



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:25 PM UTC

PDB ID : 1MNF / pdb_00001mnf
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)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

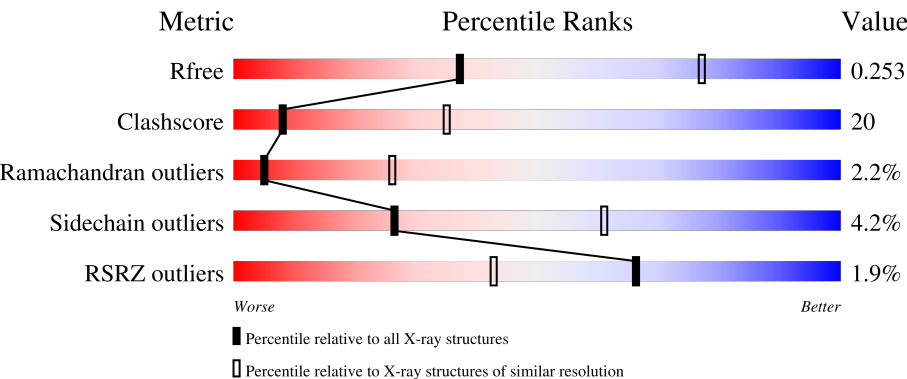
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance i

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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	547	2% 63% 28% . .
1	B	547	3% 62% 30% . .
1	C	547	% 60% 32% . .
1	D	547	2% 60% 31% . . .
1	E	547	% 62% 29% . .

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Mol	Chain	Length	Quality of chain
1	F	547	
1	G	547	
1	H	547	
1	I	547	
1	J	547	
1	K	547	
1	L	547	
1	M	547	
1	N	547	
2	1	12	
2	2	12	
2	O	12	
2	P	12	
2	Q	12	
2	R	12	
2	S	12	
2	T	12	
2	U	12	
2	V	12	
2	W	12	
2	X	12	
2	Y	12	
2	Z	12	

2 Entry composition

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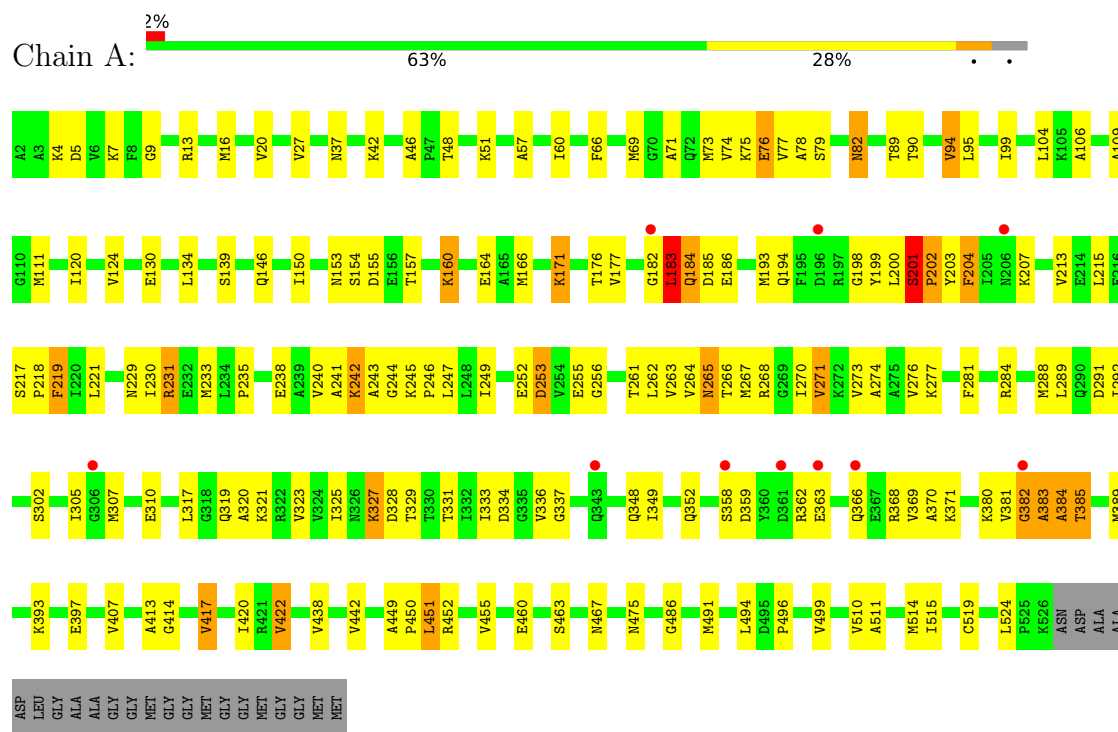
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	11	Total 11	O 11	0	0
3	H	13	Total 13	O 13	0	0
3	I	23	Total 23	O 23	0	0
3	J	10	Total 10	O 10	0	0
3	K	8	Total 8	O 8	0	0
3	L	10	Total 10	O 10	0	0
3	M	6	Total 6	O 6	0	0
3	N	15	Total 15	O 15	0	0

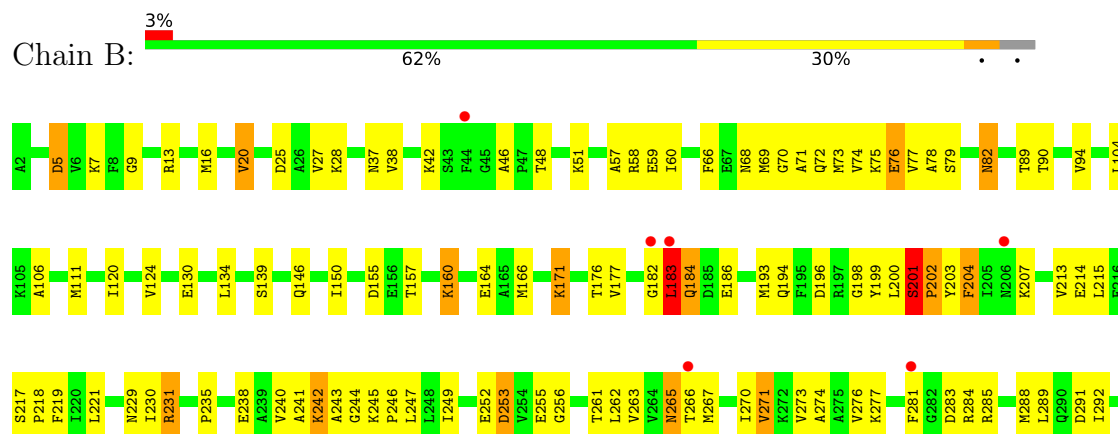
3 Residue-property plots

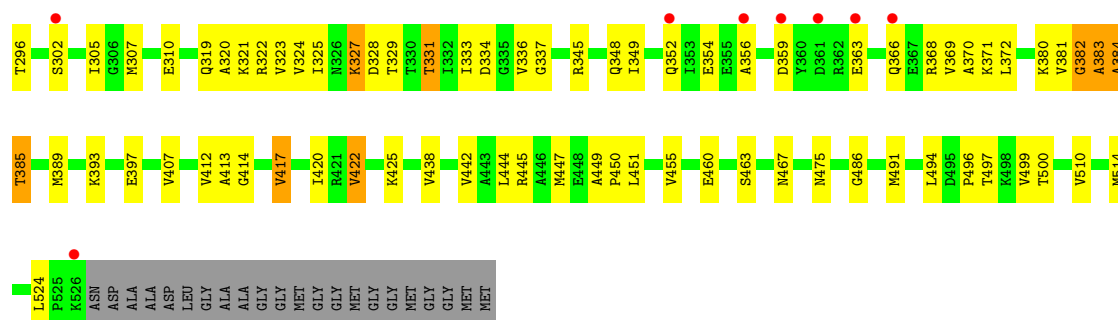
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: groEL protein

