAL:HG13	1:G:460:GLU:HB2	1.89	0.54
1:K:230:ILE:HD13	1:K:261:THR:HB	1.90	0.54
1:K:302:SER:H	1:K:307:MET:HE1	1.73	0.54
1:N:193:MET:HE3	1:N:292:ILE:HG12	1.89	0.54
1:A:213:VAL:HB	1:A:325:ILE:HB	1.89	0.54
1:I:230:ILE:HD13	1:I:261:THR:HB	1.90	0.54
1:I:455:VAL:HG13	1:I:460:GLU:HB2	1.88	0.54
1:K:5:ASP:HB2	1:K:524:LEU:HD12	1.90	0.54
1:L:349:ILE:HA	1:L:352:GLN:HG3	1.89	0.54
1:G:349:ILE:HA	1:G:352:GLN:HG3	1.89	0.54
1:A:200:LEU:HG	1:A:276:VAL:HA	1.90	0.54
1:H:413:ALA:HB2	1:H:475:ASN:HD22	1.73	0.54
1:I:383:ALA:O	1:I:384:ALA:HB3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:27:VAL:HG12	1:J:90:THR:HG23	1.90	0.54
1:K:120:ILE:O	1:K:124:VAL:HG23	2.07	0.54
1:M:200:LEU:O	1:M:201:SER:HB3	2.06	0.54
1:M:252:GLU:O	1:M:253:ASP:HB2	2.08	0.54
1:J:252:GLU:O	1:J:253:ASP:HB2	2.08	0.54
1:A:215:LEU:HB2	1:A:323:VAL:HG22	1.89	0.54
1:B:242:LYS:C	1:B:244:GLY:H	2.10	0.54
1:B:455:VAL:HG13	1:B:460:GLU:HB2	1.90	0.54
1:D:252:GLU:O	1:D:253:ASP:HB2	2.08	0.54
1:D:455:VAL:HG13	1:D:460:GLU:HB2	1.90	0.54
1:H:235:PRO:HG3	1:H:310:GLU:HA	1.90	0.54
1:H:383:ALA:CB	1:I:281:PHE:HZ	2.16	0.54
1:I:349:ILE:HA	1:I:352:GLN:HG3	1.89	0.54
1:J:414:GLY:O	1:J:417:VAL:HG13	2.08	0.54
1:N:13:ARG:HD2	1:N:104:LEU:HD22	1.88	0.54
1:D:273:VAL:HG12	1:D:274:ALA:N	2.23	0.54
1:D:414:GLY:O	1:D:417:VAL:HG13	2.08	0.54
1:E:37:ASN:ND2	1:E:51:LYS:HG3	2.23	0.54
1:G:230:ILE:HD13	1:G:261:THR:HG21	1.90	0.54
1:H:414:GLY:O	1:H:417:VAL:HG13	2.08	0.54
1:J:183:LEU:CD1	1:J:184:GLN:HG3	2.38	0.54
1:L:263:VAL:O	1:L:267:MET:HB2	2.08	0.54
1:N:455:VAL:HG13	1:N:460:GLU:HB2	1.89	0.54
1:M:265:ASN:ND2	2:1:610:LEU:H	2.01	0.53
1:D:230:ILE:HD13	1:D:261:THR:HB	1.90	0.53
1:E:183:LEU:CD1	1:E:184:GLN:HG3	2.38	0.53
1:E:266:THR:HA	1:E:271:VAL:O	2.08	0.53
1:H:266:THR:HA	1:H:271:VAL:O	2.08	0.53
1:J:200:LEU:O	1:J:201:SER:HB3	2.08	0.53
1:N:265:ASN:ND2	2:2:610:LEU:H	2.04	0.53
1:C:120:ILE:O	1:C:124:VAL:HG23	2.08	0.53
1:D:200:LEU:O	1:D:201:SER:HB3	2.07	0.53
1:D:349:ILE:HA	1:D:352:GLN:HG3	1.89	0.53
1:E:273:VAL:HG12	1:E:274:ALA:N	2.23	0.53
1:G:5:ASP:HB2	1:G:524:LEU:CD1	2.38	0.53
1:I:271:VAL:HG12	1:I:273:VAL:HG23	1.90	0.53
1:M:270:ILE:HA	1:N:229:ASN:HD22	1.73	0.53
1:A:496:PRO:HD2	1:A:499:VAL:HG11	1.90	0.53
1:C:215:LEU:HB2	1:C:323:VAL:HG22	1.91	0.53
1:C:230:ILE:HD13	1:C:261:THR:HG21	1.90	0.53
1:F:230:ILE:HD13	1:F:261:THR:CG2	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:242:LYS:C	1:F:244:GLY:H	2.12	0.53
1:L:194:GLN:O	1:L:371:LYS:HE3	2.08	0.53
1:L:383:ALA:O	1:L:384:ALA:HB3	2.07	0.53
1:L:455:VAL:HG13	1:L:460:GLU:HB2	1.90	0.53
1:L:414:GLY:H	1:L:494:LEU:HA	1.74	0.53
1:A:266:THR:HA	1:A:271:VAL:O	2.07	0.53
1:B:202:PRO:O	1:B:203:TYR:HB2	2.08	0.53
1:C:5:ASP:HB2	1:C:524:LEU:HD12	1.91	0.53
1:M:13:ARG:HD2	1:M:104:LEU:HD22	1.90	0.53
1:K:271:VAL:HG21	2:Y:607:TRP:HZ3	1.72	0.53
1:E:7:LYS:HG3	1:E:66:PHE:CZ	2.43	0.53
1:I:284:ARG:O	1:I:288:MET:HG3	2.08	0.53
1:I:291:ASP:OD2	1:I:368:ARG:HD2	2.08	0.53
1:I:414:GLY:O	1:I:417:VAL:HG13	2.07	0.53
1:F:238:GLU:O	1:F:241:ALA:HB3	2.09	0.53
1:F:414:GLY:O	1:F:417:VAL:HG13	2.08	0.53
1:H:414:GLY:H	1:H:494:LEU:HA	1.74	0.53
1:I:5:ASP:HB2	1:I:524:LEU:HD12	1.90	0.53
1:L:183:LEU:CD1	1:L:184:GLN:HG3	2.38	0.53
1:B:213:VAL:HB	1:B:325:ILE:HB	1.91	0.53
1:B:413:ALA:HB2	1:B:475:ASN:HD22	1.74	0.53
1:B:27:VAL:CG1	1:B:90:THR:HG23	2.39	0.53
1:E:5:ASP:HB2	1:E:524:LEU:HD12	1.91	0.53
1:F:413:ALA:HB2	1:F:475:ASN:HD22	1.73	0.53
1:G:202:PRO:O	1:G:204:PHE:N	2.40	0.53
1:K:37:ASN:ND2	1:K:51:LYS:HG3	2.24	0.53
1:K:413:ALA:HB2	1:K:475:ASN:HD22	1.74	0.53
1:N:130:GLU:HB3	1:N:422:VAL:HG22	1.91	0.53
1:C:271:VAL:HG21	2:Q:607:TRP:HZ3	1.72	0.53
1:I:265:ASN:ND2	2:W:610:LEU:H	2.05	0.53
1:A:349:ILE:HA	1:A:352:GLN:HG3	1.90	0.53
1:A:5:ASP:HB2	1:A:524:LEU:HD12	1.91	0.53
1:D:383:ALA:CB	1:E:281:PHE:CZ	2.89	0.53
1:B:349:ILE:HA	1:B:352:GLN:HG3	1.91	0.53
1:B:5:ASP:HB2	1:B:524:LEU:HD12	1.91	0.53
1:D:319:GLN:HB3	1:D:336:VAL:HG21	1.90	0.53
1:E:414:GLY:H	1:E:494:LEU:HA	1.73	0.53
1:G:183:LEU:CD1	1:G:184:GLN:HG3	2.39	0.53
1:A:7:LYS:HG3	1:A:66:PHE:CZ	2.44	0.53
1:C:242:LYS:C	1:C:244:GLY:H	2.10	0.53
1:F:160:LYS:O	1:F:164:GLU:HG3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:69:MET:O	1:F:73:MET:HG3	2.09	0.53
1:M:194:GLN:O	1:M:371:LYS:HE3	2.07	0.53
1:N:37:ASN:ND2	1:N:51:LYS:HG3	2.24	0.53
1:J:271:VAL:HG21	2:X:607:TRP:HZ3	1.73	0.53
1:K:183:LEU:CD1	1:K:184:GLN:HG3	2.39	0.52
1:K:213:VAL:HB	1:K:325:ILE:HB	1.92	0.52
1:L:71:ALA:O	1:L:75:LYS:HB2	2.09	0.52
1:N:238:GLU:O	1:N:241:ALA:HB3	2.09	0.52
1:N:271:VAL:HG12	1:N:273:VAL:HG23	1.91	0.52
1:F:271:VAL:HG21	2:T:607:TRP:HZ3	1.73	0.52
1:D:291:ASP:OD2	1:D:368:ARG:HD2	2.10	0.52
1:E:413:ALA:HB2	1:E:475:ASN:HD22	1.74	0.52
1:F:455:VAL:HG13	1:F:460:GLU:HB2	1.90	0.52
1:F:496:PRO:HD2	1:F:499:VAL:HG11	1.90	0.52
1:G:271:VAL:HG12	1:G:273:VAL:HG23	1.90	0.52
1:G:266:THR:CG2	1:G:273:VAL:H	2.21	0.52
1:I:71:ALA:O	1:I:75:LYS:HB2	2.09	0.52
1:K:230:ILE:HD13	1:K:261:THR:HG21	1.91	0.52
1:K:266:THR:CG2	1:K:273:VAL:H	2.22	0.52
1:K:496:PRO:HD2	1:K:499:VAL:HG11	1.91	0.52
1:C:183:LEU:CD1	1:C:184:GLN:HG3	2.39	0.52
1:E:71:ALA:O	1:E:75:LYS:HB2	2.09	0.52
1:L:13:ARG:HD2	1:L:104:LEU:HD22	1.91	0.52
1:L:266:THR:CG2	1:L:273:VAL:H	2.22	0.52
1:M:270:ILE:HG12	1:N:229:ASN:HD21	1.74	0.52
1:A:252:GLU:O	1:A:253:ASP:HB2	2.10	0.52
1:A:263:VAL:O	1:A:267:MET:HB2	2.09	0.52
1:A:27:VAL:CG1	1:A:90:THR:HG23	2.39	0.52
1:D:120:ILE:O	1:D:124:VAL:HG23	2.10	0.52
1:F:218:PRO:HB3	1:F:246:PRO:HG2	1.92	0.52
1:K:266:THR:HA	1:K:271:VAL:O	2.10	0.52
1:C:38:VAL:HG22	1:D:519:CYS:HB3	1.92	0.52
1:H:213:VAL:HB	1:H:325:ILE:HB	1.91	0.52
1:J:120:ILE:O	1:J:124:VAL:HG23	2.09	0.52
1:K:7:LYS:HG3	1:K:66:PHE:CZ	2.45	0.52
1:M:213:VAL:HB	1:M:325:ILE:HB	1.90	0.52
1:A:13:ARG:HD2	1:A:104:LEU:HD22	1.90	0.52
1:D:215:LEU:HB2	1:D:323:VAL:HG22	1.92	0.52
1:D:37:ASN:ND2	1:D:51:LYS:HG3	2.25	0.52
1:G:496:PRO:HD2	1:G:499:VAL:HG11	1.90	0.52
1:M:266:THR:CG2	1:M:273:VAL:H	2.23	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:463:SER:O	1:M:467:ASN:HB2	2.10	0.52
1:A:235:PRO:HG3	1:A:310:GLU:HA	1.90	0.52
1:B:7:LYS:HG3	1:B:66:PHE:CZ	2.45	0.52
1:D:5:ASP:HB2	1:D:524:LEU:HD12	1.92	0.52
1:M:349:ILE:HA	1:M:352:GLN:HG3	1.91	0.52
1:B:235:PRO:HG3	1:B:310:GLU:HA	1.91	0.52
1:C:265:ASN:HD21	2:Q:610:LEU:N	1.99	0.52
1:D:13:ARG:HD2	1:D:104:LEU:HD22	1.90	0.52
1:F:37:ASN:ND2	1:F:51:LYS:HG3	2.25	0.52
1:H:71:ALA:O	1:H:75:LYS:HB2	2.09	0.52
1:N:263:VAL:O	1:N:267:MET:HB2	2.10	0.52
1:I:27:VAL:HG12	1:I:90:THR:HG23	1.92	0.52
1:J:413:ALA:HB2	1:J:475:ASN:HD22	1.74	0.52
1:J:5:ASP:HB2	1:J:524:LEU:HD12	1.92	0.52
1:A:183:LEU:CD1	1:A:184:GLN:HG3	2.40	0.51
1:C:271:VAL:HG12	1:C:273:VAL:HG23	1.92	0.51
1:H:263:VAL:O	1:H:267:MET:HB2	2.10	0.51
1:J:7:LYS:HG3	1:J:66:PHE:CZ	2.46	0.51
1:L:270:ILE:HD13	2:Z:608:GLY:HA3	1.92	0.51
1:H:76:GLU:CG	1:N:46:ALA:HB2	2.38	0.51
1:K:414:GLY:H	1:K:494:LEU:HA	1.75	0.51
1:M:215:LEU:HB2	1:M:323:VAL:HG22	1.92	0.51
1:N:27:VAL:CG1	1:N:90:THR:HG23	2.41	0.51
1:B:183:LEU:CD1	1:B:184:GLN:HG3	2.40	0.51
1:B:438:VAL:O	1:B:442:VAL:HG23	2.10	0.51
1:C:252:GLU:O	1:C:253:ASP:HB2	2.11	0.51
1:F:266:THR:HA	1:F:271:VAL:O	2.10	0.51
1:G:200:LEU:O	1:G:201:SER:HB3	2.10	0.51
1:G:37:ASN:ND2	1:G:51:LYS:HG3	2.26	0.51
1:H:230:ILE:HD13	1:H:261:THR:HB	1.93	0.51
1:H:496:PRO:HD2	1:H:499:VAL:HG11	1.91	0.51
1:J:266:THR:CG2	1:J:273:VAL:H	2.22	0.51
1:A:273:VAL:HG12	1:A:274:ALA:N	2.26	0.51
1:B:496:PRO:HD2	1:B:499:VAL:HG11	1.92	0.51
1:C:266:THR:CG2	1:C:273:VAL:H	2.24	0.51
1:E:146:GLN:O	1:E:150:ILE:HG13	2.11	0.51
1:G:109:ALA:HB2	1:N:109:ALA:HB2	1.91	0.51
1:K:414:GLY:O	1:K:417:VAL:HG13	2.10	0.51
1:L:5:ASP:HB2	1:L:524:LEU:HD12	1.93	0.51
1:B:414:GLY:H	1:B:494:LEU:HA	1.76	0.51
1:G:263:VAL:O	1:G:267:MET:HB2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:455:VAL:HG13	1:H:460:GLU:HB2	1.91	0.51
1:K:27:VAL:HG12	1:K:90:THR:HG23	1.93	0.51
1:K:349:ILE:HA	1:K:352:GLN:HG3	1.91	0.51
1:M:183:LEU:CD1	1:M:184:GLN:HG3	2.40	0.51
1:M:198:GLY:HA3	1:M:328:ASP:HA	1.93	0.51
1:B:425:LYS:HD3	3:B:1203:HOH:O	2.10	0.51
1:E:414:GLY:O	1:E:417:VAL:HG13	2.11	0.51
1:I:13:ARG:HD2	1:I:104:LEU:HD22	1.91	0.51
1:M:5:ASP:HB2	1:M:524:LEU:HD12	1.93	0.51
1:A:271:VAL:HG21	2:O:607:TRP:HZ3	1.76	0.51
1:B:200:LEU:HG	1:B:276:VAL:HA	1.92	0.51
1:B:5:ASP:HB2	1:B:524:LEU:CD1	2.41	0.51
1:C:231:ARG:NH1	2:Q:612:PRO:O	2.44	0.51
1:L:413:ALA:HB2	1:L:475:ASN:HD22	1.76	0.51
1:B:445:ARG:HD3	3:B:1166:HOH:O	2.10	0.51
1:C:349:ILE:HA	1:C:352:GLN:HG3	1.92	0.51
1:E:46:ALA:HB2	1:F:76:GLU:CG	2.39	0.51
1:F:213:VAL:HB	1:F:325:ILE:HB	1.93	0.51
1:I:273:VAL:HG12	1:I:274:ALA:N	2.26	0.51
1:N:349:ILE:HA	1:N:352:GLN:HG3	1.92	0.51
1:A:230:ILE:HD13	1:A:261:THR:HB	1.93	0.51
1:D:383:ALA:CB	1:E:281:PHE:HZ	2.10	0.51
1:F:252:GLU:O	1:F:253:ASP:HB2	2.11	0.51
1:G:273:VAL:HG12	1:G:274:ALA:N	2.26	0.51
1:K:235:PRO:HG3	1:K:310:GLU:HA	1.92	0.51
1:M:245:LYS:HZ2	1:M:319:GLN:NE2	2.09	0.51
1:D:230:ILE:CD1	1:D:261:THR:HB	2.41	0.50
1:F:13:ARG:HD2	1:F:104:LEU:HD22	1.92	0.50
1:H:449:ALA:HB3	1:H:450:PRO:HD3	1.91	0.50
1:I:183:LEU:CD1	1:I:184:GLN:HG3	2.41	0.50
1:I:217:SER:N	1:I:218:PRO:CD	2.74	0.50
1:K:5:ASP:HB2	1:K:524:LEU:CD1	2.41	0.50
1:M:37:ASN:ND2	1:M:51:LYS:HG3	2.26	0.50
1:A:265:ASN:ND2	2:O:610:LEU:H	2.06	0.50
1:A:271:VAL:HG12	1:A:273:VAL:HG23	1.91	0.50
1:B:384:ALA:O	1:B:385:THR:HG23	2.12	0.50
1:D:183:LEU:CD1	1:D:184:GLN:HG3	2.40	0.50
1:E:130:GLU:HB3	1:E:422:VAL:HG22	1.93	0.50
1:E:271:VAL:HG12	1:E:273:VAL:HG23	1.93	0.50
1:F:263:VAL:O	1:F:267:MET:HB2	2.10	0.50
1:H:7:LYS:HG3	1:H:66:PHE:CZ	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:321:LYS:HD2	1:J:334:ASP:OD2	2.12	0.50
1:K:238:GLU:O	1:K:241:ALA:HB3	2.11	0.50
1:N:183:LEU:CD1	1:N:184:GLN:HG3	2.40	0.50
1:N:213:VAL:HB	1:N:325:ILE:HB	1.92	0.50
1:H:202:PRO:C	1:H:204:PHE:H	2.14	0.50
1:H:27:VAL:CG1	1:H:90:THR:HG23	2.41	0.50
1:H:302:SER:H	1:H:307:MET:HE1	1.76	0.50
1:I:414:GLY:H	1:I:494:LEU:HA	1.77	0.50
1:I:37:ASN:ND2	1:I:51:LYS:HG3	2.26	0.50
1:M:230:ILE:HD13	1:M:261:THR:HG21	1.93	0.50
1:C:200:LEU:HG	1:C:276:VAL:HA	1.93	0.50
1:C:37:ASN:ND2	1:C:51:LYS:HG3	2.27	0.50
1:E:252:GLU:O	1:E:253:ASP:HB2	2.11	0.50
1:F:183:LEU:CD1	1:F:184:GLN:HG3	2.40	0.50
1:F:200:LEU:O	1:F:201:SER:HB3	2.09	0.50
1:F:302:SER:H	1:F:307:MET:HE1	1.76	0.50
1:F:71:ALA:O	1:F:75:LYS:HB2	2.11	0.50
1:J:13:ARG:HD2	1:J:104:LEU:HD22	1.91	0.50
1:K:252:GLU:O	1:K:253:ASP:HB2	2.11	0.50
1:K:270:ILE:HD13	2:Y:608:GLY:HA3	1.92	0.50
1:L:235:PRO:HG3	1:L:310:GLU:HA	1.92	0.50
1:C:185:ASP:OD1	1:C:382:GLY:N	2.45	0.50
1:F:349:ILE:HA	1:F:352:GLN:HG3	1.94	0.50
1:H:241:ALA:HA	1:H:271:VAL:HG22	1.93	0.50
1:J:496:PRO:HD2	1:J:499:VAL:HG11	1.94	0.50
1:K:230:ILE:CD1	1:K:261:THR:HB	2.42	0.50
1:N:5:ASP:HB2	1:N:524:LEU:HD12	1.94	0.50
1:A:5:ASP:HB2	1:A:524:LEU:CD1	2.42	0.50
1:B:198:GLY:HA3	1:B:328:ASP:HA	1.92	0.50
1:B:202:PRO:C	1:B:204:PHE:H	2.15	0.50
1:B:266:THR:HA	1:B:271:VAL:O	2.12	0.50
1:B:46:ALA:HB2	1:C:76:GLU:CG	2.40	0.50
1:C:235:PRO:HG3	1:C:310:GLU:HA	1.94	0.50
1:D:7:LYS:HG3	1:D:66:PHE:CZ	2.46	0.50
1:E:270:ILE:HD13	2:S:608:GLY:HA3	1.94	0.50
1:H:183:LEU:CD1	1:H:184:GLN:HG3	2.42	0.50
1:H:37:ASN:ND2	1:H:51:LYS:HG3	2.26	0.50
1:J:37:ASN:ND2	1:J:51:LYS:HG3	2.27	0.50
1:L:238:GLU:O	1:L:241:ALA:HB3	2.11	0.50
1:N:200:LEU:HG	1:N:276:VAL:HA	1.92	0.50
1:C:463:SER:O	1:C:467:ASN:HB2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:185:ASP:OD1	1:D:382:GLY:N	2.42	0.50
1:E:200:LEU:O	1:E:201:SER:HB3	2.11	0.50
1:E:238:GLU:O	1:E:241:ALA:HB3	2.12	0.50
1:F:463:SER:O	1:F:467:ASN:HB2	2.12	0.50
1:G:13:ARG:HD2	1:G:104:LEU:HD22	1.92	0.50
1:I:155:ASP:OD1	1:I:157:THR:HB	2.12	0.50
1:J:235:PRO:HG3	1:J:310:GLU:HA	1.93	0.50
1:J:525:PRO:HG2	3:J:1175:HOH:O	2.11	0.50
1:J:270:ILE:HA	1:K:229:ASN:ND2	2.26	0.50
1:L:414:GLY:O	1:L:417:VAL:HG13	2.12	0.50
1:L:37:ASN:ND2	1:L:51:LYS:HG3	2.26	0.50
1:N:270:ILE:HD13	2:2:608:GLY:HA3	1.94	0.50
1:F:270:ILE:HG12	1:G:229:ASN:ND2	2.27	0.50
1:M:120:ILE:O	1:M:124:VAL:HG23	2.12	0.50
1:N:131:LEU:HD13	1:N:422:VAL:HG21	1.94	0.50
1:A:218:PRO:HD2	1:A:320:ALA:O	2.12	0.50
1:B:59:GLU:O	1:C:4:LYS:HG3	2.12	0.50
1:D:302:SER:H	1:D:307:MET:CE	2.25	0.50
1:F:270:ILE:HG12	1:G:229:ASN:HD21	1.77	0.50
1:H:193:MET:HG3	1:H:371:LYS:HB3	1.94	0.50
1:A:200:LEU:O	1:A:201:SER:HB3	2.11	0.49
1:B:266:THR:CG2	1:B:273:VAL:H	2.24	0.49
1:K:241:ALA:HA	1:K:271:VAL:HG22	1.94	0.49
1:L:218:PRO:HB3	1:L:246:PRO:HG2	1.94	0.49
2:1:602:TRP:NE1	2:1:612:PRO:HG3	2.27	0.49
1:A:291:ASP:OD2	1:A:368:ARG:HD2	2.12	0.49
1:E:230:ILE:HD13	1:E:261:THR:HB	1.93	0.49
1:F:235:PRO:HG3	1:F:310:GLU:HA	1.94	0.49
1:I:230:ILE:CD1	1:I:261:THR:HB	2.42	0.49
1:K:193:MET:HE3	1:K:292:ILE:HG12	1.94	0.49
1:L:302:SER:H	1:L:307:MET:HE1	1.76	0.49
1:N:193:MET:HE1	1:N:292:ILE:HG12	1.94	0.49
1:N:198:GLY:HA3	1:N:328:ASP:HA	1.94	0.49
1:C:200:LEU:O	1:C:201:SER:HB3	2.11	0.49
1:D:266:THR:CG2	1:D:273:VAL:H	2.24	0.49
1:D:384:ALA:O	1:D:385:THR:HG23	2.11	0.49
1:F:414:GLY:H	1:F:494:LEU:HA	1.77	0.49
1:E:38:VAL:HG22	1:F:519:CYS:HB3	1.94	0.49
1:H:305:ILE:O	1:H:305:ILE:HG22	2.12	0.49
1:N:252:GLU:O	1:N:253:ASP:HB2	2.11	0.49
1:B:37:ASN:ND2	1:B:51:LYS:HG3	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:291:ASP:OD2	1:E:368:ARG:HD2	2.13	0.49
1:F:200:LEU:HG	1:F:276:VAL:HA	1.93	0.49
1:L:201:SER:O	1:L:202:PRO:O	2.31	0.49
1:M:217:SER:N	1:M:218:PRO:CD	2.76	0.49
1:M:235:PRO:HG3	1:M:310:GLU:HA	1.95	0.49
1:N:414:GLY:H	1:N:494:LEU:HA	1.77	0.49
2:X:602:TRP:CE2	2:X:612:PRO:HG3	2.47	0.49
1:A:452:ARG:HD3	3:A:1012:HOH:O	2.13	0.49
1:B:273:VAL:HG12	1:B:274:ALA:N	2.28	0.49
1:C:193:MET:HE3	1:C:292:ILE:HG12	1.94	0.49
1:C:414:GLY:H	1:C:494:LEU:HA	1.78	0.49
1:C:496:PRO:HD2	1:C:499:VAL:HG11	1.95	0.49
1:D:131:LEU:HD13	1:D:422:VAL:HG21	1.94	0.49
1:D:213:VAL:HB	1:D:325:ILE:HB	1.94	0.49
1:E:185:ASP:OD1	1:E:382:GLY:N	2.45	0.49
1:I:230:ILE:HD13	1:I:261:THR:HG21	1.94	0.49
1:L:200:LEU:HG	1:L:276:VAL:HA	1.94	0.49
1:A:155:ASP:OD1	1:A:157:THR:HB	2.12	0.49
1:G:238:GLU:O	1:G:241:ALA:HB3	2.12	0.49
1:M:271:VAL:HG12	1:M:273:VAL:HG23	1.94	0.49
1:C:263:VAL:O	1:C:267:MET:HB2	2.12	0.49
1:D:182:GLY:O	1:D:183:LEU:O	2.31	0.49
1:D:235:PRO:HG3	1:D:310:GLU:HA	1.95	0.49
1:E:305:ILE:HG22	1:E:305:ILE:O	2.11	0.49
1:G:252:GLU:O	1:G:253:ASP:HB2	2.12	0.49
1:G:235:PRO:HG3	1:G:310:GLU:HA	1.93	0.49
1:I:463:SER:O	1:I:467:ASN:HB2	2.12	0.49
1:L:291:ASP:OD2	1:L:368:ARG:HD2	2.11	0.49
2:T:602:TRP:NE1	2:T:612:PRO:HG3	2.27	0.49
1:D:238:GLU:O	1:D:241:ALA:HB3	2.12	0.49
1:J:463:SER:O	1:J:467:ASN:HB2	2.12	0.49
1:L:463:SER:O	1:L:467:ASN:HB2	2.13	0.49
1:M:305:ILE:O	1:M:305:ILE:HG22	2.12	0.49
1:N:235:PRO:HG3	1:N:310:GLU:HA	1.95	0.49
1:A:231:ARG:HH22	2:O:603:MET:HE1	1.78	0.49
1:M:231:ARG:NH1	2:1:612:PRO:O	2.46	0.49
1:A:200:LEU:HD21	1:A:277:LYS:HG3	1.95	0.49
1:A:241:ALA:HA	1:A:271:VAL:HG22	1.95	0.49
1:B:146:GLN:O	1:B:150:ILE:HG13	2.13	0.49
1:B:463:SER:O	1:B:467:ASN:HB2	2.13	0.49
1:H:5:ASP:HB2	1:H:524:LEU:HD12	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:71:ALA:O	1:J:75:LYS:HB2	2.13	0.49
1:K:202:PRO:C	1:K:204:PHE:H	2.16	0.49
1:L:230:ILE:HD13	1:L:261:THR:HB	1.93	0.49
1:L:273:VAL:HG12	1:L:274:ALA:N	2.27	0.49
1:A:201:SER:O	1:A:202:PRO:O	2.30	0.49