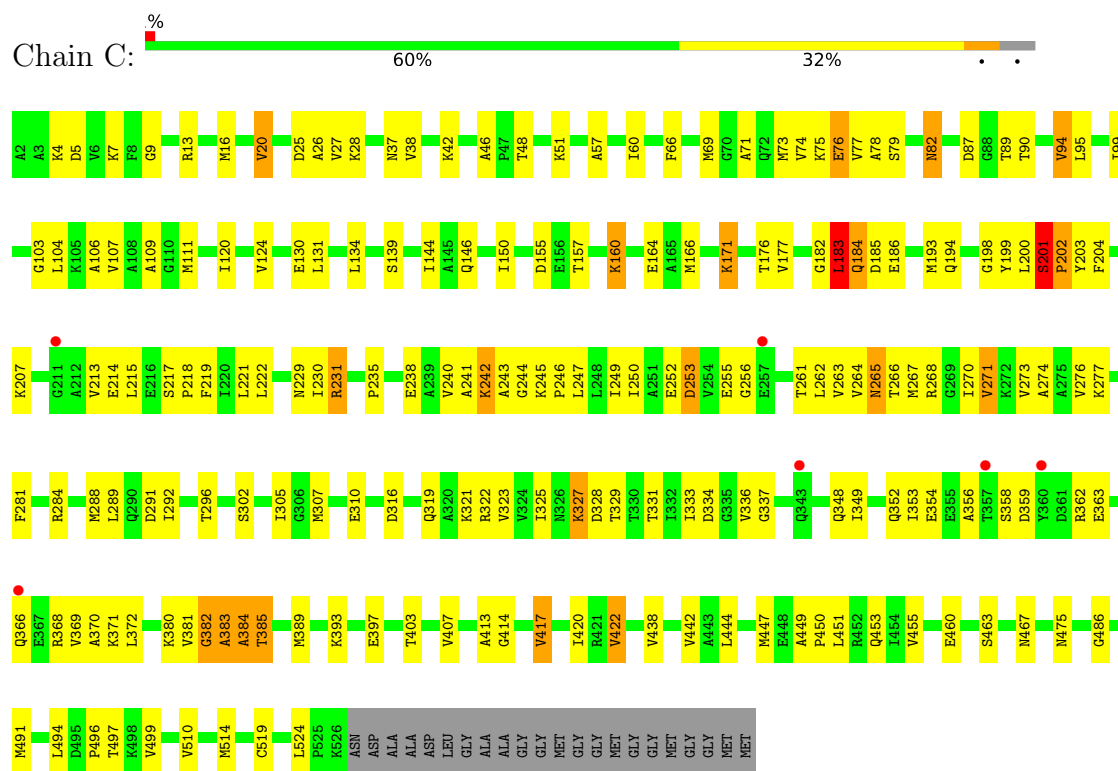


- Molecule 1: groEL protein

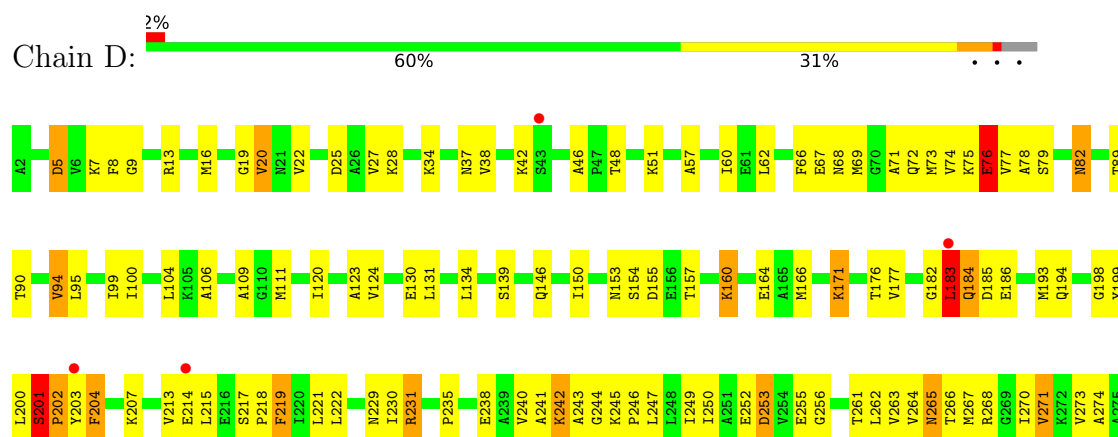


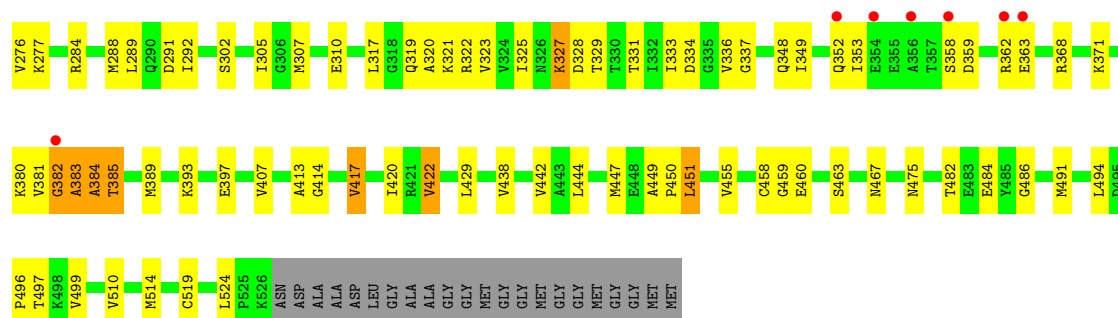


• Molecule 1: groEL protein

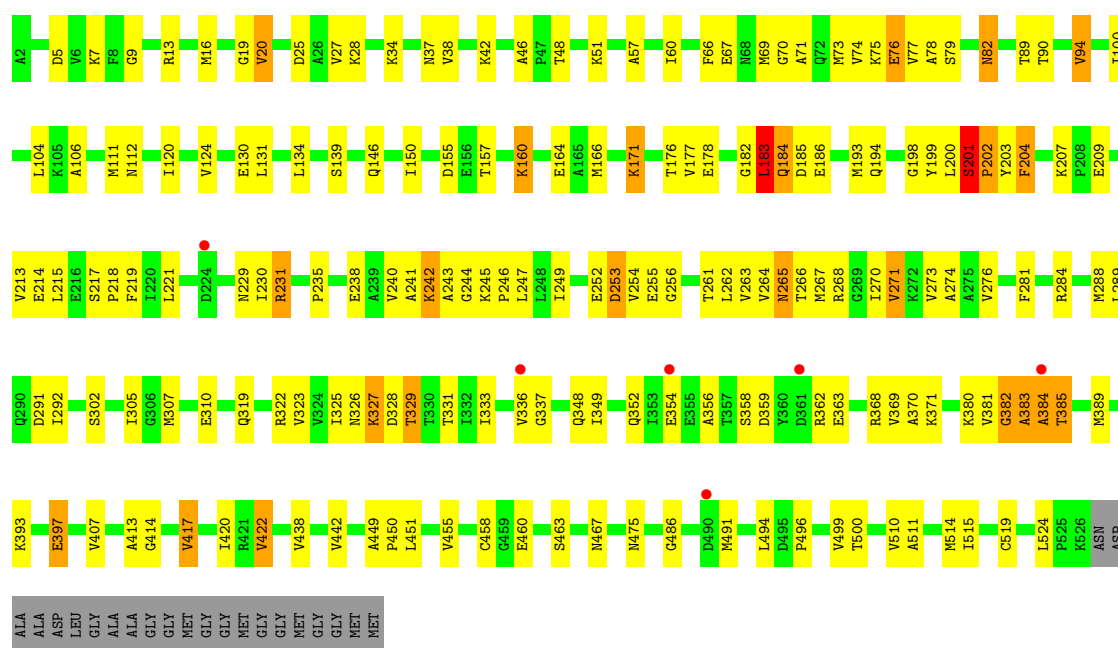


• Molecule 1: groEL protein

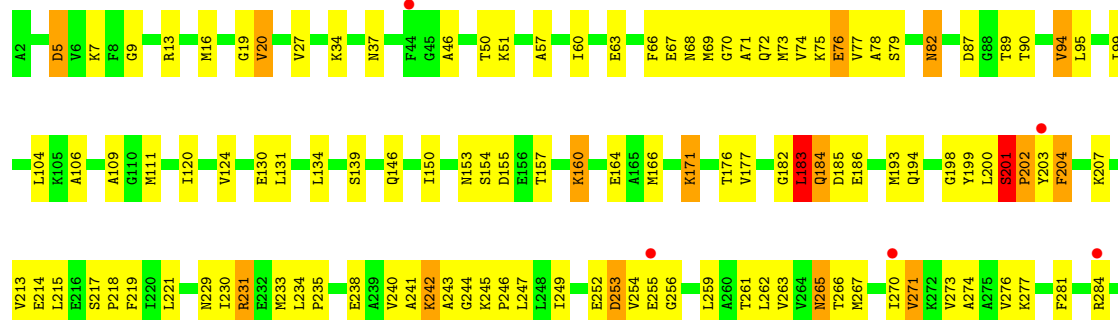




• Molecule 1: groEL protein

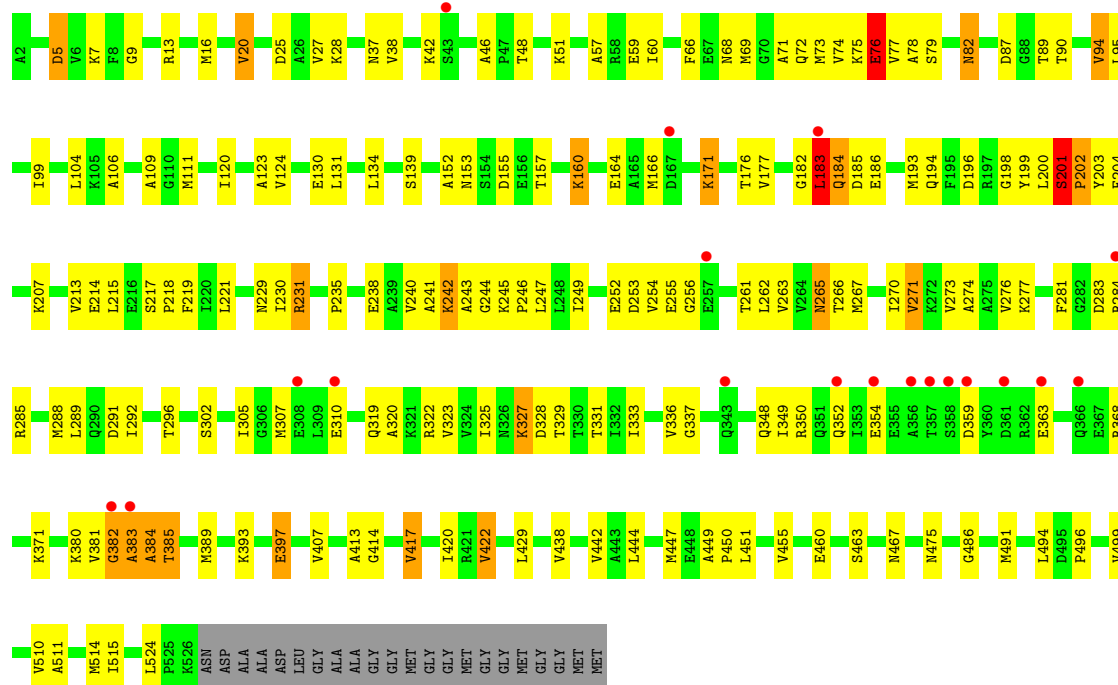


• Molecule 1: groEL protein

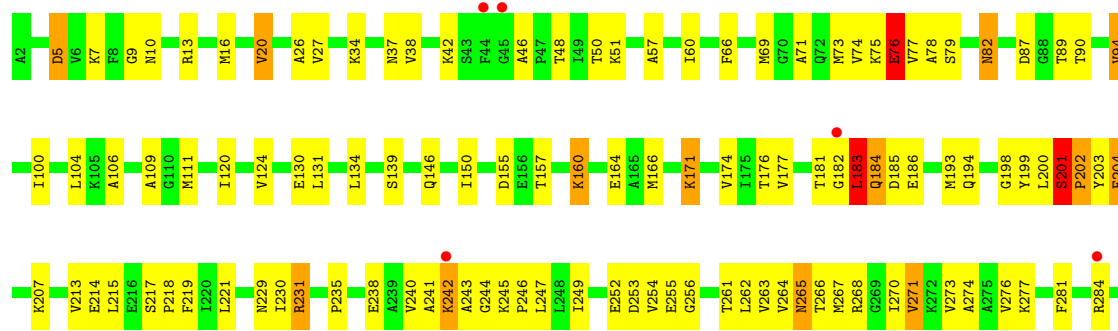


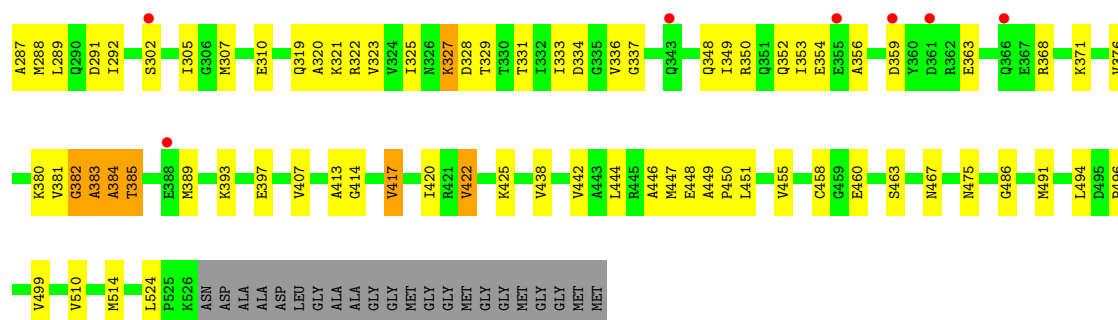


• Molecule 1: groEL protein

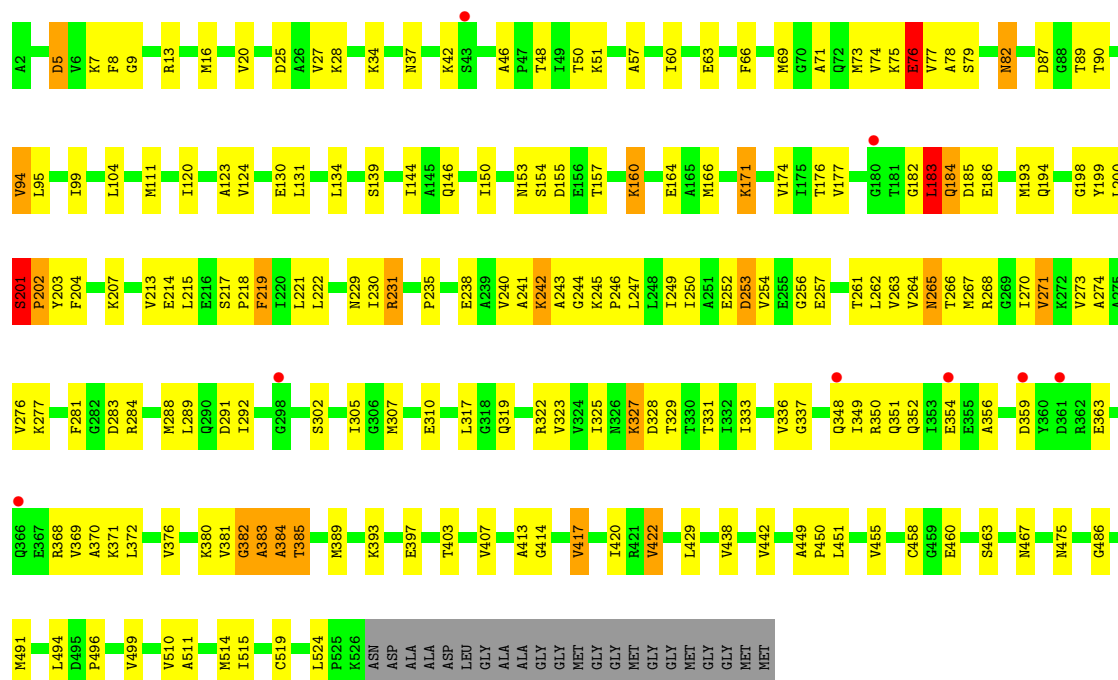


• Molecule 1: groEL protein

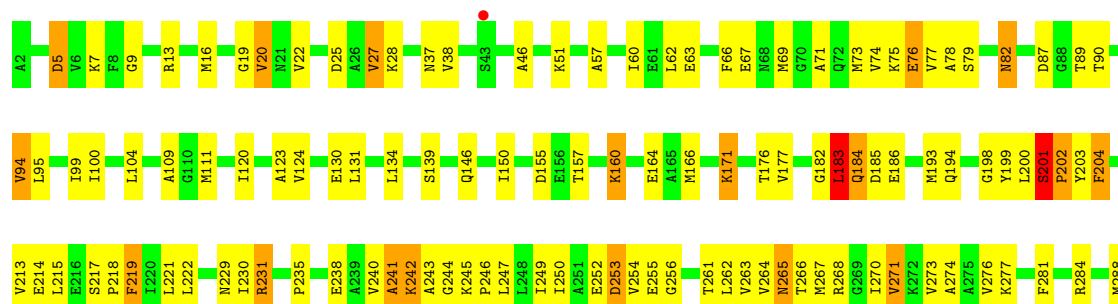


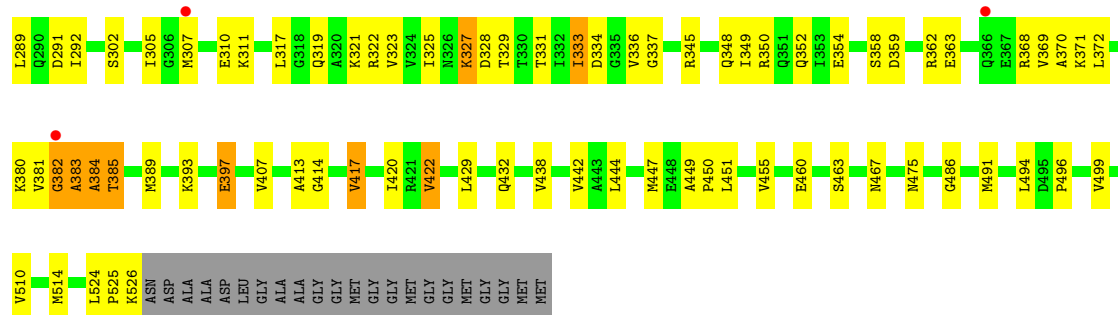


• Molecule 1: groEL protein

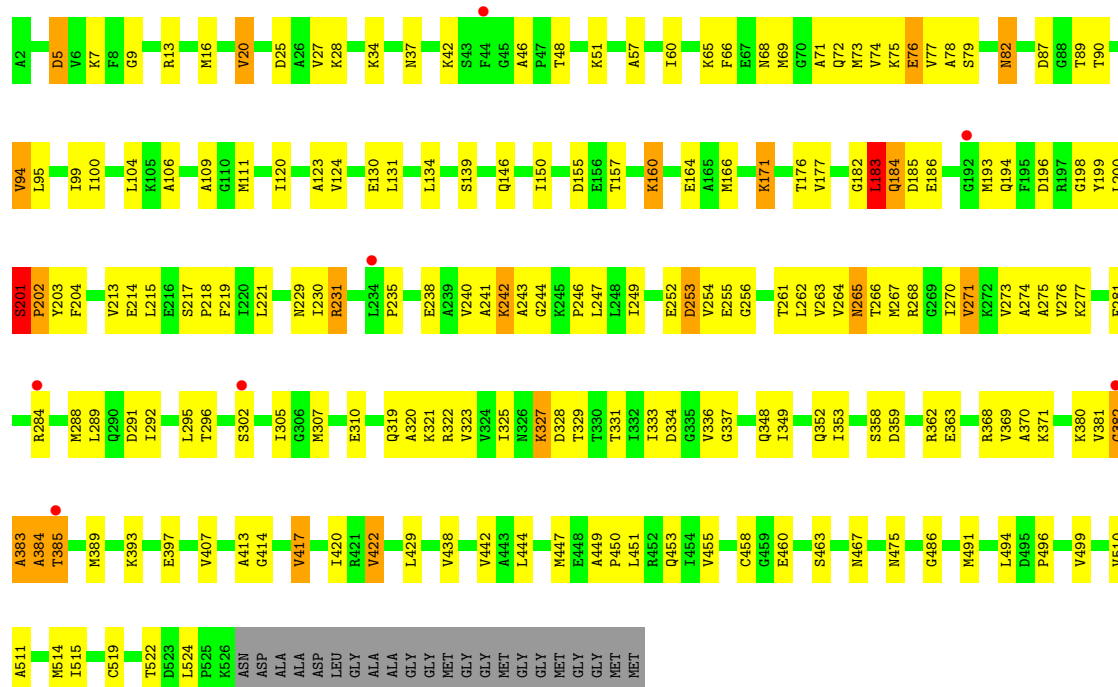


• Molecule 1: groEL protein

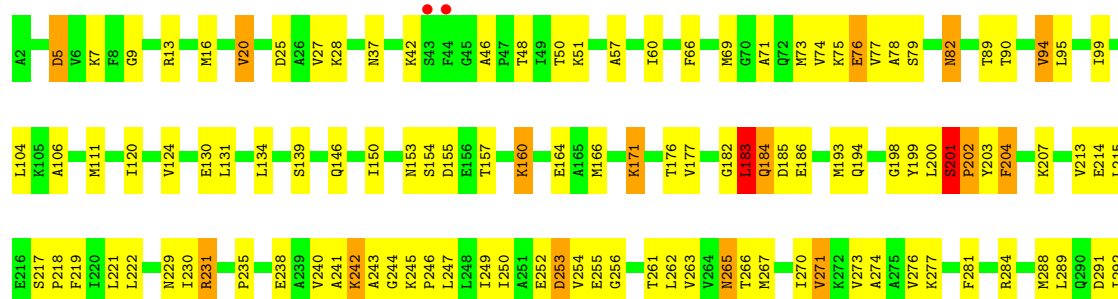


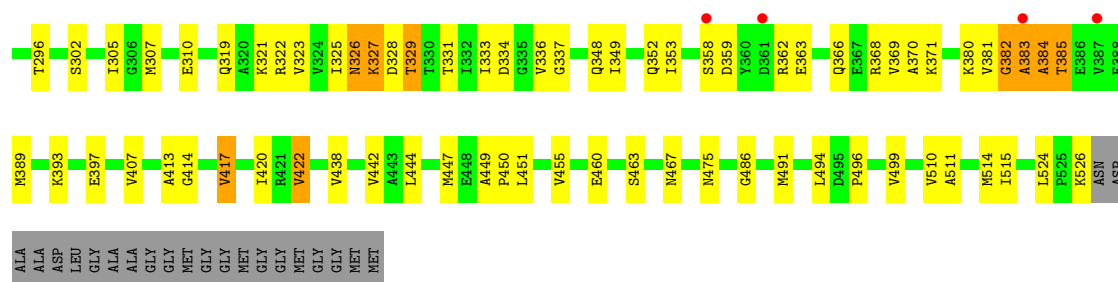


• Molecule 1: groEL protein

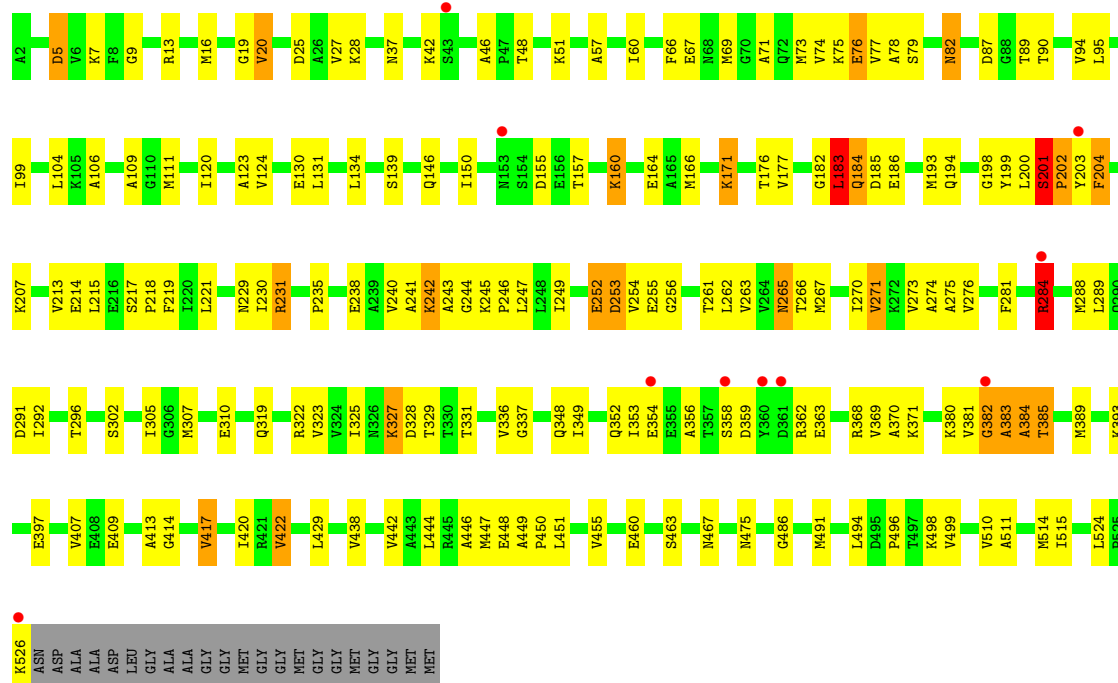


• Molecule 1: groEL protein

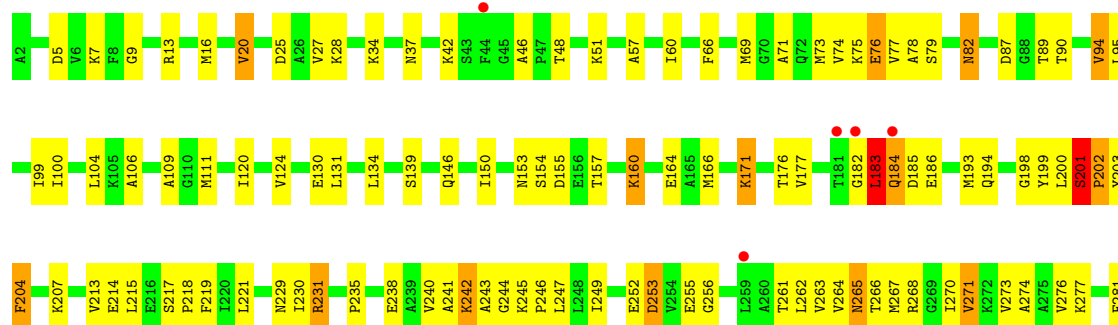


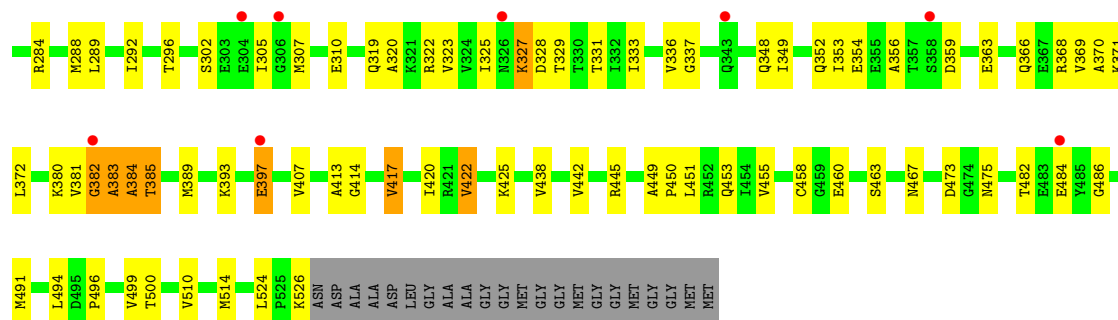


- Molecule 1: groEL protein