1:B:238:GLU:O	1:B:241:ALA:HB3	2.12	0.49
1:D:5:ASP:HB2	1:D:524:LEU:CD1	2.42	0.49
1:E:240:VAL:HG11	1:E:247:LEU:HB2	1.94	0.49
1:E:5:ASP:HB2	1:E:524:LEU:CD1	2.42	0.49
1:F:305:ILE:HG22	1:F:305:ILE:O	2.13	0.49
1:G:231:ARG:NH1	2:U:612:PRO:O	2.46	0.49
1:I:235:PRO:HG3	1:I:310:GLU:HA	1.95	0.49
1:I:302:SER:H	1:I:307:MET:HE1	1.78	0.49
1:J:146:GLN:O	1:J:150:ILE:HG13	2.13	0.49
1:N:273:VAL:HG12	1:N:274:ALA:N	2.28	0.49
1:C:213:VAL:HB	1:C:325:ILE:HB	1.94	0.48
1:C:273:VAL:HG12	1:C:274:ALA:N	2.27	0.48
1:F:27:VAL:CG1	1:F:90:THR:HG23	2.43	0.48
1:K:263:VAL:O	1:K:267:MET:HB2	2.13	0.48
1:N:241:ALA:HA	1:N:271:VAL:HG22	1.94	0.48
1:E:200:LEU:HG	1:E:276:VAL:HA	1.95	0.48
1:E:217:SER:N	1:E:218:PRO:CD	2.76	0.48
1:F:5:ASP:HB2	1:F:524:LEU:CD1	2.43	0.48
1:M:241:ALA:HA	1:M:271:VAL:HG22	1.94	0.48
1:M:27:VAL:CG1	1:M:90:THR:HG23	2.43	0.48
1:A:185:ASP:OD1	1:A:382:GLY:N	2.45	0.48
1:C:7:LYS:HG3	1:C:66:PHE:CZ	2.48	0.48
1:D:230:ILE:HD13	1:D:261:THR:HG21	1.94	0.48
1:G:384:ALA:O	1:G:385:THR:HG23	2.13	0.48
1:J:305:ILE:O	1:J:305:ILE:HG22	2.12	0.48
1:K:200:LEU:HG	1:K:276:VAL:HA	1.96	0.48
1:K:463:SER:O	1:K:467:ASN:HB2	2.13	0.48
1:L:202:PRO:C	1:L:204:PHE:H	2.17	0.48
1:L:252:GLU:O	1:L:253:ASP:HB2	2.14	0.48
1:B:193:MET:HE1	1:B:292:ILE:HG12	1.94	0.48
1:B:38:VAL:HG22	1:C:519:CYS:HB3	1.94	0.48
1:C:5:ASP:HB2	1:C:524:LEU:CD1	2.43	0.48
1:E:271:VAL:HG21	2:S:607:TRP:HZ3	1.78	0.48
1:E:27:VAL:HG12	1:E:90:THR:HG23	1.95	0.48
1:J:349:ILE:HA	1:J:352:GLN:HG3	1.95	0.48
1:J:5:ASP:HB2	1:J:524:LEU:CD1	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:198:GLY:HA3	1:K:328:ASP:HA	1.94	0.48
1:K:217:SER:N	1:K:218:PRO:CD	2.76	0.48
1:L:213:VAL:HB	1:L:325:ILE:HB	1.95	0.48
1:M:496:PRO:HD2	1:M:499:VAL:HG11	1.96	0.48
2:X:602:TRP:NE1	2:X:612:PRO:HG3	2.28	0.48
1:B:414:GLY:O	1:B:417:VAL:HG13	2.13	0.48
1:C:27:VAL:CG1	1:C:90:THR:HG23	2.43	0.48
1:G:202:PRO:C	1:G:204:PHE:H	2.16	0.48
1:N:185:ASP:OD1	1:N:382:GLY:N	2.47	0.48
2:1:602:TRP:CE2	2:1:612:PRO:HG3	2.49	0.48
1:E:155:ASP:OD1	1:E:157:THR:HB	2.14	0.48
1:E:202:PRO:O	1:E:204:PHE:N	2.45	0.48
1:G:27:VAL:CG1	1:G:90:THR:HG23	2.43	0.48
1:H:238:GLU:O	1:H:241:ALA:HB3	2.13	0.48
1:I:185:ASP:OD1	1:I:382:GLY:N	2.45	0.48
1:K:291:ASP:OD2	1:K:368:ARG:HD2	2.14	0.48
1:M:16:MET:O	1:M:20:VAL:HG13	2.14	0.48
1:N:305:ILE:O	1:N:305:ILE:HG22	2.13	0.48
1:D:200:LEU:HG	1:D:276:VAL:HA	1.95	0.48
1:I:120:ILE:O	1:I:124:VAL:HG23	2.14	0.48
1:N:266:THR:CG2	1:N:273:VAL:H	2.27	0.48
1:D:109:ALA:HB2	1:J:109:ALA:HB2	1.96	0.48
1:J:247:LEU:HD21	1:J:249:ILE:HD11	1.95	0.48
1:J:230:ILE:HD13	1:J:261:THR:HG21	1.95	0.48
1:K:230:ILE:HD13	1:K:261:THR:CB	2.43	0.48
1:N:201:SER:O	1:N:202:PRO:O	2.31	0.48
1:B:202:PRO:O	1:B:204:PHE:N	2.41	0.48
1:B:230:ILE:HD13	1:B:261:THR:HG21	1.95	0.48
1:B:305:ILE:O	1:B:305:ILE:HG22	2.12	0.48
1:E:264:VAL:O	1:E:268:ARG:HG3	2.13	0.48
1:G:305:ILE:O	1:G:305:ILE:HG22	2.14	0.48
1:I:5:ASP:HB2	1:I:524:LEU:CD1	2.44	0.48
1:K:200:LEU:O	1:K:201:SER:HB3	2.12	0.48
1:K:305:ILE:O	1:K:305:ILE:HG22	2.12	0.48
1:A:463:SER:O	1:A:467:ASN:HB2	2.14	0.48
1:B:217:SER:N	1:B:218:PRO:CD	2.76	0.48
1:C:139:SER:O	1:C:171:LYS:HE2	2.14	0.48
1:D:384:ALA:C	1:D:385:THR:HG23	2.34	0.48
1:E:199:TYR:HA	1:E:276:VAL:HG12	1.96	0.48
1:H:230:ILE:CD1	1:H:261:THR:HB	2.44	0.48
1:I:252:GLU:O	1:I:253:ASP:HB2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:185:ASP:OD1	1:K:382:GLY:N	2.47	0.48
1:N:202:PRO:C	1:N:204:PHE:H	2.17	0.48
1:N:16:MET:O	1:N:20:VAL:HG13	2.14	0.48
1:J:265:ASN:ND2	2:X:610:LEU:H	2.10	0.48
1:C:240:VAL:HG11	1:C:247:LEU:HB2	1.96	0.47
1:F:202:PRO:C	1:F:204:PHE:H	2.17	0.47
1:L:319:GLN:HB3	1:L:336:VAL:HG21	1.95	0.47
1:M:245:LYS:NZ	1:M:319:GLN:NE2	2.62	0.47
1:M:414:GLY:H	1:M:494:LEU:HA	1.79	0.47
1:A:305:ILE:O	1:A:305:ILE:HG22	2.14	0.47
1:F:155:ASP:OD1	1:F:157:THR:HB	2.13	0.47
1:F:217:SER:N	1:F:218:PRO:CD	2.77	0.47
1:F:218:PRO:HG3	1:F:323:VAL:HG13	1.95	0.47
1:G:16:MET:O	1:G:20:VAL:HG13	2.14	0.47
1:H:155:ASP:OD1	1:H:157:THR:HB	2.14	0.47
1:H:79:SER:HA	1:H:89:THR:CG2	2.44	0.47
1:I:202:PRO:O	1:I:204:PHE:N	2.45	0.47
1:I:63:GLU:HB3	3:I:1204:HOH:O	2.14	0.47
1:L:182:GLY:O	1:L:183:LEU:O	2.32	0.47
1:L:245:LYS:NZ	1:L:319:GLN:NE2	2.62	0.47
1:N:193:MET:HG3	1:N:371:LYS:HB3	1.96	0.47
1:E:263:VAL:O	1:E:267:MET:HB2	2.13	0.47
1:G:463:SER:O	1:G:467:ASN:HB2	2.14	0.47
1:I:240:VAL:HG11	1:I:247:LEU:HB2	1.96	0.47
1:J:182:GLY:O	1:J:183:LEU:O	2.32	0.47
1:K:369:VAL:HG23	1:K:370:ALA:N	2.28	0.47
1:L:200:LEU:O	1:L:201:SER:HB3	2.12	0.47
1:L:230:ILE:HD13	1:L:261:THR:HG21	1.96	0.47
1:M:5:ASP:HB2	1:M:524:LEU:CD1	2.43	0.47
1:H:229:ASN:HD22	1:N:270:ILE:HA	1.78	0.47
1:N:463:SER:O	1:N:467:ASN:HB2	2.14	0.47
1:A:198:GLY:HA3	1:A:328:ASP:HA	1.94	0.47
1:A:384:ALA:O	1:A:385:THR:HG23	2.15	0.47
1:C:241:ALA:HA	1:C:271:VAL:HG22	1.96	0.47
1:J:414:GLY:H	1:J:494:LEU:HA	1.79	0.47
1:K:200:LEU:HD21	1:K:277:LYS:HG3	1.96	0.47
1:L:384:ALA:O	1:L:385:THR:HG23	2.14	0.47
1:M:200:LEU:HD13	1:M:254:VAL:HB	1.96	0.47
1:M:263:VAL:O	1:M:267:MET:HB2	2.13	0.47
1:B:291:ASP:OD2	1:B:368:ARG:HD2	2.14	0.47
1:C:438:VAL:O	1:C:442:VAL:HG23	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:16:MET:O	1:E:20:VAL:HG13	2.14	0.47
1:E:463:SER:O	1:E:467:ASN:HB2	2.14	0.47
1:G:200:LEU:HG	1:G:276:VAL:HA	1.95	0.47
1:M:230:ILE:CD1	1:M:261:THR:HB	2.45	0.47
1:N:155:ASP:OD1	1:N:157:THR:HB	2.15	0.47
1:B:263:VAL:O	1:B:267:MET:HB2	2.14	0.47
1:D:202:PRO:C	1:D:204:PHE:H	2.17	0.47
1:D:414:GLY:H	1:D:494:LEU:HA	1.79	0.47
1:F:185:ASP:OD1	1:F:382:GLY:N	2.47	0.47
1:I:305:ILE:HG22	1:I:305:ILE:O	2.14	0.47
1:J:262:LEU:HD22	1:J:273:VAL:HG11	1.97	0.47
1:K:131:LEU:HD13	1:K:422:VAL:HG21	1.96	0.47
1:L:305:ILE:HG22	1:L:305:ILE:O	2.14	0.47
2:P:602:TRP:NE1	2:P:612:PRO:HG3	2.29	0.47
1:A:270:ILE:HG12	1:B:229:ASN:HD21	1.80	0.47
1:B:382:GLY:O	1:B:389:MET:HG2	2.14	0.47
1:D:247:LEU:HD21	1:D:249:ILE:HD11	1.95	0.47
1:G:414:GLY:H	1:G:494:LEU:HA	1.80	0.47
1:J:202:PRO:C	1:J:204:PHE:H	2.17	0.47
1:A:199:TYR:HA	1:A:276:VAL:HG12	1.97	0.47
1:F:182:GLY:O	1:F:183:LEU:O	2.33	0.47
1:F:270:ILE:HD13	2:T:608:GLY:HA3	1.97	0.47
1:G:198:GLY:HA3	1:G:328:ASP:HA	1.95	0.47
1:H:384:ALA:O	1:H:385:THR:HG23	2.14	0.47
1:H:5:ASP:HB2	1:H:524:LEU:CD1	2.45	0.47
1:I:383:ALA:HB1	1:J:281:PHE:CZ	2.44	0.47
1:K:384:ALA:O	1:K:385:THR:HG23	2.15	0.47
1:L:369:VAL:HG23	1:L:370:ALA:N	2.29	0.47
1:M:193:MET:HG2	1:M:194:GLN:N	2.29	0.47
2:V:602:TRP:NE1	2:V:612:PRO:HG3	2.29	0.47
1:A:238:GLU:O	1:A:241:ALA:HB3	2.15	0.47
1:E:266:THR:HG22	1:E:271:VAL:O	2.15	0.47
1:E:438:VAL:O	1:E:442:VAL:HG23	2.15	0.47
1:H:252:GLU:O	1:H:253:ASP:HB2	2.15	0.47
1:I:90:THR:O	1:I:94:VAL:HG13	2.14	0.47
1:J:199:TYR:CZ	1:J:327:LYS:HA	2.50	0.47
1:L:193:MET:HG2	1:L:194:GLN:N	2.29	0.47
1:M:271:VAL:HG21	2:1:607:TRP:HZ3	1.80	0.47
1:B:384:ALA:C	1:B:385:THR:HG23	2.35	0.47
1:C:26:ALA:HA	1:D:8:PHE:HE1	1.80	0.47
1:D:200:LEU:HD21	1:D:277:LYS:HG3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:235:PRO:HG3	1:E:310:GLU:HA	1.97	0.47
1:E:241:ALA:HA	1:E:271:VAL:HG22	1.96	0.47
1:F:266:THR:CG2	1:F:273:VAL:H	2.27	0.47
1:F:273:VAL:HG12	1:F:274:ALA:N	2.30	0.47
1:I:200:LEU:O	1:I:201:SER:HB3	2.13	0.47
1:I:266:THR:CG2	1:I:273:VAL:H	2.27	0.47
1:K:240:VAL:HG11	1:K:247:LEU:HB2	1.96	0.47
1:A:319:GLN:HB3	1:A:336:VAL:HG21	1.96	0.47
1:A:245:LYS:NZ	1:A:319:GLN:NE2	2.62	0.47
1:A:37:ASN:ND2	1:A:51:LYS:HG3	2.30	0.47
1:B:182:GLY:O	1:B:183:LEU:O	2.33	0.47
1:F:87:ASP:O	1:F:499:VAL:HG23	2.15	0.47
1:G:217:SER:N	1:G:218:PRO:CD	2.78	0.47
1:H:384:ALA:C	1:H:385:THR:HG23	2.36	0.47
1:M:382:GLY:O	1:M:389:MET:HG2	2.15	0.47
1:A:414:GLY:H	1:A:494:LEU:HA	1.79	0.46
1:B:321:LYS:HD2	1:B:334:ASP:OD2	2.15	0.46
1:E:245:LYS:NZ	1:E:319:GLN:NE2	2.63	0.46
1:F:198:GLY:HA3	1:F:328:ASP:HA	1.97	0.46
1:G:155:ASP:OD1	1:G:157:THR:HB	2.14	0.46
1:H:266:THR:CG2	1:H:273:VAL:H	2.28	0.46
1:K:155:ASP:OD1	1:K:157:THR:HB	2.15	0.46
1:L:130:GLU:HG3	3:L:1115:HOH:O	2.14	0.46
1:L:199:TYR:HA	1:L:276:VAL:HG12	1.97	0.46
1:L:5:ASP:HB2	1:L:524:LEU:CD1	2.45	0.46
1:L:95:LEU:O	1:L:99:ILE:HG13	2.15	0.46
1:M:199:TYR:HA	1:M:276:VAL:HG12	1.98	0.46
1:M:384:ALA:C	1:M:385:THR:HG23	2.36	0.46
1:B:193:MET:HG3	1:B:371:LYS:HB3	1.96	0.46
1:D:463:SER:O	1:D:467:ASN:HB2	2.15	0.46
1:D:27:VAL:CG1	1:D:90:THR:HG23	2.45	0.46
1:F:131:LEU:HD13	1:F:422:VAL:HG21	1.97	0.46
1:F:266:THR:HG22	1:F:271:VAL:O	2.15	0.46
1:H:463:SER:O	1:H:467:ASN:HB2	2.16	0.46
1:J:185:ASP:OD1	1:J:382:GLY:N	2.48	0.46
1:J:27:VAL:CG1	1:J:90:THR:HG23	2.45	0.46
1:I:270:ILE:CD1	2:W:608:GLY:HA3	2.45	0.46
1:A:230:ILE:CD1	1:A:261:THR:HB	2.46	0.46
1:D:199:TYR:CZ	1:D:327:LYS:HA	2.51	0.46
1:D:90:THR:O	1:D:94:VAL:HG13	2.15	0.46
1:E:202:PRO:C	1:E:204:PHE:H	2.18	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:231:ARG:NH1	2:S:612:PRO:O	2.48	0.46
1:E:131:LEU:HD13	1:E:422:VAL:HG21	1.97	0.46
1:F:199:TYR:HA	1:F:276:VAL:HG12	1.97	0.46
1:F:296:THR:HB	1:F:319:GLN:H	1.79	0.46
1:G:193:MET:HE1	1:G:292:ILE:HG12	1.97	0.46
1:H:38:VAL:HG22	1:I:519:CYS:HB3	1.96	0.46
1:I:384:ALA:O	1:I:385:THR:HG23	2.15	0.46
1:I:95:LEU:O	1:I:99:ILE:HG13	2.16	0.46
1:J:384:ALA:O	1:J:385:THR:HG23	2.15	0.46
1:L:230:ILE:CD1	1:L:261:THR:HB	2.46	0.46
1:M:182:GLY:O	1:M:183:LEU:O	2.34	0.46
1:M:200:LEU:HG	1:M:276:VAL:HA	1.97	0.46
1:N:245:LYS:NZ	1:N:319:GLN:NE2	2.63	0.46
1:C:182:GLY:O	1:C:183:LEU:O	2.33	0.46
1:C:217:SER:N	1:C:218:PRO:CD	2.78	0.46
1:G:131:LEU:HD13	1:G:422:VAL:HG21	1.97	0.46
1:G:79:SER:HA	1:G:89:THR:HG22	1.97	0.46
1:I:139:SER:O	1:I:171:LYS:HE2	2.16	0.46
1:I:193:MET:HG2	1:I:194:GLN:N	2.30	0.46
1:A:321:LYS:HD2	1:A:334:ASP:OD2	2.15	0.46
1:E:193:MET:HG2	1:E:194:GLN:N	2.31	0.46
1:J:200:LEU:HD21	1:J:277:LYS:HG3	1.98	0.46
1:K:79:SER:HA	1:K:89:THR:HG22	1.98	0.46
1:K:79:SER:HA	1:K:89:THR:CG2	2.46	0.46
1:L:265:ASN:HD21	2:Z:610:LEU:N	2.00	0.46
1:L:79:SER:HA	1:L:89:THR:HG22	1.98	0.46
1:M:247:LEU:HD21	1:M:249:ILE:HD11	1.96	0.46
1:M:384:ALA:O	1:M:385:THR:HG23	2.14	0.46
2:Y:604:THR:HG22	2:Y:605:THR:O	2.16	0.46
1:A:266:THR:CG2	1:A:273:VAL:H	2.28	0.46
1:B:200:LEU:HD21	1:B:277:LYS:HG3	1.98	0.46
1:C:202:PRO:C	1:C:204:PHE:H	2.18	0.46
1:E:182:GLY:O	1:E:183:LEU:O	2.34	0.46
1:I:131:LEU:HD13	1:I:422:VAL:HG21	1.97	0.46
1:M:230:ILE:HD13	1:M:261:THR:HB	1.96	0.46
1:K:270:ILE:CD1	2:Y:608:GLY:HA3	2.45	0.46
1:A:193:MET:HG2	1:A:194:GLN:N	2.30	0.46
1:C:176:THR:HG22	1:C:177:VAL:N	2.31	0.46
1:H:79:SER:HA	1:H:89:THR:HG22	1.97	0.46
1:I:241:ALA:HA	1:I:271:VAL:HG22	1.98	0.46
1:M:240:VAL:HG11	1:M:247:LEU:HB2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:201:SER:C	1:N:202:PRO:O	2.54	0.46
2:V:602:TRP:CE2	2:V:612:PRO:HG3	2.51	0.46
1:A:176:THR:HG22	1:A:177:VAL:N	2.31	0.46
1:A:182:GLY:O	1:A:183:LEU:O	2.33	0.46
1:A:218:PRO:CB	1:A:246:PRO:HG2	2.46	0.46
1:A:90:THR:O	1:A:94:VAL:HG13	2.14	0.46
1:B:199:TYR:CZ	1:B:327:LYS:HA	2.51	0.46
1:C:90:THR:O	1:C:94:VAL:HG13	2.15	0.46
1:G:241:ALA:HA	1:G:271:VAL:HG22	1.98	0.46
1:G:245:LYS:NZ	1:G:319:GLN:NE2	2.63	0.46
1:H:182:GLY:O	1:H:183:LEU:O	2.34	0.46
1:I:146:GLN:O	1:I:150:ILE:HG13	2.16	0.46
1:J:200:LEU:HG	1:J:276:VAL:HA	1.97	0.46
1:K:264:VAL:O	1:K:268:ARG:HG3	2.15	0.46
1:L:79:SER:HA	1:L:89:THR:CG2	2.46	0.46
2:P:602:TRP:CE2	2:P:612:PRO:HG3	2.50	0.46
1:C:270:ILE:CD1	2:Q:608:GLY:HA3	2.45	0.46
1:A:230:ILE:HD13	1:A:261:THR:HG21	1.98	0.46
1:B:245:LYS:NZ	1:B:319:GLN:NE2	2.64	0.46
1:F:270:ILE:HA	1:G:229:ASN:HD22	1.81	0.46
1:H:198:GLY:HA3	1:H:328:ASP:HA	1.97	0.46
1:J:217:SER:N	1:J:218:PRO:CD	2.79	0.46
1:J:230:ILE:HD13	1:J:261:THR:HB	1.98	0.46
1:J:384:ALA:C	1:J:385:THR:HG23	2.36	0.46
1:J:131:LEU:HD13	1:J:422:VAL:HG21	1.97	0.46
1:N:199:TYR:HA	1:N:276:VAL:HG12	1.98	0.46
1:N:5:ASP:HB2	1:N:524:LEU:CD1	2.46	0.46
1:B:270:ILE:HD13	2:P:608:GLY:HA3	1.97	0.46
1:B:199:TYR:HA	1:B:276:VAL:HG12	1.98	0.46
1:B:524:LEU:HD12	1:B:524:LEU:HA	1.84	0.46
1:C:238:GLU:O	1:C:241:ALA:HB3	2.16	0.46
1:F:265:ASN:HD21	2:T:610:LEU:N	2.06	0.46
1:G:266:THR:HG22	1:G:271:VAL:O	2.16	0.46
1:H:199:TYR:HA	1:H:276:VAL:HG12	1.98	0.46
1:H:199:TYR:CZ	1:H:327:LYS:HA	2.50	0.46
1:H:321:LYS:HD2	1:H:334:ASP:OD2	2.15	0.46
1:K:182:GLY:O	1:K:183:LEU:O	2.34	0.46
1:K:193:MET:HG2	1:K:194:GLN:N	2.31	0.46
1:K:273:VAL:HG12	1:K:274:ALA:N	2.31	0.46
1:M:202:PRO:C	1:M:204:PHE:H	2.18	0.46
2:R:602:TRP:CE2	2:R:612:PRO:HG3	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:265:ASN:HD21	2:R:610:LEU:N	2.03	0.45
1:G:384:ALA:C	1:G:385:THR:HG23	2.36	0.45
1:G:90:THR:O	1:G:94:VAL:HG13	2.15	0.45
1:J:198:GLY:HA3	1:J:328:ASP:HA	1.96	0.45
1:K:16:MET:O	1:K:20:VAL:HG13	2.16	0.45
1:K:90:THR:O	1:K:94:VAL:HG13	2.16	0.45
2:T:602:TRP:CE2	2:T:612:PRO:HG3	2.52	0.45
1:C:245:LYS:NZ	1:C:319:GLN:NE2	2.64	0.45
1:F:90:THR:O	1:F:94:VAL:HG13	2.16	0.45
1:G:193:MET:HG2	1:G:194:GLN:N	2.31	0.45
1:H:185:ASP:OD1	1:H:382:GLY:N	2.46	0.45
1:H:349:ILE:O	1:H:353:ILE:HG13	2.16	0.45
1:H:87:ASP:O	1:H:499:VAL:HG23	2.16	0.45
1:I:302:SER:H	1:I:307:MET:CE	2.28	0.45
1:I:384:ALA:C	1:I:385:THR:HG23	2.35	0.45
1:J:230:ILE:CD1	1:J:261:THR:HB	2.46	0.45
1:J:266:THR:HG22	1:J:271:VAL:O	2.16	0.45
1:K:384:ALA:C	1:K:385:THR:HG23	2.37	0.45
1:L:200:LEU:HD13	1:L:254:VAL:HB	1.98	0.45
1:L:218:PRO:HG3	1:L:323:VAL:HG13	1.96	0.45
2:Q:602:TRP:NE1	2:Q:612:PRO:HG3	2.31	0.45
1:D:270:ILE:CD1	2:R:608:GLY:HA3	2.46	0.45
1:B:240:VAL:HG11	1:B:247:LEU:HB2	1.98	0.45
1:C:200:LEU:HD21	1:C:277:LYS:HG3	1.97	0.45
1:E:90:THR:O	1:E:94:VAL:HG13	2.16	0.45
1:F:247:LEU:HD21	1:F:249:ILE:HD11	1.98	0.45
1:F:270:ILE:HA	1:G:229:ASN:ND2	2.32	0.45
1:G:240:VAL:HG11	1:G:247:LEU:HB2	1.97	0.45
1:G:270:ILE:HD13	2:U:608:GLY:HA3	1.98	0.45
1:H:193:MET:HG2	1:H:194:GLN:N	2.32	0.45
1:J:263:VAL:O	1:J:267:MET:HB2	2.17	0.45
1:J:95:LEU:O	1:J:99:ILE:HG13	2.17	0.45
1:K:217:SER:N	1:K:218:PRO:HD3	2.32	0.45
1:L:185:ASP:OD1	1:L:382:GLY:N	2.48	0.45
1:L:384:ALA:C	1:L:385:THR:HG23	2.36	0.45
1:M:238:GLU:O	1:M:241:ALA:HB3	2.16	0.45
1:M:291:ASP:OD2	1:M:368:ARG:HD2	2.15	0.45
1:N:240:VAL:HG11	1:N:247:LEU:HB2	1.98	0.45
1:B:155:ASP:OD1	1:B:157:THR:HB	2.16	0.45
1:C:321:LYS:HD2	1:C:334:ASP:OD2	2.15	0.45
1:D:230:ILE:HD13	1:D:261:THR:CB	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:79:SER:HA	1:G:89:THR:CG2	2.46	0.45
1:H:444:LEU:HD23	1:H:447:MET:CE	2.46	0.45
1:I:222:LEU:HD23	1:I:250:ILE:HB	1.98	0.45
1:I:199:TYR:CZ	1:I:327:LYS:HA	2.51	0.45
1:J:199:TYR:HA	1:J:276:VAL:HG12	1.99	0.45
1:J:241:ALA:HA	1:J:271:VAL:HG22	1.99	0.45
1:M:217:SER:N	1:M:218:PRO:HD3	2.31	0.45
1:N:445:ARG:HD3	3:N:1133:HOH:O	2.15	0.45
2:W:604:THR:HG22	2:W:605:THR:O	2.16	0.45
1:A:146:GLN:O	1:A:150:ILE:HG13	2.16	0.45
1:B:241:ALA:HA	1:B:271:VAL:HG22	1.98	0.45
1:C:199:TYR:HA	1:C:276:VAL:HG12	1.99	0.45
1:C:384:ALA:O	1:C:385:THR:HG23	2.16	0.45
1:F:241:ALA:HA	1:F:271:VAL:HG22	1.98	0.45
1:F:7:LYS:HG3	1:F:66:PHE:CZ	2.51	0.45
1:H:231:ARG:NH1	2:V:612:PRO:O	2.50	0.45
1:I:202:PRO:C	1:I:204:PHE:H	2.20	0.45
1:I:230:ILE:HD13	1:I:261:THR:CB	2.45	0.45
1:L:382:GLY:O	1:L:389:MET:HG2	2.16	0.45
1:N:42:LYS:HE3	1:N:48:THR:OG1	2.17	0.45
1:B:25:ASP:HA	1:B:28:LYS:HE2	1.97	0.45
1:B:218:PRO:HD2	1:B:320:ALA:O	2.17	0.45
1:C:186:GLU:HB2	1:C:380:LYS:HB2	1.98	0.45
1:D:240:VAL:HG11	1:D:247:LEU:HB2	1.97	0.45
1:D:218:PRO:HD2	1:D:320:ALA:O	2.16	0.45