- Molecule 1: groEL protein





- Molecule 2: 12-residue peptide substrate



- Molecule 2: 12-residue peptide substrate



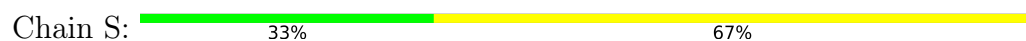
- Molecule 2: 12-residue peptide substrate



- Molecule 2: 12-residue peptide substrate



- Molecule 2: 12-residue peptide substrate



- Molecule 2: 12-residue peptide substrate





- Molecule 2: 12-residue peptide substrate



- Molecule 2: 12-residue peptide substrate



- Molecule 2: 12-residue peptide substrate



- Molecule 2: 12-residue peptide substrate



- Molecule 2: 12-residue peptide substrate



- Molecule 2: 12-residue peptide substrate



- Molecule 2: 12-residue peptide substrate





● Molecule 2: 12-residue peptide substrate



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	135.41 Å 260.69 Å 148.69 Å 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) 83.2 (20.01-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.84 (at 2.98 Å)	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 , 37.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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	0.49	0/3892	0.92	11/5254 (0.2%)
1	B	0.51	0/3892	1.00	17/5254 (0.3%)
1	C	0.48	0/3892	0.92	10/5254 (0.2%)
1	D	0.52	0/3892	0.92	12/5254 (0.2%)
1	E	0.52	0/3892	0.92	11/5254 (0.2%)
1	F	0.51	0/3892	0.92	13/5254 (0.2%)
1	G	0.52	0/3892	0.91	12/5254 (0.2%)
1	H	0.48	0/3892	0.92	13/5254 (0.2%)
1	I	0.48	0/3892	0.92	12/5254 (0.2%)
1	J	0.47	0/3892	0.91	11/5254 (0.2%)
1	K	0.49	0/3892	0.92	10/5254 (0.2%)
1	L	0.51	0/3892	0.92	13/5254 (0.2%)
1	M	0.46	0/3892	0.94	14/5254 (0.3%)
1	N	0.47	0/3892	0.93	14/5254 (0.3%)
2	1	0.38	0/111	0.82	1/152 (0.7%)
2	2	0.42	0/111	0.90	1/152 (0.7%)
2	O	0.41	0/111	0.87	1/152 (0.7%)
2	P	0.44	0/111	0.91	1/152 (0.7%)
2	Q	0.44	0/111	0.89	1/152 (0.7%)
2	R	0.37	0/111	0.91	1/152 (0.7%)
2	S	0.38	0/111	0.89	1/152 (0.7%)
2	T	0.40	0/111	0.83	1/152 (0.7%)
2	U	0.45	0/111	0.89	1/152 (0.7%)
2	V	0.42	0/111	0.89	1/152 (0.7%)
2	W	0.38	0/111	0.89	1/152 (0.7%)
2	X	0.37	0/111	0.90	1/152 (0.7%)
2	Y	0.40	0/111	0.90	1/152 (0.7%)
2	Z	0.37	0/111	0.88	1/152 (0.7%)
All	All	0.49	0/56042	0.92	187/75684 (0.2%)

There are no bond length outliers.

All (187) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	58	ARG	NE-CZ-NH2	16.13	133.72	119.20
1	B	58	ARG	NE-CZ-NH1	-15.44	106.06	121.50
1	B	58	ARG	CD-NE-CZ	14.10	144.15	124.40
1	N	368	ARG	NE-CZ-NH2	9.08	127.37	119.20
1	N	368	ARG	NE-CZ-NH1	-8.72	112.78	121.50
1	M	284	ARG	NE-CZ-NH2	8.70	127.03	119.20
1	B	242	LYS	N-CA-C	-8.44	99.72	110.19
1	C	242	LYS	N-CA-C	-8.19	100.04	110.19
1	L	242	LYS	N-CA-C	-8.10	100.15	110.19
1	F	242	LYS	N-CA-C	-8.08	100.17	110.19
1	G	242	LYS	N-CA-C	-8.03	100.23	110.19
1	I	242	LYS	N-CA-C	-7.99	100.28	110.19
1	K	242	LYS	N-CA-C	-7.83	100.48	110.19
1	D	242	LYS	N-CA-C	-7.72	100.62	110.19
1	M	284	ARG	NE-CZ-NH1	-7.61	113.89	121.50
1	J	242	LYS	N-CA-C	-7.57	100.81	110.19
1	M	242	LYS	N-CA-C	-7.55	100.82	110.19
1	N	242	LYS	N-CA-C	-7.48	100.91	110.19
1	A	242	LYS	N-CA-C	-7.47	100.93	110.19
2	X	611	HIS	N-CA-C	7.46	114.94	108.22
1	E	242	LYS	N-CA-C	-7.43	100.97	110.19
2	Y	611	HIS	N-CA-C	7.43	114.91	108.22
2	Z	611	HIS	N-CA-C	7.22	114.72	108.22
2	R	611	HIS	N-CA-C	7.21	114.71	108.22
2	S	611	HIS	N-CA-C	7.16	114.67	108.22
1	B	58	ARG	CG-CD-NE	-7.16	96.26	112.00
1	L	219	PHE	N-CA-C	-7.16	100.22	110.59
2	2	611	HIS	N-CA-C	7.15	114.66	108.22
1	H	242	LYS	N-CA-C	-7.11	101.38	110.19
2	P	611	HIS	N-CA-C	7.05	114.57	108.22
2	U	611	HIS	N-CA-C	7.04	114.56	108.22
2	W	611	HIS	N-CA-C	6.92	114.45	108.22
2	Q	611	HIS	N-CA-C	6.90	114.43	108.22
1	F	219	PHE	N-CA-C	-6.88	100.62	110.59
1	D	60	ILE	N-CA-C	6.85	118.32	107.98
2	V	611	HIS	N-CA-C	6.83	114.37	108.22
2	O	611	HIS	N-CA-C	6.83	114.36	108.22
1	N	219	PHE	N-CA-C	-6.75	100.81	110.59
1	C	219	PHE	N-CA-C	-6.72	101.48	110.55
2	T	611	HIS	N-CA-C	6.60	114.16	108.22
1	K	219	PHE	N-CA-C	-6.50	101.16	110.59
1	G	219	PHE	N-CA-C	-6.48	101.19	110.59
1	K	333	ILE	N-CA-C	6.46	117.17	107.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	219	PHE	N-CA-C	-6.37	101.36	110.59
1	F	265	ASN	N-CA-C	6.33	118.18	111.28
1	B	333	ILE	N-CA-C	6.30	116.94	107.80
1	H	219	PHE	N-CA-C	-6.24	101.28	110.52
1	E	219	PHE	N-CA-C	-6.22	101.32	110.52
1	J	219	PHE	N-CA-C	-6.21	101.59	110.59
1	A	333	ILE	N-CA-C	6.19	116.78	107.80
1	K	327	LYS	N-CA-C	-6.17	104.61	111.71
1	L	327	LYS	N-CA-C	-6.11	104.73	111.82
1	I	60	ILE	N-CA-C	6.10	117.57	108.54
1	L	207	LYS	CA-C-N	6.10	126.54	119.47
1	L	207	LYS	C-N-CA	6.10	126.54	119.47
1	K	60	ILE	N-CA-C	6.07	117.52	108.54
1	I	219	PHE	N-CA-C	-6.06	101.56	110.52
1	N	333	ILE	N-CA-C	6.06	116.58	107.80
1	J	60	ILE	N-CA-C	6.02	117.45	108.54
1	A	60	ILE	N-CA-C	6.02	117.45	108.54
1	L	60	ILE	N-CA-C	6.01	117.43	108.54
1	N	60	ILE	N-CA-C	6.01	117.44	108.54
1	A	219	PHE	N-CA-C	-5.96	101.69	110.52
1	F	60	ILE	N-CA-C	5.94	117.33	108.54
1	G	60	ILE	N-CA-C	5.94	117.33	108.54
1	H	60	ILE	N-CA-C	5.94	117.33	108.54
1	L	265	ASN	N-CA-C	5.93	117.75	111.28
1	B	219	PHE	N-CA-C	-5.88	102.07	110.59
2	1	611	HIS	N-CA-C	5.87	113.51	108.22
1	B	255	GLU	N-CA-C	5.84	118.24	110.53
1	C	207	LYS	CA-C-N	5.80	126.20	119.47
1	C	207	LYS	C-N-CA	5.80	126.20	119.47
1	D	333	ILE	N-CA-C	5.77	116.16	107.80
1	M	76	GLU	N-CA-C	5.75	117.35	111.14
1	M	60	ILE	N-CA-C	5.75	117.05	108.54
1	B	327	LYS	N-CA-C	-5.75	105.37	112.38
1	C	327	LYS	N-CA-C	-5.74	105.54	112.54
1	E	333	ILE	N-CA-C	5.73	116.10	107.80
1	A	327	LYS	N-CA-C	-5.70	105.58	112.54
1	C	60	ILE	N-CA-C	5.70	116.97	108.54
1	G	327	LYS	N-CA-C	-5.70	105.59	112.54
1	A	265	ASN	N-CA-C	5.68	117.48	111.28
1	M	327	LYS	N-CA-C	-5.66	105.64	112.54
1	E	76	GLU	N-CA-C	5.63	117.22	111.14
1	D	327	LYS	N-CA-C	-5.63	105.24	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	327	LYS	N-CA-C	-5.61	105.53	112.38
1	N	327	LYS	N-CA-C	-5.61	105.26	111.71
1	J	204	PHE	N-CA-C	-5.60	105.27	111.71
1	B	60	ILE	N-CA-C	5.60	116.82	108.54
1	C	333	ILE	N-CA-C	5.59	115.91	107.80
1	I	5	ASP	N-CA-C	-5.58	99.31	108.41
1	G	333	ILE	N-CA-C	5.58	115.89	107.80
1	E	60	ILE	N-CA-C	5.57	116.79	108.54
1	E	204	PHE	N-CA-C	-5.57	105.31	111.71
1	G	255	GLU	N-CA-C	5.57	117.88	110.53
1	I	265	ASN	N-CA-C	5.57	117.35	111.28
1	L	255	GLU	N-CA-C	5.56	117.88	110.53
1	D	219	PHE	N-CA-C	-5.53	102.34	110.52
1	H	76	GLU	N-CA-C	5.52	117.16	111.03
1	E	207	LYS	CA-C-N	5.50	125.84	119.47
1	E	207	LYS	C-N-CA	5.50	125.84	119.47
1	E	265	ASN	N-CA-C	5.50	117.27	111.28