1:H:217:SER:N	1:H:218:PRO:CD	2.80	0.45
1:J:193:MET:HG2	1:J:194:GLN:N	2.31	0.45
1:K:139:SER:O	1:K:171:LYS:HE2	2.17	0.45
1:L:155:ASP:OD1	1:L:157:THR:HB	2.16	0.45
1:N:176:THR:HG22	1:N:177:VAL:N	2.32	0.45
1:C:302:SER:H	1:C:307:MET:CE	2.29	0.45
1:C:199:TYR:CZ	1:C:327:LYS:HA	2.52	0.45
1:F:16:MET:O	1:F:20:VAL:HG13	2.17	0.45
1:L:146:GLN:O	1:L:150:ILE:HG13	2.17	0.45
1:L:270:ILE:O	1:L:271:VAL:HB	2.16	0.45
1:M:409:GLU:OE2	1:M:498:LYS:HG3	2.15	0.45
2:U:602:TRP:NE1	2:U:612:PRO:HG3	2.31	0.45
1:M:270:ILE:HD13	2:1:608:GLY:HA3	1.99	0.45
1:A:384:ALA:C	1:A:385:THR:HG23	2.36	0.45
1:C:384:ALA:C	1:C:385:THR:HG23	2.37	0.45
1:D:16:MET:O	1:D:20:VAL:HG13	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:176:THR:HG22	1:D:177:VAL:N	2.32	0.45
1:E:381:VAL:O	1:E:382:GLY:O	2.34	0.45
1:F:217:SER:N	1:F:218:PRO:HD3	2.32	0.45
1:F:245:LYS:NZ	1:F:319:GLN:NE2	2.65	0.45
1:G:217:SER:N	1:G:218:PRO:HD3	2.32	0.45
1:I:182:GLY:O	1:I:183:LEU:O	2.35	0.45
1:I:198:GLY:HA3	1:I:328:ASP:HA	1.98	0.45
1:I:369:VAL:HG23	1:I:370:ALA:N	2.32	0.45
1:J:193:MET:HG3	1:J:371:LYS:HB3	1.98	0.45
1:J:238:GLU:O	1:J:241:ALA:HB3	2.16	0.45
1:K:46:ALA:HB2	1:L:76:GLU:CG	2.43	0.45
1:M:302:SER:H	1:M:307:MET:CE	2.29	0.45
1:E:139:SER:O	1:E:171:LYS:HE2	2.17	0.45
1:F:384:ALA:C	1:F:385:THR:HG23	2.37	0.45
1:J:291:ASP:OD2	1:J:368:ARG:HD2	2.17	0.45
1:L:444:LEU:HD23	1:L:447:MET:CE	2.47	0.45
1:N:319:GLN:HB3	1:N:336:VAL:HG21	1.98	0.45
1:C:155:ASP:OD1	1:C:157:THR:HB	2.16	0.45
1:D:263:VAL:O	1:D:267:MET:HB2	2.16	0.45
1:D:319:GLN:HB3	1:D:336:VAL:CG2	2.46	0.45
1:F:146:GLN:O	1:F:150:ILE:HG13	2.17	0.45
1:F:176:THR:HG22	1:F:177:VAL:N	2.32	0.45
1:H:218:PRO:HD2	1:H:320:ALA:O	2.17	0.45
1:J:273:VAL:HG12	1:J:274:ALA:N	2.31	0.45
1:J:219:PHE:HB3	1:J:317:LEU:HD23	1.99	0.45
1:L:217:SER:N	1:L:218:PRO:CD	2.80	0.45
1:M:155:ASP:OD1	1:M:157:THR:HB	2.17	0.45
1:N:384:ALA:O	1:N:385:THR:HG23	2.16	0.45
1:N:79:SER:HA	1:N:89:THR:CG2	2.46	0.45
1:A:240:VAL:HG11	1:A:247:LEU:HB2	1.98	0.44
1:B:302:SER:H	1:B:307:MET:CE	2.30	0.44
1:C:264:VAL:O	1:C:268:ARG:HG3	2.17	0.44
1:E:384:ALA:C	1:E:385:THR:HG23	2.37	0.44
1:G:185:ASP:OD1	1:G:382:GLY:N	2.50	0.44
1:H:90:THR:O	1:H:94:VAL:HG13	2.17	0.44
1:I:193:MET:HG3	1:I:371:LYS:HB3	1.98	0.44
1:J:201:SER:O	1:J:202:PRO:O	2.35	0.44
1:L:245:LYS:HZ2	1:L:319:GLN:NE2	2.15	0.44
1:L:414:GLY:N	1:L:494:LEU:HA	2.32	0.44
1:N:218:PRO:HG3	1:N:323:VAL:HG13	1.98	0.44
1:A:202:PRO:O	1:A:204:PHE:N	2.45	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:302:SER:H	1:B:307:MET:HE1	1.82	0.44
1:D:305:ILE:O	1:D:305:ILE:HG22	2.16	0.44
1:D:382:GLY:O	1:D:389:MET:HG2	2.17	0.44
1:E:183:LEU:O	1:E:184:GLN:CB	2.65	0.44
1:E:217:SER:N	1:E:218:PRO:HD3	2.32	0.44
1:E:384:ALA:O	1:E:385:THR:HG23	2.16	0.44
1:G:68:ASN:O	1:G:72:GLN:HG2	2.17	0.44
1:H:146:GLN:O	1:H:150:ILE:HG13	2.17	0.44
1:J:240:VAL:HG11	1:J:247:LEU:HB2	1.98	0.44
1:J:222:LEU:HD23	1:J:250:ILE:HB	1.99	0.44
1:M:25:ASP:HA	1:M:28:LYS:HE2	2.00	0.44
1:N:384:ALA:C	1:N:385:THR:HG23	2.37	0.44
1:A:202:PRO:C	1:A:204:PHE:H	2.18	0.44
1:D:217:SER:N	1:D:218:PRO:CD	2.81	0.44
1:D:321:LYS:HD2	1:D:334:ASP:OD2	2.17	0.44
1:F:384:ALA:O	1:F:385:THR:HG23	2.16	0.44
1:I:199:TYR:HA	1:I:276:VAL:HG12	2.00	0.44
1:I:263:VAL:O	1:I:267:MET:HB2	2.16	0.44
1:I:264:VAL:O	1:I:268:ARG:HG3	2.16	0.44
1:J:369:VAL:HG23	1:J:370:ALA:N	2.32	0.44
1:K:319:GLN:HB3	1:K:336:VAL:HG21	1.98	0.44
1:L:240:VAL:HG11	1:L:247:LEU:HB2	1.99	0.44
1:E:100:ILE:HD13	1:E:514:MET:CE	2.47	0.44
1:F:230:ILE:HD13	1:F:261:THR:HG21	2.00	0.44
1:F:302:SER:H	1:F:307:MET:CE	2.29	0.44
1:F:383:ALA:HB1	1:G:281:PHE:HZ	1.83	0.44
1:H:200:LEU:HG	1:H:276:VAL:HA	1.98	0.44
1:H:247:LEU:HD21	1:H:249:ILE:HD11	1.98	0.44
1:I:79:SER:HA	1:I:89:THR:HG22	1.99	0.44
1:K:511:ALA:O	1:K:515:ILE:HG13	2.18	0.44
1:N:200:LEU:O	1:N:201:SER:HB3	2.17	0.44
1:N:230:ILE:HD13	1:N:261:THR:HG21	2.00	0.44
1:N:425:LYS:CE	3:N:1053:HOH:O	2.66	0.44
2:S:602:TRP:CE2	2:S:612:PRO:HG3	2.52	0.44
2:W:602:TRP:NE1	2:W:612:PRO:HG3	2.32	0.44
1:A:217:SER:N	1:A:218:PRO:CD	2.81	0.44
1:A:193:MET:HE1	1:A:292:ILE:HG12	2.00	0.44
1:A:305:ILE:HD12	1:A:307:MET:HE2	1.99	0.44
1:C:201:SER:C	1:C:202:PRO:O	2.56	0.44
1:C:291:ASP:OD2	1:C:368:ARG:HD2	2.18	0.44
1:D:198:GLY:HA3	1:D:328:ASP:HA	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:198:GLY:HA3	1:E:328:ASP:HA	2.00	0.44
1:F:336:VAL:O	1:F:337:GLY:C	2.56	0.44
1:G:182:GLY:O	1:G:183:LEU:O	2.35	0.44
1:G:383:ALA:O	1:G:384:ALA:CB	2.65	0.44
1:H:186:GLU:HB2	1:H:380:LYS:HB2	1.99	0.44
1:H:245:LYS:NZ	1:H:319:GLN:NE2	2.65	0.44
1:I:217:SER:N	1:I:218:PRO:HD3	2.32	0.44
1:J:100:ILE:HD13	1:J:514:MET:CE	2.47	0.44
1:K:146:GLN:O	1:K:150:ILE:HG13	2.17	0.44
1:K:382:GLY:O	1:K:389:MET:HG2	2.17	0.44
1:K:95:LEU:O	1:K:99:ILE:HG13	2.17	0.44
1:M:79:SER:HA	1:M:89:THR:CG2	2.47	0.44
1:N:193:MET:HG2	1:N:194:GLN:N	2.32	0.44
2:S:602:TRP:NE1	2:S:612:PRO:HG3	2.33	0.44
1:A:366:GLN:O	1:A:369:VAL:HG22	2.17	0.44
1:B:176:THR:HG22	1:B:177:VAL:N	2.33	0.44
1:D:146:GLN:O	1:D:150:ILE:HG13	2.17	0.44
1:D:271:VAL:HG21	2:R:607:TRP:CZ3	2.49	0.44
1:E:302:SER:H	1:E:307:MET:CE	2.30	0.44
1:F:369:VAL:HG23	1:F:370:ALA:N	2.33	0.44
1:G:438:VAL:O	1:G:442:VAL:HG23	2.17	0.44
1:H:266:THR:HG22	1:H:271:VAL:O	2.17	0.44
1:J:176:THR:HG21	1:J:333:ILE:HD11	1.99	0.44
1:J:319:GLN:HB3	1:J:336:VAL:HG21	1.98	0.44
1:K:202:PRO:O	1:K:204:PHE:N	2.48	0.44
1:K:87:ASP:O	1:K:499:VAL:HG23	2.17	0.44
1:L:193:MET:HE3	1:L:292:ILE:HG12	1.96	0.44
1:M:111:MET:SD	1:M:438:VAL:HG21	2.58	0.44
1:M:146:GLN:O	1:M:150:ILE:HG13	2.18	0.44
1:M:87:ASP:O	1:M:499:VAL:HG23	2.18	0.44
1:N:349:ILE:O	1:N:353:ILE:HG13	2.18	0.44
1:N:87:ASP:O	1:N:499:VAL:HG23	2.17	0.44
2:S:604:THR:HG22	2:S:605:THR:O	2.17	0.44
2:Y:602:TRP:NE1	2:Y:612:PRO:HG3	2.33	0.44
1:C:305:ILE:O	1:C:305:ILE:HG22	2.18	0.44
1:D:241:ALA:HA	1:D:271:VAL:HG22	1.99	0.44
1:F:231:ARG:NH1	2:T:612:PRO:O	2.51	0.44
1:F:68:ASN:O	1:F:72:GLN:HG2	2.17	0.44
1:H:201:SER:C	1:H:202:PRO:O	2.56	0.44
1:H:302:SER:H	1:H:307:MET:CE	2.30	0.44
1:J:139:SER:O	1:J:171:LYS:HE2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:183:LEU:O	1:N:184:GLN:CB	2.64	0.44
1:N:217:SER:N	1:N:218:PRO:CD	2.80	0.44
2:Q:604:THR:HG22	2:Q:605:THR:O	2.18	0.44
2:R:602:TRP:NE1	2:R:612:PRO:HG3	2.33	0.44
2:U:602:TRP:CE2	2:U:612:PRO:HG3	2.52	0.44
1:B:247:LEU:HD21	1:B:249:ILE:HD11	1.99	0.44
1:H:111:MET:SD	1:H:438:VAL:HG21	2.58	0.44
1:J:155:ASP:OD1	1:J:157:THR:HB	2.17	0.44
1:M:193:MET:HE3	1:M:292:ILE:HG12	1.98	0.44
1:B:217:SER:N	1:B:218:PRO:HD3	2.33	0.44
1:B:79:SER:HA	1:B:89:THR:HG22	2.00	0.44
1:C:198:GLY:HA3	1:C:328:ASP:HA	1.99	0.44
1:D:79:SER:HA	1:D:89:THR:CG2	2.48	0.44
1:F:202:PRO:O	1:F:204:PHE:N	2.45	0.44
1:F:218:PRO:HD2	1:F:320:ALA:O	2.18	0.44
1:G:291:ASP:OD2	1:G:368:ARG:HD2	2.18	0.44
1:K:199:TYR:CZ	1:K:327:LYS:HA	2.53	0.44
1:K:321:LYS:HD2	1:K:334:ASP:OD2	2.18	0.44
1:A:139:SER:O	1:A:171:LYS:HE2	2.17	0.43
1:A:231:ARG:NH1	2:O:612:PRO:O	2.51	0.43
1:E:186:GLU:HB2	1:E:380:LYS:HB2	1.99	0.43
1:F:95:LEU:O	1:F:99:ILE:HG13	2.17	0.43
1:G:245:LYS:HZ2	1:G:319:GLN:NE2	2.16	0.43
1:H:438:VAL:O	1:H:442:VAL:HG23	2.17	0.43
1:I:238:GLU:O	1:I:241:ALA:HB3	2.18	0.43
1:J:87:ASP:O	1:J:499:VAL:HG23	2.17	0.43
1:K:186:GLU:HB2	1:K:380:LYS:HB2	1.99	0.43
1:N:302:SER:H	1:N:307:MET:HE1	1.83	0.43
1:N:90:THR:O	1:N:94:VAL:HG13	2.17	0.43
2:W:602:TRP:CE2	2:W:612:PRO:HG3	2.53	0.43
1:A:369:VAL:HG23	1:A:370:ALA:N	2.33	0.43
1:D:155:ASP:OD1	1:D:157:THR:HB	2.18	0.43
1:D:266:THR:HG22	1:D:271:VAL:O	2.18	0.43
1:G:247:LEU:HD21	1:G:249:ILE:HD11	1.99	0.43
1:K:200:LEU:HD13	1:K:254:VAL:HB	1.99	0.43
1:L:198:GLY:HA3	1:L:328:ASP:HA	2.00	0.43
1:M:186:GLU:HB2	1:M:380:LYS:HB2	1.99	0.43
2:O:604:THR:HG22	2:O:605:THR:O	2.18	0.43
1:A:524:LEU:HD12	1:A:524:LEU:HA	1.85	0.43
1:B:218:PRO:HG3	1:B:323:VAL:HG13	2.00	0.43
1:D:193:MET:HG3	1:D:371:LYS:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:511:ALA:O	1:E:515:ILE:HG13	2.19	0.43
1:F:382:GLY:O	1:F:389:MET:HG2	2.17	0.43
1:H:425:LYS:HE2	3:H:1084:HOH:O	2.18	0.43
1:I:27:VAL:CG1	1:I:90:THR:HG23	2.48	0.43
1:J:176:THR:HG22	1:J:177:VAL:N	2.34	0.43
1:L:139:SER:O	1:L:171:LYS:HE2	2.18	0.43
1:L:241:ALA:HA	1:L:271:VAL:HG22	1.99	0.43
1:M:202:PRO:O	1:M:204:PHE:N	2.46	0.43
1:N:79:SER:HA	1:N:89:THR:HG22	1.99	0.43
2:X:604:THR:HG22	2:X:605:THR:O	2.18	0.43
1:B:200:LEU:O	1:B:201:SER:HB3	2.18	0.43
1:A:270:ILE:HG12	1:B:229:ASN:ND2	2.32	0.43
1:B:381:VAL:O	1:B:382:GLY:O	2.37	0.43
1:C:193:MET:HG3	1:C:371:LYS:HB3	2.00	0.43
1:C:42:LYS:HE3	1:C:48:THR:OG1	2.18	0.43
1:D:183:LEU:O	1:D:184:GLN:CB	2.66	0.43
1:D:264:VAL:O	1:D:268:ARG:HG3	2.18	0.43
1:E:230:ILE:CD1	1:E:261:THR:HB	2.47	0.43
1:E:42:LYS:HE3	1:E:48:THR:OG1	2.19	0.43
1:F:230:ILE:HD13	1:F:261:THR:HB	2.00	0.43
1:I:200:LEU:HD21	1:I:277:LYS:HG3	2.00	0.43
1:K:295:LEU:O	1:K:295:LEU:HD13	2.18	0.43
1:K:381:VAL:O	1:K:382:GLY:O	2.37	0.43
1:M:79:SER:HA	1:M:89:THR:HG22	2.00	0.43
2:Q:602:TRP:CE2	2:Q:612:PRO:HG3	2.53	0.43
1:A:247:LEU:HD21	1:A:249:ILE:HD11	2.00	0.43
1:A:199:TYR:CZ	1:A:327:LYS:HA	2.53	0.43
1:B:186:GLU:HB2	1:B:380:LYS:HB2	2.00	0.43
1:F:186:GLU:HB2	1:F:380:LYS:HB2	1.99	0.43
1:F:79:SER:HA	1:F:89:THR:CG2	2.48	0.43
1:I:496:PRO:HD2	1:I:499:VAL:CG1	2.48	0.43
1:J:444:LEU:HD23	1:J:447:MET:CE	2.49	0.43
1:L:230:ILE:HD13	1:L:261:THR:CB	2.49	0.43
1:N:182:GLY:O	1:N:183:LEU:O	2.37	0.43
1:A:201:SER:C	1:A:202:PRO:O	2.55	0.43
1:A:79:SER:HA	1:A:89:THR:CG2	2.49	0.43
1:D:193:MET:HG2	1:D:194:GLN:N	2.33	0.43
1:E:100:ILE:HD13	1:E:514:MET:HE2	2.01	0.43
1:E:171:LYS:H	1:E:171:LYS:HG2	1.68	0.43
1:E:200:LEU:HD13	1:E:254:VAL:HB	2.00	0.43
1:E:34:LYS:HG3	1:E:458:CYS:SG	2.59	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:193:MET:HG3	1:E:371:LYS:HB3	2.01	0.43
1:F:139:SER:O	1:F:171:LYS:HE2	2.18	0.43
1:I:202:PRO:O	1:I:203:TYR:CB	2.66	0.43
1:L:302:SER:H	1:L:307:MET:CE	2.31	0.43
1:M:200:LEU:HD12	1:M:275:ALA:CB	2.48	0.43
1:C:382:GLY:O	1:C:389:MET:HG2	2.18	0.43
1:D:438:VAL:O	1:D:442:VAL:HG23	2.18	0.43
1:D:451:LEU:HD22	1:D:455:VAL:HG23	2.00	0.43
1:E:19:GLY:HA3	1:E:67:GLU:O	2.19	0.43
1:G:177:VAL:HG21	1:G:397:GLU:HG3	2.00	0.43
1:H:131:LEU:HD13	1:H:422:VAL:HG21	2.00	0.43
1:I:111:MET:SD	1:I:438:VAL:HG21	2.59	0.43
1:J:438:VAL:O	1:J:442:VAL:HG23	2.18	0.43
1:K:218:PRO:HD2	1:K:320:ALA:O	2.19	0.43
1:L:438:VAL:O	1:L:442:VAL:HG23	2.17	0.43
1:M:176:THR:HG22	1:M:177:VAL:N	2.33	0.43
1:N:153:ASN:O	1:N:154:SER:HB2	2.19	0.43
1:N:230:ILE:HD13	1:N:261:THR:HB	2.00	0.43
2:Y:602:TRP:CE2	2:Y:612:PRO:HG3	2.53	0.43
1:D:68:ASN:O	1:D:72:GLN:HG2	2.18	0.43
1:E:414:GLY:N	1:E:494:LEU:HA	2.34	0.43
1:G:199:TYR:HA	1:G:276:VAL:HG12	2.01	0.43
1:H:291:ASP:OD2	1:H:368:ARG:HD2	2.19	0.43
1:J:201:SER:C	1:J:202:PRO:O	2.56	0.43
1:K:199:TYR:HA	1:K:276:VAL:HG12	2.01	0.43
1:L:202:PRO:O	1:L:204:PHE:N	2.44	0.43
1:N:171:LYS:HG2	1:N:171:LYS:H	1.68	0.43
1:A:230:ILE:HD13	1:A:261:THR:CB	2.48	0.43
1:C:25:ASP:HA	1:C:28:LYS:HE2	2.01	0.43
1:D:139:SER:O	1:D:171:LYS:HE2	2.19	0.43
1:H:230:ILE:HD13	1:H:261:THR:HG21	2.01	0.43
1:I:200:LEU:HG	1:I:276:VAL:HA	2.00	0.43
1:I:214:GLU:CD	1:I:322:ARG:HH21	2.22	0.43
1:M:201:SER:O	1:M:202:PRO:O	2.37	0.43
1:M:201:SER:C	1:M:202:PRO:O	2.57	0.43
1:N:25:ASP:HA	1:N:28:LYS:HE2	2.00	0.43
1:N:438:VAL:O	1:N:442:VAL:HG23	2.18	0.43
2:P:604:THR:HG22	2:P:605:THR:O	2.18	0.43
2:2:602:TRP:NE1	2:2:612:PRO:HG3	2.34	0.43
1:C:201:SER:O	1:C:202:PRO:O	2.36	0.43
1:D:214:GLU:CD	1:D:322:ARG:HH21	2.22	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:27:VAL:CG1	1:E:90:THR:HG23	2.49	0.43
1:F:230:ILE:CD1	1:F:261:THR:HB	2.49	0.43
1:H:381:VAL:O	1:H:382:GLY:O	2.37	0.43
1:L:201:SER:C	1:L:202:PRO:O	2.55	0.43
1:L:326:ASN:HB2	1:L:329:THR:HG22	2.01	0.43
1:L:321:LYS:HD2	1:L:334:ASP:OD2	2.18	0.43
1:L:381:VAL:O	1:L:382:GLY:O	2.37	0.43
1:N:146:GLN:O	1:N:150:ILE:HG13	2.18	0.43
1:B:16:MET:O	1:B:20:VAL:HG13	2.19	0.42
1:F:358:SER:O	1:F:362:ARG:HB2	2.19	0.42
1:H:16:MET:O	1:H:20:VAL:HG13	2.19	0.42
1:H:264:VAL:O	1:H:268:ARG:HG3	2.19	0.42
1:I:382:GLY:O	1:I:389:MET:HG2	2.18	0.42
1:J:214:GLU:CD	1:J:322:ARG:HH21	2.22	0.42
1:J:524:LEU:HD12	1:J:524:LEU:HA	1.87	0.42
1:K:65:LYS:HE3	1:K:522:THR:OG1	2.19	0.42
1:L:100:ILE:HD13	1:L:514:MET:HE2	2.01	0.42
1:M:95:LEU:O	1:M:99:ILE:HG13	2.19	0.42
2:2:604:THR:HG22	2:2:605:THR:O	2.19	0.42
1:A:264:VAL:O	1:A:268:ARG:HG3	2.18	0.42
1:A:42:LYS:HE3	1:A:48:THR:OG1	2.19	0.42
1:B:231:ARG:NH1	2:P:612:PRO:O	2.52	0.42
1:B:345:ARG:HG2	1:B:372:LEU:HD21	2.02	0.42
1:E:178:GLU:OE2	1:E:322:ARG:HD3	2.20	0.42
1:F:193:MET:HG2	1:F:194:GLN:N	2.34	0.42
1:F:444:LEU:HD23	1:F:447:MET:CE	2.49	0.42
1:G:186:GLU:HB2	1:G:380:LYS:HB2	2.01	0.42
1:H:200:LEU:HD21	1:H:277:LYS:HG3	2.00	0.42
1:I:79:SER:HA	1:I:89:THR:CG2	2.48	0.42
1:J:264:VAL:O	1:J:268:ARG:HG3	2.19	0.42
1:J:245:LYS:NZ	1:J:319:GLN:NE2	2.66	0.42
1:J:79:SER:HA	1:J:89:THR:CG2	2.49	0.42
1:J:79:SER:HA	1:J:89:THR:HG22	2.01	0.42
1:L:131:LEU:HD13	1:L:422:VAL:HG21	2.00	0.42
1:L:176:THR:HG22	1:L:177:VAL:N	2.34	0.42
1:L:222:LEU:HD23	1:L:250:ILE:HB	2.01	0.42
1:M:139:SER:O	1:M:171:LYS:HE2	2.19	0.42
1:M:230:ILE:HD13	1:M:261:THR:CB	2.50	0.42
1:M:296:THR:HB	1:M:319:GLN:H	1.83	0.42
1:G:261:THR:HG23	2:U:610:LEU:O	2.19	0.42
1:A:221:LEU:HD23	1:A:249:ILE:CD1	2.47	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:GLU:HB2	1:A:380:LYS:HB2	2.01	0.42
1:B:183:LEU:O	1:B:184:GLN:CB	2.64	0.42
1:C:79:SER:HA	1:C:89:THR:CG2	2.49	0.42
1:D:186:GLU:HB2	1:D:380:LYS:HB2	2.01	0.42
1:D:199:TYR:HA	1:D:276:VAL:HG12	2.01	0.42
1:D:42:LYS:HE3	1:D:48:THR:OG1	2.19	0.42
1:D:22:VAL:HG11	1:D:62:LEU:HD21	2.00	0.42
1:E:230:ILE:HD13	1:E:261:THR:HG21	2.00	0.42
1:F:79:SER:HA	1:F:89:THR:HG22	2.00	0.42
1:G:176:THR:HG22	1:G:177:VAL:N	2.34	0.42
1:H:202:PRO:O	1:H:204:PHE:N	2.46	0.42
1:K:524:LEU:HD12	1:K:524:LEU:HA	1.87	0.42
1:K:27:VAL:CG1	1:K:90:THR:HG23	2.49	0.42
1:L:171:LYS:H	1:L:171:LYS:HG2	1.68	0.42
1:L:524:LEU:HA	1:L:524:LEU:HD12	1.88	0.42
1:N:266:THR:HG22	1:N:271:VAL:O	2.19	0.42
1:N:95:LEU:O	1:N:99:ILE:HG13	2.20	0.42
1:B:230:ILE:HD13	1:B:261:THR:HB	2.00	0.42
1:C:524:LEU:HA	1:C:524:LEU:HD12	1.89	0.42
1:D:245:LYS:NZ	1:D:319:GLN:NE2	2.67	0.42
1:H:240:VAL:HG11	1:H:247:LEU:HB2	2.00	0.42
1:H:383:ALA:CB	1:I:281:PHE:CZ	2.96	0.42
1:M:218:PRO:CB	1:M:246:PRO:HG2	2.46	0.42
1:M:193:MET:HG3	1:M:371:LYS:HB3	2.01	0.42
1:N:372:LEU:HA	1:N:372:LEU:HD12	1.87	0.42
1:G:271:VAL:HG21	2:U:607:TRP:HZ3	1.83	0.42
1:A:336:VAL:O	1:A:337:GLY:C	2.56	0.42
1:B:139:SER:O	1:B:171:LYS:HE2	2.20	0.42
1:C:214:GLU:CD	1:C:322:ARG:HH21	2.23	0.42
1:E:201:SER:O	1:E:202:PRO:O	2.38	0.42
1:E:245:LYS:HZ3	1:E:319:GLN:HE21	1.68	0.42
1:E:336:VAL:O	1:E:337:GLY:C	2.58	0.42
1:E:358:SER:O	1:E:362:ARG:HB2	2.19	0.42
1:F:153:ASN:O	1:F:154:SER:HB2	2.20	0.42
1:F:366:GLN:O	1:F:369:VAL:HG22	2.20	0.42
1:F:383:ALA:O	1:F:384:ALA:CB	2.68	0.42
1:H:217:SER:N	1:H:218:PRO:HD3	2.34	0.42
1:J:25:ASP:HA	1:J:28:LYS:HE2	2.00	0.42
1:K:266:THR:HG22	1:K:271:VAL:O	2.20	0.42
1:K:438:VAL:O	1:K:442:VAL:HG23	2.19	0.42
1:N:100:ILE:HD13	1:N:514:MET:CE	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:218:PRO:HD2	1:N:320:ALA:O	2.19	0.42
1:N:336:VAL:O	1:N:337:GLY:C	2.58	0.42
1:A:111:MET:SD	1:A:438:VAL:HG21	2.60	0.42