1	A	207	LYS	CA-C-N	5.49	125.84	119.47
1	A	207	LYS	C-N-CA	5.49	125.84	119.47
1	E	327	LYS	N-CA-C	-5.49	105.39	111.71
1	F	207	LYS	CA-C-N	5.49	125.84	119.47
1	F	207	LYS	C-N-CA	5.49	125.84	119.47
1	J	333	ILE	N-CA-C	5.48	115.75	107.80
1	E	255	GLU	N-CA-C	5.47	117.94	110.55
1	G	265	ASN	N-CA-C	5.47	117.25	111.28
1	B	265	ASN	N-CA-C	5.43	117.20	111.28
1	K	196	ASP	N-CA-C	5.43	118.03	109.39
1	M	207	LYS	CA-C-N	5.42	125.76	119.47
1	M	207	LYS	C-N-CA	5.42	125.76	119.47
1	I	207	LYS	CA-C-N	5.41	125.75	119.47
1	I	207	LYS	C-N-CA	5.41	125.75	119.47
1	F	204	PHE	N-CA-C	-5.41	105.55	111.82
1	G	207	LYS	CA-C-N	5.40	125.74	119.47
1	G	207	LYS	C-N-CA	5.40	125.74	119.47
1	D	265	ASN	N-CA-C	5.40	117.16	111.28
1	I	333	ILE	N-CA-C	5.39	115.62	107.80
1	B	5	ASP	N-CA-C	-5.38	99.74	108.52
1	H	255	GLU	N-CA-C	5.37	117.62	110.53
1	K	5	ASP	N-CA-C	-5.37	99.78	108.52
1	N	255	GLU	N-CA-C	5.36	117.60	110.53
1	N	368	ARG	CD-NE-CZ	5.33	131.86	124.40
1	L	5	ASP	N-CA-C	-5.33	99.72	108.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	333	ILE	N-CA-C	5.33	115.53	107.80
1	I	327	LYS	N-CA-C	-5.33	105.58	111.71
1	B	196	ASP	N-CA-C	5.31	117.59	109.62
1	N	204	PHE	N-CA-C	-5.31	105.60	111.71
1	L	333	ILE	N-CA-C	5.30	115.49	107.80
1	K	265	ASN	N-CA-C	5.30	117.06	111.28
1	A	76	GLU	N-CA-C	5.30	116.86	111.14
1	L	204	PHE	N-CA-C	-5.29	105.62	111.71
1	N	207	LYS	CA-C-N	5.29	125.61	119.47
1	N	207	LYS	C-N-CA	5.29	125.61	119.47
1	M	5	ASP	N-CA-C	-5.29	99.90	108.52
1	K	255	GLU	N-CA-C	5.28	117.49	110.53
1	B	207	LYS	CA-C-N	5.27	125.58	119.47
1	B	207	LYS	C-N-CA	5.27	125.58	119.47
1	D	255	GLU	N-CA-C	5.26	117.48	110.53
1	K	76	GLU	N-CA-C	5.26	116.83	111.14
1	M	204	PHE	N-CA-C	-5.26	105.66	111.71
1	J	327	LYS	N-CA-C	-5.26	105.66	111.71
1	C	265	ASN	N-CA-C	5.25	117.00	111.28
1	D	204	PHE	N-CA-C	-5.25	105.68	111.71
1	D	76	GLU	N-CA-C	5.24	116.80	111.14
1	H	204	PHE	N-CA-C	-5.24	105.69	111.71
1	J	265	ASN	N-CA-C	5.24	116.99	111.28
1	H	207	LYS	CA-C-N	5.23	125.54	119.47
1	H	207	LYS	C-N-CA	5.23	125.54	119.47
1	H	5	ASP	N-CA-C	-5.20	100.05	108.52
1	C	255	GLU	N-CA-C	5.19	117.56	110.55
1	B	76	GLU	N-CA-C	5.18	116.73	111.14
1	J	255	GLU	N-CA-C	5.18	117.37	110.53
1	H	50	THR	N-CA-C	5.17	117.05	109.24
1	M	265	ASN	N-CA-C	5.17	116.92	111.28
1	G	76	GLU	N-CA-C	5.17	116.72	111.14
1	A	204	PHE	N-CA-C	-5.16	105.78	111.71
1	C	76	GLU	N-CA-C	5.15	116.75	111.03
1	D	5	ASP	N-CA-C	-5.15	100.12	108.52
1	F	76	GLU	N-CA-C	5.15	116.70	111.14
1	N	76	GLU	N-CA-C	5.14	116.74	111.03
1	I	50	THR	N-CA-C	5.14	117.00	109.24
1	J	27	VAL	N-CA-C	5.14	115.81	110.82
1	A	255	GLU	N-CA-C	5.13	117.30	110.53
1	F	327	LYS	N-CA-C	-5.12	105.83	111.71
1	M	252	GLU	N-CA-C	-5.11	106.14	112.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	255	GLU	N-CA-C	5.11	117.70	110.50
1	G	196	ASP	N-CA-C	5.10	117.27	109.62
1	I	76	GLU	N-CA-C	5.10	116.65	111.14
1	N	265	ASN	N-CA-C	5.09	116.83	111.28
1	F	5	ASP	N-CA-C	-5.08	100.23	108.52
1	I	351	GLN	N-CA-C	-5.08	105.83	112.23
1	F	333	ILE	N-CA-C	5.08	115.16	107.80
1	H	265	ASN	N-CA-C	5.07	116.81	111.28
1	J	241	ALA	N-CA-C	-5.06	105.45	110.97
1	D	207	LYS	CA-C-N	5.05	125.33	119.47
1	D	207	LYS	C-N-CA	5.05	125.33	119.47
1	F	255	GLU	N-CA-C	5.04	117.36	110.55
1	J	5	ASP	N-CA-C	-5.03	100.21	108.41
1	B	204	PHE	N-CA-C	-5.02	105.94	111.71
1	L	50	THR	N-CA-C	5.02	116.82	109.24
1	L	76	GLU	N-CA-C	5.01	116.59	111.03
1	G	5	ASP	N-CA-C	-5.01	100.36	108.52
1	F	50	THR	N-CA-C	5.00	116.80	109.24

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3864	0	3989	155	0
1	B	3864	0	3989	155	0
1	C	3864	0	3989	160	1
1	D	3864	0	3989	172	0
1	E	3864	0	3989	159	0
1	F	3864	0	3989	160	0
1	G	3864	0	3989	156	1
1	H	3864	0	3989	164	1
1	I	3864	0	3989	166	0
1	J	3864	0	3989	169	2
1	K	3864	0	3989	167	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	3864	0	3989	155	1
1	M	3864	0	3989	158	0
1	N	3864	0	3989	163	0
2	1	104	0	91	9	0
2	2	104	0	91	9	0
2	O	104	0	91	9	0
2	P	104	0	91	10	0
2	Q	104	0	91	11	0
2	R	104	0	91	12	0
2	S	104	0	91	10	0
2	T	104	0	91	10	0
2	U	104	0	91	10	0
2	V	104	0	91	11	0
2	W	104	0	91	10	0
2	X	104	0	91	9	0
2	Y	104	0	91	11	0
2	Z	104	0	91	7	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	2200	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 20.