1:B:201:SER:O	1:B:202:PRO:O	2.37	0.42
1:B:221:LEU:HD23	1:B:249:ILE:CD1	2.47	0.42
1:B:79:SER:HA	1:B:89:THR:CG2	2.49	0.42
1:C:369:VAL:HG23	1:C:370:ALA:N	2.35	0.42
1:D:171:LYS:H	1:D:171:LYS:HG2	1.68	0.42
1:D:79:SER:HA	1:D:89:THR:HG22	2.01	0.42
1:E:199:TYR:CZ	1:E:327:LYS:HA	2.55	0.42
1:E:79:SER:HA	1:E:89:THR:CG2	2.48	0.42
1:H:181:THR:HB	1:I:283:ASP:OD2	2.20	0.42
1:H:319:GLN:HB3	1:H:336:VAL:HG21	2.00	0.42
1:H:382:GLY:O	1:H:389:MET:HG2	2.19	0.42
1:I:25:ASP:HA	1:I:28:LYS:HE2	2.00	0.42
1:I:42:LYS:HE3	1:I:48:THR:OG1	2.19	0.42
1:I:63:GLU:OE1	1:J:524:LEU:HD21	2.20	0.42
1:L:349:ILE:O	1:L:353:ILE:HG13	2.20	0.42
1:L:42:LYS:HE3	1:L:48:THR:OG1	2.20	0.42
1:M:185:ASP:OD1	1:M:382:GLY:N	2.47	0.42
1:M:524:LEU:HA	1:M:524:LEU:HD12	1.86	0.42
1:N:230:ILE:CD1	1:N:261:THR:HB	2.50	0.42
2:1:604:THR:HG22	2:1:605:THR:O	2.20	0.42
1:A:219:PHE:HB3	1:A:317:LEU:HD23	2.02	0.42
1:A:383:ALA:O	1:A:384:ALA:CB	2.66	0.42
1:C:146:GLN:O	1:C:150:ILE:HG13	2.20	0.42
1:C:28:LYS:HB2	1:C:453:GLN:HG2	2.02	0.42
1:E:369:VAL:HG23	1:E:370:ALA:N	2.35	0.42
1:G:302:SER:H	1:G:307:MET:CE	2.32	0.42
1:G:42:LYS:HE3	1:G:48:THR:OG1	2.19	0.42
1:H:245:LYS:HZ2	1:H:319:GLN:NE2	2.18	0.42
1:I:319:GLN:HB3	1:I:336:VAL:HG21	2.00	0.42
1:I:438:VAL:O	1:I:442:VAL:HG23	2.19	0.42
1:J:382:GLY:O	1:J:389:MET:HG2	2.18	0.42
1:J:111:MET:SD	1:J:438:VAL:HG21	2.60	0.42
1:K:233:MET:HB3	1:K:233:MET:HE3	1.93	0.42
1:M:131:LEU:HD13	1:M:422:VAL:HG21	2.01	0.42
1:A:217:SER:N	1:A:218:PRO:HD3	2.35	0.42
1:F:319:GLN:HB3	1:F:336:VAL:HG21	2.02	0.42
1:G:200:LEU:HD21	1:G:277:LYS:HG3	2.02	0.42
1:G:201:SER:O	1:G:202:PRO:O	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:176:THR:HG22	1:H:177:VAL:N	2.35	0.42
1:I:414:GLY:N	1:I:494:LEU:HA	2.35	0.42
1:K:218:PRO:CB	1:K:246:PRO:HG2	2.49	0.42
1:K:247:LEU:HD21	1:K:249:ILE:HD11	2.01	0.42
1:K:42:LYS:HE3	1:K:48:THR:OG1	2.20	0.42
1:L:296:THR:HB	1:L:319:GLN:H	1.84	0.42
1:L:186:GLU:HB2	1:L:380:LYS:HB2	2.01	0.42
1:N:217:SER:N	1:N:218:PRO:HD3	2.35	0.42
1:N:199:TYR:CZ	1:N:327:LYS:HA	2.54	0.42
1:N:186:GLU:HB2	1:N:380:LYS:HB2	2.01	0.42
1:N:34:LYS:HG3	1:N:458:CYS:SG	2.59	0.42
1:B:500:THR:HB	3:B:1206:HOH:O	2.20	0.42
1:D:349:ILE:O	1:D:353:ILE:HG13	2.20	0.42
1:D:95:LEU:O	1:D:99:ILE:HG13	2.20	0.42
1:G:350:ARG:O	1:G:354:GLU:HG2	2.19	0.42
1:H:369:VAL:HG23	1:H:370:ALA:N	2.35	0.42
1:H:42:LYS:HE3	1:H:48:THR:OG1	2.20	0.42
1:L:200:LEU:HD21	1:L:277:LYS:HG3	2.01	0.42
1:L:271:VAL:HG21	2:Z:607:TRP:CZ3	2.52	0.42
1:L:90:THR:O	1:L:94:VAL:HG13	2.20	0.42
1:N:202:PRO:O	1:N:204:PHE:N	2.42	0.42
1:N:302:SER:H	1:N:307:MET:CE	2.33	0.42
1:D:271:VAL:CG2	2:R:607:TRP:HZ3	2.30	0.42
1:B:230:ILE:CD1	1:B:261:THR:HB	2.50	0.42
1:C:202:PRO:O	1:C:204:PHE:N	2.45	0.42
1:C:217:SER:N	1:C:218:PRO:HD3	2.35	0.42
1:C:79:SER:HA	1:C:89:THR:HG22	2.02	0.42
1:D:100:ILE:HD13	1:D:514:MET:HE2	2.02	0.42
1:E:176:THR:HG22	1:E:177:VAL:N	2.35	0.42
1:E:230:ILE:HD13	1:E:261:THR:CB	2.50	0.42
1:E:302:SER:H	1:E:307:MET:HE1	1.85	0.42
1:G:218:PRO:HD2	1:G:320:ALA:O	2.20	0.42
1:H:139:SER:O	1:H:171:LYS:HE2	2.20	0.42
1:I:200:LEU:HD13	1:I:254:VAL:HB	2.00	0.42
1:I:245:LYS:NZ	1:I:319:GLN:NE2	2.68	0.42
1:I:144:ILE:HG23	1:I:403:THR:CG2	2.50	0.42
1:J:302:SER:H	1:J:307:MET:HE3	1.84	0.42
1:J:358:SER:O	1:J:362:ARG:HB2	2.20	0.42
1:J:19:GLY:HA3	1:J:67:GLU:O	2.19	0.42
1:J:63:GLU:OE1	1:K:524:LEU:HD21	2.20	0.42
1:M:183:LEU:O	1:M:184:GLN:CB	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:42:LYS:HE3	1:M:48:THR:OG1	2.20	0.42
1:M:270:ILE:HG12	1:N:229:ASN:ND2	2.34	0.42
2:2:602:TRP:CE2	2:2:612:PRO:HG3	2.55	0.41
1:A:153:ASN:O	1:A:154:SER:HB2	2.20	0.41
1:A:383:ALA:HB1	1:B:281:PHE:HZ	1.85	0.41
1:C:366:GLN:O	1:C:369:VAL:HG22	2.20	0.41
1:D:131:LEU:HD12	1:D:131:LEU:HA	1.95	0.41
1:F:177:VAL:HG21	1:F:397:GLU:HG3	2.02	0.41
1:G:139:SER:O	1:G:171:LYS:HE2	2.19	0.41
1:G:230:ILE:CD1	1:G:261:THR:HB	2.49	0.41
1:H:230:ILE:HD13	1:H:261:THR:CB	2.50	0.41
1:H:414:GLY:N	1:H:494:LEU:HA	2.35	0.41
1:I:153:ASN:O	1:I:154:SER:HB2	2.20	0.41
1:I:201:SER:C	1:I:202:PRO:O	2.58	0.41
1:I:524:LEU:HA	1:I:524:LEU:HD12	1.87	0.41
1:J:186:GLU:HB2	1:J:380:LYS:HB2	2.01	0.41
1:J:200:LEU:HD13	1:J:254:VAL:HB	2.01	0.41
1:J:381:VAL:O	1:J:382:GLY:O	2.38	0.41
1:J:383:ALA:O	1:J:384:ALA:CB	2.67	0.41
1:K:176:THR:HG22	1:K:177:VAL:N	2.35	0.41
1:L:183:LEU:O	1:L:184:GLN:CB	2.67	0.41
1:M:319:GLN:HB3	1:M:336:VAL:HG21	2.01	0.41
1:M:438:VAL:O	1:M:442:VAL:HG23	2.19	0.41
1:E:270:ILE:CD1	2:S:608:GLY:HA3	2.50	0.41
1:C:381:VAL:O	1:C:382:GLY:O	2.38	0.41
1:D:270:ILE:O	1:D:271:VAL:HB	2.20	0.41
1:D:482:THR:O	1:D:484:GLU:HG2	2.20	0.41
1:F:193:MET:HG3	1:F:371:LYS:HB3	2.02	0.41
1:F:240:VAL:HG11	1:F:247:LEU:HB2	2.01	0.41
1:F:321:LYS:HD2	1:F:334:ASP:OD2	2.20	0.41
1:H:524:LEU:HA	1:H:524:LEU:HD12	1.84	0.41
1:J:270:ILE:HD13	2:X:608:GLY:HA3	2.02	0.41
1:K:242:LYS:C	1:K:244:GLY:N	2.73	0.41
1:K:25:ASP:HA	1:K:28:LYS:HE2	2.01	0.41
1:K:68:ASN:O	1:K:72:GLN:HG2	2.21	0.41
1:L:217:SER:N	1:L:218:PRO:HD3	2.35	0.41
1:L:358:SER:O	1:L:362:ARG:HB2	2.21	0.41
2:O:602:TRP:NE1	2:O:612:PRO:HG3	2.35	0.41
2:R:604:THR:HG22	2:R:605:THR:O	2.21	0.41
1:A:270:ILE:O	1:A:271:VAL:HB	2.20	0.41
1:A:193:MET:HG3	1:A:371:LYS:HB3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:LYS:HG3	1:G:59:GLU:O	2.21	0.41
1:B:202:PRO:C	1:B:204:PHE:N	2.73	0.41
1:B:369:VAL:HG23	1:B:370:ALA:N	2.35	0.41
1:C:230:ILE:CD1	1:C:261:THR:HB	2.51	0.41
1:D:201:SER:C	1:D:202:PRO:O	2.59	0.41
1:D:219:PHE:HB3	1:D:317:LEU:HD23	2.01	0.41
1:E:326:ASN:HB2	1:E:329:THR:HG22	2.02	0.41
1:G:382:GLY:O	1:G:389:MET:HG2	2.20	0.41
1:H:201:SER:O	1:H:202:PRO:O	2.37	0.41
1:I:176:THR:HG22	1:I:177:VAL:N	2.35	0.41
1:H:268:ARG:O	1:I:257:GLU:HG2	2.20	0.41
1:J:22:VAL:HG11	1:J:62:LEU:HD21	2.02	0.41
1:L:242:LYS:C	1:L:244:GLY:N	2.73	0.41
1:L:25:ASP:HA	1:L:28:LYS:HE2	2.02	0.41
1:L:444:LEU:HD23	1:L:447:MET:HE1	2.02	0.41
1:N:270:ILE:O	1:N:271:VAL:HB	2.21	0.41
1:N:369:VAL:HG23	1:N:370:ALA:N	2.35	0.41
1:A:79:SER:HA	1:A:89:THR:HG22	2.02	0.41
1:D:202:PRO:O	1:D:204:PHE:N	2.48	0.41
1:D:217:SER:N	1:D:218:PRO:HD3	2.35	0.41
1:D:242:LYS:C	1:D:244:GLY:N	2.74	0.41
1:E:79:SER:HA	1:E:89:THR:HG22	2.02	0.41
1:F:200:LEU:HD21	1:F:277:LYS:HG3	2.02	0.41
1:G:230:ILE:HD13	1:G:261:THR:HB	2.03	0.41
1:H:193:MET:HE3	1:H:292:ILE:HG12	2.02	0.41
1:H:287:ALA:HB1	1:H:368:ARG:NH1	2.35	0.41
1:J:217:SER:N	1:J:218:PRO:HD3	2.35	0.41
1:K:349:ILE:O	1:K:353:ILE:HG13	2.21	0.41
1:M:336:VAL:O	1:M:337:GLY:C	2.59	0.41
1:M:358:SER:O	1:M:362:ARG:HB2	2.20	0.41
1:M:383:ALA:O	1:M:384:ALA:CB	2.68	0.41
1:N:305:ILE:HD12	1:N:307:MET:HE2	2.02	0.41
1:N:296:THR:HB	1:N:319:GLN:H	1.84	0.41
1:H:270:ILE:CD1	2:V:608:GLY:HA3	2.49	0.41
1:B:242:LYS:O	1:B:243:ALA:CB	2.69	0.41
1:C:358:SER:O	1:C:362:ARG:HB2	2.20	0.41
1:E:383:ALA:O	1:E:384:ALA:CB	2.69	0.41
1:G:123:ALA:HA	1:G:429:LEU:CD2	2.51	0.41
1:G:201:SER:C	1:G:202:PRO:O	2.59	0.41
1:H:46:ALA:HB2	1:I:76:GLU:CG	2.49	0.41
1:J:16:MET:O	1:J:20:VAL:HG13	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:358:SER:O	1:K:362:ARG:HB2	2.21	0.41
1:N:139:SER:O	1:N:171:LYS:HE2	2.19	0.41
1:N:382:GLY:O	1:N:389:MET:HG2	2.20	0.41
1:B:42:LYS:HE3	1:B:48:THR:OG1	2.20	0.41
1:C:131:LEU:HD13	1:C:422:VAL:HG21	2.03	0.41
1:C:202:PRO:O	1:C:203:TYR:CB	2.67	0.41
1:C:16:MET:O	1:C:20:VAL:HG13	2.20	0.41
1:C:221:LEU:HD23	1:C:249:ILE:CD1	2.48	0.41
1:D:100:ILE:HD13	1:D:514:MET:CE	2.50	0.41
1:D:111:MET:SD	1:D:438:VAL:HG21	2.61	0.41
1:D:369:VAL:HG23	1:D:370:ALA:N	2.36	0.41
1:F:349:ILE:O	1:F:353:ILE:HG13	2.21	0.41
1:G:218:PRO:HG3	1:G:323:VAL:HG13	2.02	0.41
1:G:87:ASP:O	1:G:499:VAL:HG23	2.20	0.41
1:H:218:PRO:CB	1:H:246:PRO:HG2	2.50	0.41
1:I:270:ILE:O	1:I:271:VAL:HB	2.21	0.41
1:I:511:ALA:O	1:I:515:ILE:HG13	2.20	0.41
1:J:242:LYS:C	1:J:244:GLY:N	2.74	0.41
1:K:270:ILE:O	1:K:271:VAL:HB	2.20	0.41
1:K:336:VAL:O	1:K:337:GLY:C	2.58	0.41
1:K:123:ALA:HA	1:K:429:LEU:CD2	2.50	0.41
1:M:199:TYR:CZ	1:M:327:LYS:HA	2.55	0.41
1:B:366:GLN:O	1:B:369:VAL:HG22	2.21	0.41
1:C:183:LEU:O	1:C:184:GLN:CB	2.66	0.41
1:D:202:PRO:O	1:D:203:TYR:CB	2.66	0.41
1:D:25:ASP:HA	1:D:28:LYS:HE2	2.03	0.41
1:D:358:SER:O	1:D:362:ARG:HB2	2.21	0.41
1:D:383:ALA:O	1:D:384:ALA:CB	2.67	0.41
1:D:38:VAL:HG22	1:E:519:CYS:HB3	2.03	0.41
1:D:19:GLY:HA3	1:D:67:GLU:O	2.20	0.41
1:F:193:MET:HE3	1:F:292:ILE:HG12	2.00	0.41
1:F:19:GLY:HA3	1:F:67:GLU:O	2.20	0.41
1:G:202:PRO:C	1:G:204:PHE:N	2.74	0.41
1:I:186:GLU:HB2	1:I:380:LYS:HB2	2.02	0.41
1:I:34:LYS:HG3	1:I:458:CYS:SG	2.61	0.41
1:I:87:ASP:O	1:I:499:VAL:HG23	2.20	0.41
1:J:90:THR:O	1:J:94:VAL:HG13	2.20	0.41
1:K:296:THR:HB	1:K:319:GLN:H	1.86	0.41
1:C:95:LEU:O	1:C:99:ILE:HG13	2.20	0.41
1:D:444:LEU:HD23	1:D:447:MET:CE	2.50	0.41
1:E:221:LEU:HD23	1:E:249:ILE:CD1	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:199:TYR:CZ	1:F:327:LYS:HA	2.56	0.41
1:G:16:MET:HB3	1:G:514:MET:CE	2.51	0.41
1:I:123:ALA:HA	1:I:429:LEU:CD2	2.51	0.41
1:I:242:LYS:O	1:I:243:ALA:CB	2.69	0.41
1:J:202:PRO:O	1:J:204:PHE:N	2.48	0.41
1:L:153:ASN:O	1:L:154:SER:HB2	2.21	0.41
1:M:171:LYS:H	1:M:171:LYS:HG2	1.69	0.41
1:N:177:VAL:HG21	1:N:397:GLU:HG3	2.03	0.41
2:O:602:TRP:CE2	2:O:612:PRO:HG3	2.55	0.41
1:A:451:LEU:HD22	1:A:455:VAL:HG23	2.02	0.41
1:A:95:LEU:O	1:A:99:ILE:HG13	2.21	0.41
1:B:201:SER:C	1:B:202:PRO:O	2.58	0.41
1:C:455:VAL:CG1	1:C:460:GLU:HB2	2.50	0.41
1:D:524:LEU:HD12	1:D:524:LEU:HA	1.88	0.41
1:E:242:LYS:C	1:E:244:GLY:N	2.74	0.41
1:F:201:SER:HB3	1:F:259:LEU:HD21	2.02	0.41
1:G:336:VAL:O	1:G:337:GLY:C	2.59	0.41
1:H:100:ILE:HD13	1:H:514:MET:CE	2.51	0.41
1:I:350:ARG:O	1:I:354:GLU:HG2	2.21	0.41
1:J:350:ARG:O	1:J:354:GLU:HG2	2.21	0.41
1:K:193:MET:HG3	1:K:371:LYS:HB3	2.02	0.41
1:J:38:VAL:HG22	1:K:519:CYS:HB3	2.03	0.41
1:L:16:MET:O	1:L:20:VAL:HG13	2.21	0.41
2:T:604:THR:HG22	2:T:605:THR:O	2.20	0.41
2:V:604:THR:HG22	2:V:605:THR:O	2.21	0.41
1:A:381:VAL:O	1:A:382:GLY:O	2.39	0.41
1:A:438:VAL:O	1:A:442:VAL:HG23	2.20	0.41
1:C:103:GLY:O	1:C:107:VAL:HG23	2.19	0.41
1:C:111:MET:SD	1:C:438:VAL:HG21	2.61	0.41
1:C:414:GLY:N	1:C:494:LEU:HA	2.36	0.41
1:C:87:ASP:O	1:C:499:VAL:HG23	2.20	0.41
1:D:153:ASN:O	1:D:154:SER:HB2	2.21	0.41
1:D:221:LEU:HD23	1:D:249:ILE:CD1	2.49	0.41
1:E:201:SER:C	1:E:202:PRO:O	2.59	0.41
1:F:200:LEU:HD13	1:F:254:VAL:HB	2.02	0.41
1:J:176:THR:HG21	1:J:333:ILE:CD1	2.51	0.41
1:K:214:GLU:CD	1:K:322:ARG:HH21	2.24	0.41
1:K:100:ILE:HD13	1:K:514:MET:CE	2.51	0.41
1:L:199:TYR:CZ	1:L:327:LYS:HA	2.56	0.41
1:M:123:ALA:HA	1:M:429:LEU:CD2	2.51	0.41
1:N:383:ALA:O	1:N:384:ALA:CB	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:482:THR:O	1:N:484:GLU:HG2	2.21	0.41
1:B:271:VAL:HG21	2:P:607:TRP:HZ3	1.86	0.41
1:A:519:CYS:HB3	1:G:38:VAL:HG22	2.03	0.41
1:B:270:ILE:O	1:B:271:VAL:HB	2.21	0.41
1:C:349:ILE:O	1:C:353:ILE:HG13	2.21	0.41
1:C:372:LEU:HD12	1:C:372:LEU:HA	1.93	0.41
1:D:336:VAL:O	1:D:337:GLY:C	2.58	0.41
1:E:25:ASP:HA	1:E:28:LYS:HE2	2.03	0.41
1:E:382:GLY:O	1:E:389:MET:HG2	2.21	0.41
1:F:201:SER:C	1:F:202:PRO:O	2.60	0.41
1:G:25:ASP:HA	1:G:28:LYS:HE2	2.02	0.41
1:H:34:LYS:HG3	1:H:458:CYS:SG	2.60	0.41
1:I:372:LEU:HA	1:I:372:LEU:HD12	1.91	0.41
1:J:183:LEU:O	1:J:184:GLN:CB	2.66	0.41
1:J:240:VAL:O	1:J:242:LYS:O	2.38	0.41
1:L:233:MET:HB3	1:L:233:MET:HE3	1.93	0.41
1:M:302:SER:H	1:M:307:MET:HE1	1.85	0.41
1:N:264:VAL:O	1:N:268:ARG:HG3	2.21	0.41
1:N:381:VAL:O	1:N:382:GLY:O	2.39	0.41
1:A:77:VAL:CG2	1:A:510:VAL:HB	2.48	0.40
1:C:144:ILE:HG23	1:C:403:THR:CG2	2.51	0.40
1:D:245:LYS:HZ2	1:D:319:GLN:NE2	2.19	0.40
1:A:229:ASN:HD22	1:G:270:ILE:HA	1.83	0.40
1:G:296:THR:HB	1:G:319:GLN:H	1.85	0.40
1:G:511:ALA:O	1:G:515:ILE:HG13	2.20	0.40
1:H:202:PRO:C	1:H:204:PHE:N	2.74	0.40
1:H:200:LEU:HD13	1:H:254:VAL:HB	2.02	0.40
1:J:177:VAL:HG21	1:J:397:GLU:HG3	2.02	0.40
1:J:19:GLY:HA2	1:J:62:LEU:CD1	2.51	0.40
1:M:19:GLY:HA3	1:M:67:GLU:O	2.20	0.40
1:M:349:ILE:O	1:M:353:ILE:HG13	2.20	0.40
1:M:369:VAL:HG23	1:M:370:ALA:N	2.36	0.40
1:M:511:ALA:O	1:M:515:ILE:HG13	2.21	0.40
1:B:270:ILE:CD1	2:P:608:GLY:HA3	2.51	0.40
1:C:222:LEU:HD23	1:C:250:ILE:HB	2.03	0.40
1:C:444:LEU:HD23	1:C:447:MET:CE	2.50	0.40
1:G:152:ALA:O	1:G:153:ASN:HB3	2.21	0.40
1:G:111:MET:SD	1:G:438:VAL:HG21	2.62	0.40
1:G:444:LEU:HD23	1:G:447:MET:CE	2.52	0.40
1:G:95:LEU:O	1:G:99:ILE:HG13	2.21	0.40
1:L:511:ALA:O	1:L:515:ILE:HG13	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:200:LEU:HD21	1:N:277:LYS:HG3	2.03	0.40
2:U:604:THR:HG22	2:U:605:THR:O	2.21	0.40
1:A:358:SER:O	1:A:362:ARG:HB2	2.21	0.40
1:A:382:GLY:O	1:A:389:MET:HG2	2.21	0.40
1:A:414:GLY:N	1:A:494:LEU:HA	2.36	0.40
1:B:296:THR:HB	1:B:319:GLN:H	1.86	0.40
1:B:324:VAL:HB	1:B:331:THR:HG23	2.03	0.40
1:B:444:LEU:HD23	1:B:447:MET:CE	2.52	0.40
1:B:68:ASN:O	1:B:72:GLN:HG2	2.22	0.40
1:C:171:LYS:H	1:C:171:LYS:HG2	1.70	0.40
1:D:222:LEU:HD23	1:D:250:ILE:HB	2.03	0.40
1:D:34:LYS:HG3	1:D:458:CYS:SG	2.61	0.40
1:D:46:ALA:HB2	1:E:76:GLU:CG	2.51	0.40
1:E:131:LEU:HD21	1:E:500:THR:HG22	2.03	0.40
1:E:177:VAL:HG21	1:E:397:GLU:HG3	2.03	0.40
1:F:291:ASP:OD2	1:F:368:ARG:HD2	2.20	0.40
1:F:524:LEU:HA	1:F:524:LEU:HD12	1.88	0.40
1:I:16:MET:HB3	1:I:514:MET:CE	2.52	0.40
1:I:201:SER:O	1:I:202:PRO:O	2.39	0.40
1:I:336:VAL:O	1:I:337:GLY:C	2.58	0.40
1:K:242:LYS:O	1:K:243:ALA:CB	2.70	0.40
1:K:271:VAL:HG21	2:Y:607:TRP:CZ3	2.55	0.40
1:K:444:LEU:HD23	1:K:447:MET:CE	2.52	0.40
1:M:266:THR:HG22	1:M:271:VAL:O	2.21	0.40
1:M:444:LEU:HD23	1:M:447:MET:CE	2.50	0.40
1:A:511:ALA:O	1:A:515:ILE:HG13	2.22	0.40
1:B:214:GLU:CD	1:B:322:ARG:HH21	2.25	0.40
1:C:296:THR:HB	1:C:319:GLN:H	1.87	0.40
1:C:319:GLN:HB3	1:C:336:VAL:HG21	2.03	0.40
1:D:218:PRO:HG3	1:D:323:VAL:HG13	2.03	0.40
1:D:123:ALA:HA	1:D:429:LEU:CD2	2.51	0.40
1:F:414:GLY:N	1:F:494:LEU:HA	2.37	0.40
1:G:302:SER:H	1:G:307:MET:HE1	1.87	0.40
1:G:199:TYR:CZ	1:G:327:LYS:HA	2.56	0.40
1:H:174:VAL:HB	1:H:376:VAL:HG22	2.04	0.40
1:H:271:VAL:HG12	1:H:273:VAL:CG2	2.52	0.40
1:I:218:PRO:CB	1:I:246:PRO:HG2	2.51	0.40
1:I:270:ILE:HA	1:J:229:ASN:HD22	1.84	0.40
1:J:336:VAL:O	1:J:337:GLY:C	2.58	0.40
1:J:123:ALA:HA	1:J:429:LEU:CD2	2.52	0.40
1:J:414:GLY:N	1:J:494:LEU:HA	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:383:ALA:O	1:K:384:ALA:CB	2.68	0.40
1:K:494:LEU:O	1:K:494:LEU:HD12	2.21	0.40
1:L:366:GLN:O	1:L:369:VAL:HG22	2.22	0.40
1:N:473:ASP:HB2	3:N:1053:HOH:O	2.20	0.40
1:A:245:LYS:HZ2	1:A:319:GLN:NE2	2.20	0.40
1:D:459:GLY:HA3	1:E:112:ASN:ND2	2.36	0.40
1:F:233:MET:HB3	1:F:233:MET:HE3	1.95	0.40
1:F:34:LYS:HG3	1:F:458:CYS:SG	2.61	0.40
1:G:200:LEU:HD13	1:G:254:VAL:HB	2.03	0.40
1:H:350:ARG:O	1:H:354:GLU:HG2	2.21	0.40
1:I:174:VAL:HB	1:I:376:VAL:HG22	2.03	0.40
1:I:219:PHE:HB3	1:I:317:LEU:HD23	2.04	0.40
1:H:26:ALA:HA	1:I:8:PHE:HE1	1.85	0.40
1:J:345:ARG:HG2	1:J:372:LEU:HD21	2.03	0.40
1:K:131:LEU:HA	1:K:131:LEU:HD12	1.92	0.40
1:K:183:LEU:O	1:K:184:GLN:CB	2.66	0.40
1:K:200:LEU:HD12	1:K:275:ALA:CB	2.52	0.40
1:K:270:ILE:HA	1:L:229:ASN:ND2	2.36	0.40
1:K:28:LYS:HB2	1:K:453:GLN:HG2	2.04	0.40
1:K:34:LYS:HG3	1:K:458:CYS:SG	2.62	0.40
1:L:46:ALA:HB2	1:M:76:GLU:CG	2.49	0.40
1:N:366:GLN:O	1:N:369:VAL:HG22	2.22	0.40
1:N:28:LYS:HD2	1:N:453:GLN:NE2	2.37	0.40
1:N:131:LEU:HD21	1:N:500:THR:HG22	2.04	0.40

All (3) 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)
1:G:354:GLU:OE1	1:J:432:GLN:O[2_655]	1.90	0.30
1:H:166:MET:O	1:L:359:ASP:OD2[1_455]	2.13	0.07
1:C:316:ASP:OD1	1:J:311:LYS:NZ[1_554]	2.13	0.07

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	523/547 (96%)	495 (95%)	16 (3%)	12 (2%)	6	30
1	B	523/547 (96%)	496 (95%)	15 (3%)	12 (2%)	6	30
1	C	523/547 (96%)	493 (94%)	18 (3%)	12 (2%)	6	30
1	D	523/547 (96%)	494 (94%)	17 (3%)	12 (2%)	6	30
1	E	523/547 (96%)	495 (95%)	16 (3%)	12 (2%)	6	30
1	F	523/547 (96%)	492 (94%)	19 (4%)	12 (2%)	6	30
1	G	523/547 (96%)	495 (95%)	17 (3%)	11 (2%)	7	33
1	H	523/547 (96%)	495 (95%)	17 (3%)	11 (2%)	7	33
1	I	523/547 (96%)	494 (94%)	17 (3%)	12 (2%)	6	30
1	J	523/547 (96%)	493 (94%)	18 (3%)	12 (2%)	6	30
1	K	523/547 (96%)	494 (94%)	17 (3%)	12 (2%)	6	30
1	L	523/547 (96%)	494 (94%)	17 (3%)	12 (2%)	6	30
1	M	523/547 (96%)	495 (95%)	16 (3%)	12 (2%)	6	30
1	N	523/547 (96%)	495 (95%)	16 (3%)	12 (2%)	6	30
2	1	10/12 (83%)	10 (100%)	0	0	100	100
2	2	10/12 (83%)	10 (100%)	0	0	100	100
2	O	10/12 (83%)	10 (100%)	0	0	100	100
2	P	10/12 (83%)	10 (100%)	0	0	100	100
2	Q	10/12 (83%)	10 (100%)	0	0	100	100
2	R	10/12 (83%)	10 (100%)	0	0	100	100
2	S	10/12 (83%)	10 (100%)	0	0	100	100
2	T	10/12 (83%)	10 (100%)	0	0	100	100
2	U	10/12 (83%)	10 (100%)	0	0	100	100
2	V	10/12 (83%)	10 (100%)	0	0	100	100
2	W	10/12 (83%)	10 (100%)	0	0	100	100
2	X	10/12 (83%)	10 (100%)	0	0	100	100
2	Y	10/12 (83%)	10 (100%)	0	0	100	100
2	Z	10/12 (83%)	10 (100%)	0	0	100	100
All	All	7462/7826 (95%)	7060 (95%)	236 (3%)	166 (2%)	6	31