All (2200) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:193:MET:HE1	1:F:292:ILE:HG12	1.26	1.11
1:D:193:MET:HE1	1:D:292:ILE:HG12	1.30	1.11
1:F:183:LEU:H	1:F:383:ALA:HB3	1.12	1.10
1:C:193:MET:HE1	1:C:292:ILE:HG12	1.26	1.10
1:E:183:LEU:H	1:E:383:ALA:HB3	1.05	1.10
1:D:183:LEU:H	1:D:383:ALA:HB3	1.02	1.10
1:H:193:MET:HE1	1:H:292:ILE:HG12	1.34	1.10
1:A:183:LEU:H	1:A:383:ALA:HB3	1.11	1.09
1:J:193:MET:HE1	1:J:292:ILE:HG12	1.28	1.09
1:I:193:MET:HE1	1:I:292:ILE:HG12	1.35	1.07
1:E:193:MET:HE1	1:E:292:ILE:HG12	1.33	1.07
1:A:193:MET:HE1	1:A:292:ILE:HG12	1.37	1.06
1:G:183:LEU:H	1:G:383:ALA:HB3	1.10	1.05
1:M:193:MET:HE1	1:M:292:ILE:HG12	1.33	1.05
1:B:193:MET:HE1	1:B:292:ILE:HG12	1.32	1.05
1:K:193:MET:HE1	1:K:292:ILE:HG12	1.34	1.05
1:G:193:MET:HE1	1:G:292:ILE:HG12	1.36	1.03
1:L:193:MET:HE1	1:L:292:ILE:HG12	1.35	1.03
1:N:193:MET:HE1	1:N:292:ILE:HG12	1.35	1.03
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:302:SER:H	1:D:307:MET:HE3	1.44	0.81
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
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:F:302:SER:H	1:F:307:MET:HE3	1.47	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:B:302:SER:H	1:B:307:MET:HE3	1.47	0.79
1:C:193:MET:HE1	1:C:292:ILE:CG1	2.11	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:H:302:SER:H	1:H:307:MET:HE3	1.49	0.78
1:F:229:ASN:OD1	1:F:231:ARG:HB2	1.84	0.78
1:E:302:SER:H	1:E:307:MET:HE3	1.48	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:L:302:SER:H	1:L:307:MET:HE3	1.49	0.78
1:B:82:ASN:HB2	1:B:89:THR:HG23	1.66	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:302:SER:H	1:C:307:MET:HE3	1.47	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:E:46:ALA:CB	1:F:76:GLU:HG3	2.13	0.77
1:M:265:ASN:HD21	2:1:610:LEU:H	1.32	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:J:193:MET:HE1	1:J:292:ILE:CG1	2.12	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:G:302:SER:H	1:G:307:MET:HE3	1.50	0.77
1:K:302:SER:H	1:K:307:MET:HE3	1.50	0.77
1:E:183:LEU:HD23	1:E:384:ALA:HB2	1.66	0.77
1:I:302:SER:H	1:I:307:MET:HE3	1.50	0.77
1:N:82:ASN:HB2	1:N:89:THR:HG23	1.66	0.77
1:N:229:ASN:OD1	1:N:231:ARG:HB2	1.85	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
1:N:183:LEU:N	1:N:383:ALA:HB3	1.95	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:M:302:SER:H	1:M:307:MET:HE3	1.48	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:J:302:SER:H	1:J:307:MET:HE3	1.51	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:193:MET:HE1	1:F:292:ILE:CG1	2.12	0.75
1:F:381:VAL:HG21	1:F:393:LYS:HA	1.68	0.75
1:N:302:SER:H	1:N:307:MET:HE3	1.51	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:A:265:ASN:HD21	2:O:610:LEU:H	1.34	0.75
1:F:183:LEU:HD23	1:F:384:ALA:HB2	1.69	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:M:193:MET:HE1	1:M:292:ILE:CG1	2.16	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: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:A:302:SER:H	1:A:307:MET:HE3	1.53	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:265:ASN:HD21	2:2:610:LEU:H	1.34	0.73
1:N:381:VAL:HG21	1:N:393:LYS:HA	1.71	0.73
1:E:171:LYS:HB2	1:E:407:VAL:HG11	1.70	0.73
1:E:381:VAL:HG21	1:E:393:LYS:HA	1.71	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:I:265:ASN:HD21	2:W:610:LEU:H	1.35	0.72
1:K:171:LYS:HB2	1:K:407:VAL:HG11	1.72	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:171:LYS:HB2	1:J:407:VAL:HG11	1.73	0.70
1:J:183:LEU:H	1:J:383:ALA:CB	1.97	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:77:VAL:HG21	1:E:510:VAL:HB	1.75	0.68
1:D:46:ALA:CB	1:E:76:GLU:HG3	2.23	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:193:MET:HE1	1:D:292:ILE:CG1	2.17	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:N:16:MET:SD	1:N:73:MET:HE1	2.34	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: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:I:193:MET:HE1	1:I:292:ILE:CG1	2.20	0.66
1:M:16:MET:SD	1:M:73:MET:HE1	2.36	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:F:183:LEU:H	1:F:383:ALA:CB	2.02	0.65
1:K:78:ALA:O	1:K:89:THR:HG22	1.96	0.65
1:H:193:MET:HE1	1:H:292:ILE:CG1	2.21	0.65
1:K:383:ALA:HB1	1:L:281:PHE:HZ	1.61	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
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:57:ALA:O	1:I:75:LYS:HE3	1.95	0.65
1:I:348:GLN:O	1:I:352:GLN:HG2	1.97	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:E:262:LEU:O	1:E:266:THR:HG23	1.97	0.64
1:K:183:LEU:O	1:K:184:GLN:HB2	1.97	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:B:183:LEU:O	1:B:184:GLN:HB2	1.97	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:I:16:MET:SD	1:I:73:MET:HE1	2.38	0.64
1:N:348:GLN:O	1:N:352:GLN:HG2	1.98	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:N:193:MET:HE1	1:N:292:ILE:CG1	2.20	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:J:183:LEU:O	1:J:184:GLN:HB2	1.98	0.63
1:K:77:VAL:HG21	1:K:510:VAL:HB	1.81	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: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:E:193:MET:HE1	1:E:292:ILE:CG1	2.18	0.63
1:G:193:MET:HE1	1:G:292:ILE:CG1	2.21	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:B:193:MET:HE1	1:B:292:ILE:CG1	2.18	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:K:242:LYS:C	1:K:244:GLY:H	2.07	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:K:193:MET:HE1	1:K:292:ILE:CG1	2.20	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: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:218:PRO:HB3	1:M:246:PRO:HG2	1.81	0.62
1:F:16:MET:SD	1:F:73:MET:HE1	2.40	0.62
1:L:183:LEU:O	1:L:184:GLN:HB2	2.00	0.62
1:H:183:LEU:O	1:H:184:GLN:HB2	1.99	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:16:MET:SD	1:D:73:MET:HE1	2.40	0.61
1:D:266:THR:HG21	1:D:273:VAL:H	1.65	0.61
1:E:242:LYS:C	1:E:244:GLY:H	2.08	0.61
1:F:193:MET:CE	1:F:292:ILE:HG12	2.17	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:J:242:LYS:C	1:J:244:GLY:H	2.08	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:A:82:ASN:HB2	1:A:89:THR:CG2	2.30	0.61
1:A:193:MET:HE1	1:A:292:ILE:CG1	2.24	0.61
1:C:417:VAL:HA	1:C:420:ILE:HG22	1.82	0.61
1:D:242:LYS:C	1:D:244:GLY:H	2.08	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:H:16:MET:SD	1:H:73:MET:HE1	2.40	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:A:231:ARG:HH22	2:O:603:MET:HE1	1.65	0.60
1:E:270:ILE:HA	1:F:229:ASN:ND2	2.15	0.60
1:F:215:LEU:HB2	1:F:323:VAL:HG22	1.83	0.60
1:H:242:LYS:C	1:H:244:GLY:H	2.09	0.60
1:K:348:GLN:O	1:K:352:GLN:HG2	2.01	0.60