All (166) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	183	LEU
1	B	183	LEU
1	C	183	LEU
1	D	183	LEU
1	E	183	LEU
1	F	183	LEU
1	G	183	LEU
1	H	183	LEU
1	I	183	LEU
1	J	183	LEU
1	K	183	LEU
1	L	183	LEU
1	M	183	LEU
1	N	183	LEU
1	A	9	GLY
1	A	256	GLY
1	A	382	GLY
1	B	9	GLY
1	B	256	GLY
1	B	382	GLY
1	C	9	GLY
1	C	256	GLY
1	C	382	GLY
1	D	9	GLY
1	D	256	GLY
1	D	382	GLY
1	E	256	GLY
1	E	382	GLY
1	F	9	GLY
1	F	256	GLY
1	F	382	GLY
1	G	9	GLY
1	G	256	GLY
1	G	382	GLY
1	H	9	GLY
1	H	256	GLY
1	H	382	GLY
1	I	9	GLY
1	I	382	GLY
1	J	9	GLY
1	J	382	GLY
1	K	9	GLY
1	K	256	GLY

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Mol	Chain	Res	Type
1	K	382	GLY
1	L	9	GLY
1	L	256	GLY
1	L	382	GLY
1	M	9	GLY
1	M	256	GLY
1	M	382	GLY
1	N	9	GLY
1	N	256	GLY
1	N	382	GLY
1	A	202	PRO
1	A	383	ALA
1	B	202	PRO
1	B	383	ALA
1	C	202	PRO
1	D	202	PRO
1	E	9	GLY
1	E	202	PRO
1	F	202	PRO
1	G	202	PRO
1	G	383	ALA
1	H	202	PRO
1	H	383	ALA
1	I	202	PRO
1	I	256	GLY
1	J	202	PRO
1	J	256	GLY
1	K	202	PRO
1	L	202	PRO
1	L	383	ALA
1	M	202	PRO
1	M	383	ALA
1	N	202	PRO
1	N	383	ALA
1	A	271	VAL
1	A	384	ALA
1	A	385	THR
1	B	271	VAL
1	B	385	THR
1	C	271	VAL
1	C	383	ALA
1	C	385	THR

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Mol	Chain	Res	Type
1	D	253	ASP
1	D	271	VAL
1	D	383	ALA
1	D	384	ALA
1	D	385	THR
1	E	271	VAL
1	E	383	ALA
1	E	385	THR
1	F	271	VAL
1	F	383	ALA
1	F	385	THR
1	G	271	VAL
1	G	384	ALA
1	G	385	THR
1	H	271	VAL
1	H	385	THR
1	I	271	VAL
1	I	383	ALA
1	I	385	THR
1	J	253	ASP
1	J	271	VAL
1	J	383	ALA
1	J	385	THR
1	K	253	ASP
1	K	271	VAL
1	K	383	ALA
1	K	385	THR
1	L	271	VAL
1	L	385	THR
1	M	253	ASP
1	M	271	VAL
1	M	385	THR
1	N	271	VAL
1	N	385	THR
1	A	184	GLN
1	A	253	ASP
1	B	184	GLN
1	B	253	ASP
1	B	384	ALA
1	C	184	GLN
1	C	253	ASP
1	C	384	ALA

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Mol	Chain	Res	Type
1	D	184	GLN
1	E	184	GLN
1	E	253	ASP
1	E	384	ALA
1	F	184	GLN
1	F	253	ASP
1	F	384	ALA
1	G	184	GLN
1	H	184	GLN
1	H	384	ALA
1	I	184	GLN
1	I	253	ASP
1	I	384	ALA
1	J	184	GLN
1	J	384	ALA
1	K	184	GLN
1	K	384	ALA
1	L	184	GLN
1	L	253	ASP
1	L	384	ALA
1	M	184	GLN
1	M	384	ALA
1	N	184	GLN
1	N	253	ASP
1	N	384	ALA
1	A	201	SER
1	D	201	SER
1	F	201	SER
1	M	201	SER
1	C	201	SER
1	E	201	SER
1	G	201	SER
1	H	201	SER
1	J	201	SER
1	K	201	SER
1	I	201	SER
1	L	201	SER
1	B	201	SER
1	N	201	SER

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	405/414 (98%)	390 (96%)	15 (4%)	34	70
1	B	405/414 (98%)	390 (96%)	15 (4%)	34	70
1	C	405/414 (98%)	390 (96%)	15 (4%)	34	70
1	D	405/414 (98%)	390 (96%)	15 (4%)	34	70
1	E	405/414 (98%)	390 (96%)	15 (4%)	34	70
1	F	405/414 (98%)	390 (96%)	15 (4%)	34	70
1	G	405/414 (98%)	389 (96%)	16 (4%)	31	68
1	H	405/414 (98%)	389 (96%)	16 (4%)	31	68
1	I	405/414 (98%)	390 (96%)	15 (4%)	34	70
1	J	405/414 (98%)	390 (96%)	15 (4%)	34	70
1	K	405/414 (98%)	390 (96%)	15 (4%)	34	70
1	L	405/414 (98%)	390 (96%)	15 (4%)	34	70
1	M	405/414 (98%)	389 (96%)	16 (4%)	31	68
1	N	405/414 (98%)	390 (96%)	15 (4%)	34	70
2	1	11/11 (100%)	11 (100%)	0	100	100
2	2	11/11 (100%)	11 (100%)	0	100	100
2	O	11/11 (100%)	11 (100%)	0	100	100
2	P	11/11 (100%)	11 (100%)	0	100	100
2	Q	11/11 (100%)	11 (100%)	0	100	100
2	R	11/11 (100%)	11 (100%)	0	100	100
2	S	11/11 (100%)	11 (100%)	0	100	100
2	T	11/11 (100%)	11 (100%)	0	100	100
2	U	11/11 (100%)	11 (100%)	0	100	100
2	V	11/11 (100%)	11 (100%)	0	100	100
2	W	11/11 (100%)	11 (100%)	0	100	100
2	X	11/11 (100%)	11 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	Y	11/11 (100%)	11 (100%)	0	100	100
2	Z	11/11 (100%)	11 (100%)	0	100	100
All	All	5824/5950 (98%)	5611 (96%)	213 (4%)	34	70

All (213) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	VAL
1	A	74	VAL
1	A	94	VAL
1	A	134	LEU
1	A	171	LYS
1	A	183	LEU
1	A	201	SER
1	A	231	ARG
1	A	289	LEU
1	A	326	ASN
1	A	329	THR
1	A	331	THR
1	A	417	VAL
1	A	422	VAL
1	A	451	LEU
1	B	20	VAL
1	B	74	VAL
1	B	94	VAL
1	B	134	LEU
1	B	171	LYS
1	B	183	LEU
1	B	201	SER
1	B	231	ARG
1	B	289	LEU
1	B	326	ASN
1	B	329	THR
1	B	331	THR
1	B	417	VAL
1	B	422	VAL
1	B	451	LEU
1	C	20	VAL
1	C	74	VAL
1	C	94	VAL
1	C	134	LEU

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Mol	Chain	Res	Type
1	C	171	LYS
1	C	183	LEU
1	C	201	SER
1	C	231	ARG
1	C	289	LEU
1	C	326	ASN
1	C	329	THR
1	C	331	THR
1	C	417	VAL
1	C	422	VAL
1	C	451	LEU
1	D	20	VAL
1	D	74	VAL
1	D	94	VAL
1	D	134	LEU
1	D	171	LYS
1	D	183	LEU
1	D	201	SER
1	D	231	ARG
1	D	289	LEU
1	D	326	ASN
1	D	329	THR
1	D	331	THR
1	D	417	VAL
1	D	422	VAL
1	D	451	LEU
1	E	20	VAL
1	E	74	VAL
1	E	94	VAL
1	E	134	LEU
1	E	171	LYS
1	E	183	LEU
1	E	201	SER
1	E	231	ARG
1	E	289	LEU
1	E	326	ASN
1	E	329	THR
1	E	331	THR
1	E	417	VAL
1	E	422	VAL
1	E	451	LEU
1	F	20	VAL

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Mol	Chain	Res	Type
1	F	74	VAL
1	F	94	VAL
1	F	134	LEU
1	F	171	LYS
1	F	183	LEU
1	F	201	SER
1	F	231	ARG
1	F	289	LEU
1	F	326	ASN
1	F	329	THR
1	F	331	THR
1	F	417	VAL
1	F	422	VAL
1	F	451	LEU
1	G	20	VAL
1	G	74	VAL
1	G	82	ASN
1	G	94	VAL
1	G	134	LEU
1	G	171	LYS
1	G	183	LEU
1	G	201	SER
1	G	231	ARG
1	G	289	LEU
1	G	326	ASN
1	G	329	THR
1	G	331	THR
1	G	417	VAL
1	G	422	VAL
1	G	451	LEU
1	H	20	VAL
1	H	74	VAL
1	H	82	ASN
1	H	94	VAL
1	H	134	LEU
1	H	171	LYS
1	H	183	LEU
1	H	201	SER
1	H	231	ARG
1	H	289	LEU
1	H	326	ASN
1	H	329	THR

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Mol	Chain	Res	Type
1	H	331	THR
1	H	417	VAL
1	H	422	VAL
1	H	451	LEU
1	I	20	VAL
1	I	74	VAL
1	I	94	VAL
1	I	134	LEU
1	I	171	LYS
1	I	183	LEU
1	I	201	SER
1	I	231	ARG
1	I	289	LEU
1	I	326	ASN
1	I	329	THR
1	I	331	THR
1	I	417	VAL
1	I	422	VAL
1	I	451	LEU
1	J	20	VAL
1	J	74	VAL
1	J	94	VAL
1	J	134	LEU
1	J	171	LYS
1	J	183	LEU
1	J	201	SER
1	J	231	ARG
1	J	289	LEU
1	J	326	ASN
1	J	329	THR
1	J	331	THR
1	J	417	VAL
1	J	422	VAL
1	J	451	LEU
1	K	20	VAL
1	K	74	VAL
1	K	94	VAL
1	K	134	LEU
1	K	171	LYS
1	K	183	LEU
1	K	201	SER
1	K	231	ARG

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Mol	Chain	Res	Type
1	K	289	LEU
1	K	326	ASN
1	K	329	THR
1	K	331	THR
1	K	417	VAL
1	K	422	VAL
1	K	451	LEU
1	L	20	VAL
1	L	74	VAL
1	L	94	VAL
1	L	134	LEU
1	L	171	LYS
1	L	183	LEU
1	L	201	SER
1	L	231	ARG
1	L	289	LEU
1	L	326	ASN
1	L	329	THR
1	L	331	THR
1	L	417	VAL
1	L	422	VAL
1	L	451	LEU
1	M	20	VAL
1	M	74	VAL
1	M	94	VAL
1	M	134	LEU
1	M	171	LYS
1	M	183	LEU
1	M	201	SER
1	M	231	ARG
1	M	284	ARG
1	M	289	LEU
1	M	326	ASN
1	M	329	THR
1	M	331	THR
1	M	417	VAL
1	M	422	VAL
1	M	451	LEU
1	N	20	VAL
1	N	74	VAL
1	N	94	VAL
1	N	134	LEU

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Mol	Chain	Res	Type
1	N	171	LYS
1	N	183	LEU
1	N	201	SER
1	N	231	ARG
1	N	289	LEU
1	N	326	ASN
1	N	329	THR
1	N	331	THR
1	N	417	VAL
1	N	422	VAL
1	N	451	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (113) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	ASN
1	A	146	GLN
1	A	265	ASN
1	A	319	GLN
1	A	351	GLN
1	A	366	GLN
1	A	453	GLN
1	A	475	ASN
1	B	37	ASN
1	B	146	GLN
1	B	265	ASN
1	B	319	GLN
1	B	351	GLN
1	B	366	GLN
1	B	453	GLN
1	B	475	ASN
1	C	37	ASN
1	C	146	GLN
1	C	265	ASN
1	C	319	GLN
1	C	351	GLN
1	C	366	GLN
1	C	401	HIS
1	C	453	GLN
1	C	475	ASN
1	D	37	ASN
1	D	146	GLN

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Mol	Chain	Res	Type
1	D	265	ASN
1	D	319	GLN
1	D	351	GLN
1	D	366	GLN
1	D	453	GLN
1	D	475	ASN
1	E	37	ASN
1	E	146	GLN
1	E	265	ASN
1	E	319	GLN
1	E	351	GLN
1	E	366	GLN
1	E	453	GLN
1	E	475	ASN
1	F	37	ASN
1	F	146	GLN
1	F	265	ASN
1	F	319	GLN
1	F	351	GLN
1	F	366	GLN
1	F	453	GLN
1	F	475	ASN
1	G	37	ASN
1	G	146	GLN
1	G	265	ASN
1	G	319	GLN
1	G	351	GLN
1	G	366	GLN
1	G	453	GLN
1	G	475	ASN
1	H	37	ASN
1	H	146	GLN
1	H	265	ASN
1	H	319	GLN
1	H	351	GLN
1	H	366	GLN
1	H	453	GLN
1	H	475	ASN
1	I	37	ASN
1	I	146	GLN
1	I	265	ASN
1	I	319	GLN

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Mol	Chain	Res	Type
1	I	351	GLN
1	I	366	GLN
1	I	453	GLN
1	I	475	ASN
1	J	37	ASN
1	J	146	GLN
1	J	265	ASN
1	J	319	GLN
1	J	351	GLN
1	J	366	GLN
1	J	453	GLN
1	J	475	ASN
1	K	37	ASN
1	K	146	GLN
1	K	265	ASN
1	K	319	GLN
1	K	351	GLN
1	K	366	GLN
1	K	453	GLN
1	K	475	ASN
1	L	37	ASN
1	L	146	GLN
1	L	265	ASN
1	L	319	GLN
1	L	351	GLN
1	L	366	GLN
1	L	453	GLN
1	L	475	ASN
1	M	37	ASN
1	M	146	GLN
1	M	265	ASN
1	M	319	GLN
1	M	351	GLN
1	M	366	GLN
1	M	453	GLN
1	M	475	ASN
1	N	37	ASN
1	N	146	GLN
1	N	265	ASN
1	N	319	GLN
1	N	351	GLN
1	N	366	GLN

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Mol	Chain	Res	Type
1	N	453	GLN
1	N	475	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 carbohydrates in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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(Å²)	Q<0.9
1	A	525/547 (95%)	-0.45	2 (0%)	92	79	12, 36, 70, 88	0
1	B	525/547 (95%)	-0.43	2 (0%)	92	79	12, 36, 70, 88	0
1	C	525/547 (95%)	-0.49	3 (0%)	89	72	12, 36, 69, 88	0
1	D	525/547 (95%)	-0.46	1 (0%)	95	87	12, 36, 69, 88	0
1	E	525/547 (95%)	-0.45	4 (0%)	86	65	12, 36, 69, 88	0
1	F	525/547 (95%)	-0.46	5 (0%)	82	59	13, 36, 69, 88	0
1	G	525/547 (95%)	-0.48	1 (0%)	95	87	11, 35, 69, 88	0
1	H	525/547 (95%)	-0.45	3 (0%)	89	72	12, 36, 71, 88	0
1	I	525/547 (95%)	-0.44	4 (0%)	86	65	12, 36, 71, 88	0
1	J	525/547 (95%)	-0.49	4 (0%)	86	65	13, 37, 69, 88	0
1	K	525/547 (95%)	-0.45	2 (0%)	92	79	12, 36, 70, 88	0
1	L	525/547 (95%)	-0.46	2 (0%)	92	79	12, 36, 69, 88	0
1	M	525/547 (95%)	-0.49	5 (0%)	82	59	12, 37, 70, 88	0
1	N	525/547 (95%)	-0.46	5 (0%)	82	59	12, 36, 70, 88	0
2	1	12/12 (100%)	-0.04	1 (8%)	11	3	42, 55, 70, 74	0
2	2	12/12 (100%)	-0.08	0	100	100	43, 55, 71, 74	0
2	O	12/12 (100%)	-0.09	1 (8%)	11	3	43, 55, 70, 74	0
2	P	12/12 (100%)	-0.18	0	100	100	42, 55, 70, 74	0
2	Q	12/12 (100%)	-0.17	0	100	100	43, 55, 70, 74	0
2	R	12/12 (100%)	0.15	0	100	100	43, 55, 70, 74	0
2	S	12/12 (100%)	0.22	1 (8%)	11	3	43, 54, 70, 74	0
2	T	12/12 (100%)	-0.38	0	100	100	43, 54, 70, 74	0
2	U	12/12 (100%)	0.03	0	100	100	43, 54, 70, 74	0
2	V	12/12 (100%)	0.01	0	100	100	43, 54, 71, 74	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
2	W	12/12 (100%)	-0.17	0	100	100	44, 55, 71, 74	0
2	X	12/12 (100%)	-0.18	0	100	100	43, 55, 70, 74	0
2	Y	12/12 (100%)	0.08	0	100	100	44, 55, 70, 74	0
2	Z	12/12 (100%)	-0.10	0	100	100	43, 55, 70, 74	0
All	All	7518/7826 (96%)	-0.46	46 (0%)	89	72	11, 37, 71, 88	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	N	44	PHE	4.2
1	J	43	SER	4.0
1	I	43	SER	3.7
1	M	526	LYS	3.6
1	G	43	SER	3.5
1	F	44	PHE	3.3
1	M	43	SER	3.2
1	D	43	SER	3.1
1	F	306	GLY	3.0
1	J	44	PHE	3.0
1	F	43	SER	2.7
1	L	44	PHE	2.7
2	O	601	SER	2.7
1	E	43	SER	2.6
1	N	358	SER	2.6
1	B	44	PHE	2.6
1	C	357	THR	2.5
2	S	606	PRO	2.5
1	N	43	SER	2.5
1	H	357	THR	2.4
1	H	44	PHE	2.4
1	F	357	THR	2.4
1	E	304	GLU	2.3
1	H	43	SER	2.3
1	I	354	GLU	2.3
1	A	357	THR	2.3
1	N	357	THR	2.3
1	K	43	SER	2.3
1	L	43	SER	2.3
1	B	526	LYS	2.3
1	N	181	THR	2.2
1	C	526	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	J	357	THR	2.2
1	M	153	ASN	2.2
1	C	358	SER	2.1
1	M	305	ILE	2.1
1	E	44	PHE	2.1
1	J	243	ALA	2.1
1	K	44	PHE	2.1
1	M	172	GLU	2.1
1	E	351	GLN	2.1
1	F	172	GLU	2.0
1	I	315	GLU	2.0
2	1	601	SER	2.0
1	A	44	PHE	2.0
1	I	355	GLU	2.0

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

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

6.3 Carbohydrates (i)

There are no 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.