1:A:76:GLU:HG3	1:G:46:ALA:HB2	1.83	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: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:J:193:MET:CE	1:J:292:ILE:HG12	2.18	0.60
1:K:194:GLN:O	1:K:371:LYS:HE3	2.00	0.60
1:L:271:VAL:HG21	2:Z:607:TRP:HZ3	1.66	0.60
1:L:417:VAL:HA	1:L:420:ILE:HG22	1.83	0.60
1:D:271:VAL:HG21	2:R: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:L:242:LYS:C	1:L:244:GLY:H	2.07	0.60
1:M:270:ILE:HA	1:N:229:ASN:ND2	2.16	0.60
1:D:265:ASN:ND2	2:R:610:LEU:H	1.94	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: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:27:VAL:HG12	1:B:90:THR:HG23	1.84	0.60
1:B:215:LEU:HB2	1:B:323:VAL:HG22	1.82	0.60
1:B:266:THR:HG21	1:B:273:VAL:H	1.66	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:I:242:LYS:C	1:I:244:GLY:H	2.10	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:230:ILE:HD13	1:D:261:THR:CG2	2.32	0.59
1:D:242:LYS:O	1:D:243:ALA:HB3	2.02	0.59
1:F:359:ASP:O	1:F:363:GLU:HG2	2.02	0.59
1:G:242:LYS:C	1:G:244:GLY:H	2.10	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:K:16:MET:SD	1:K:73:MET:HE1	2.42	0.59
1:L:193:MET:HE1	1:L:292:ILE:CG1	2.21	0.59
1:M:242:LYS:C	1:M:244:GLY:H	2.10	0.59
1:A:27:VAL:HG12	1:A:90:THR:HG23	1.84	0.59
1:A:69:MET:O	1:A:73:MET:HG3	2.02	0.59
1:A:242:LYS:C	1:A:244:GLY:H	2.10	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:69:MET:O	1:N:73:MET:HG3	2.02	0.59
1:E:16:MET:SD	1:E:73:MET:HE1	2.42	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
1:N:242:LYS:C	1:N:244:GLY:H	2.09	0.59
1:D:486:GLY:C	1:D:491:MET:HE2	2.28	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:C:16:MET:SD	1:C:73:MET:HE1	2.43	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:82:ASN:HB2	1:J:89:THR:CG2	2.32	0.59
1:J:455:VAL:HG13	1:J:460:GLU:HB2	1.85	0.59
1:K:218:PRO:HB3	1:K:246:PRO:HG2	1.84	0.59
1:B:160:LYS:O	1:B:164:GLU:HG3	2.02	0.58
1:G:16:MET:SD	1:G:73:MET:HE1	2.43	0.58
1:G:69:MET:O	1:G:73:MET:HG3	2.03	0.58
1:G:183:LEU:HD13	1:G:184:GLN:HG3	1.84	0.58
1:H:160:LYS:O	1:H:164:GLU:HG3	2.03	0.58
1:H:271:VAL:HG21	2:V:607:TRP:HZ3	1.68	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:B:242:LYS:C	1:B:244:GLY:H	2.10	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:C:242:LYS:C	1:C:244:GLY:H	2.10	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:F:242:LYS:C	1:F:244:GLY:H	2.12	0.58
1:N:486:GLY:C	1:N:491:MET:HE2	2.28	0.58
1:A:57:ALA:O	1:A:75:LYS:HE3	2.04	0.58
1:A:383:ALA:O	1:A:384:ALA:HB3	2.04	0.58
1:D:183:LEU:HD13	1:D:184:GLN:HG3	1.84	0.58
1:I:7:LYS:HG3	1:I:66:PHE:CZ	2.38	0.58
1:I:194:GLN:O	1:I:371:LYS:HE3	2.03	0.58
1:I:270:ILE:HD13	2:W:608:GLY:HA3	1.85	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:M:383:ALA:HB1	1:N:281:PHE:HZ	1.69	0.58
1:N:266:THR:HG21	1:N:273:VAL:H	1.68	0.58
1:N:284:ARG:O	1:N:288:MET:HG3	2.01	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:G:120:ILE:O	1:G:124:VAL:HG23	2.03	0.58
1:C:218:PRO:HB3	1:C:246:PRO:HG2	1.86	0.58
1:G:383:ALA:O	1:G:384:ALA:HB3	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:L:183:LEU:HD13	1:L:184:GLN:HG3	1.85	0.57
1:B:486:GLY:C	1:B:491:MET:HE2	2.29	0.57
1:F:417:VAL:HA	1:F:420:ILE:HG22	1.85	0.57
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:K:486:GLY:C	1:K:491:MET:HE2	2.29	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:27:VAL:HG12	1:F:90:THR:HG23	1.86	0.57
1:F:266:THR:HG21	1:F:273:VAL:H	1.68	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:E:215:LEU:HB2	1:E:323:VAL:HG22	1.86	0.57
1:F:486:GLY:C	1:F:491:MET:HE2	2.30	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:L:16:MET:SD	1:L:73:MET:HE1	2.44	0.57
1:G:218:PRO:HB3	1:G:246:PRO:HG2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:486:GLY:C	1:G:491:MET:HE2	2.30	0.57
1:J:194:GLN:O	1:J:371:LYS:HE3	2.05	0.57
1:C:69:MET:O	1:C:73:MET:HG3	2.05	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:57:ALA:O	1:M:75:LYS:HE3	2.03	0.57
1:M:413:ALA:HB2	1:M:475:ASN:HD22	1.70	0.57
1:M:486:GLY:C	1:M:491:MET:HE2	2.30	0.57
1:J:46:ALA:HB2	1:K:76:GLU:CG	2.35	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:L:383:ALA:HB1	1:M:281:PHE:CZ	2.38	0.57
1:L:486:GLY:C	1:L:491:MET:HE2	2.30	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:E:265:ASN:ND2	2:S:610:LEU:H	2.00	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: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: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
2:P:607:TRP:CD1	2:P:607:TRP:H	2.23	0.56
1:C:46:ALA:HB2	1:D:76:GLU:CG	2.27	0.56
1:C:455:VAL:HG13	1:C:460:GLU:HB2	1.88	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: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: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:71:ALA:O	1:G:75:LYS:HB2	2.05	0.56
1:G:215:LEU:HB2	1:G:323:VAL:HG22	1.87	0.56
1:H:349:ILE:HA	1:H:352:GLN:HG3	1.87	0.56
1:J:16:MET:SD	1:J:73:MET:HE1	2.45	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:I:271:VAL:HG21	2:W:607:TRP:HZ3	1.71	0.56
1:N:449:ALA:HB3	1:N:450:PRO:HD3	1.86	0.56
1:A:16:MET:SD	1:A:73:MET:HE1	2.45	0.56
1:B:265:ASN:ND2	2:P:610:LEU:H	2.01	0.56
1:M:202:PRO:O	1:M:203:TYR:HB2	2.05	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:H:486:GLY:C	1:H:491:MET:HE2	2.31	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: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: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:N:71:ALA:O	1:N:75:LYS:HB2	2.06	0.55
1:N:166:MET:HE2	1:N:171:LYS:HA	1.89	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: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:M:414:GLY:O	1:M:417:VAL:HG13	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:202:PRO:C	1:H:204:PHE:H	2.14	0.55
1:H:383:ALA:O	1:H:384:ALA:HB3	2.07	0.55
1:J:486:GLY:C	1:J:491:MET:HE2	2.32	0.55
1:M:69:MET:O	1:M:73:MET:HG3	2.07	0.55
1:B:69:MET:O	1:B:73:MET:HG3	2.06	0.55
1:B:120:ILE:O	1:B:124:VAL:HG23	2.07	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
2:R:607:TRP:CD1	2:R:607:TRP:H	2.24	0.55
1:L:7:LYS:HG3	1:L:66:PHE:CZ	2.42	0.55
1:L:284:ARG:O	1:L:288:MET:HG3	2.06	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:B:202:PRO:C	1:B:204:PHE:H	2.15	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: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:265:ASN:ND2	2:U:610:LEU:H	2.02	0.55
1:G:284:ARG:O	1:G:288:MET:HG3	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:C:193:MET:CE	1:C:292:ILE:HG12	2.18	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:I:486:GLY:C	1:I:491:MET:HE2	2.32	0.54
2:X:607:TRP:CD1	2:X:607:TRP:H	2.24	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:B:16:MET:SD	1:B:73:MET:HE1	2.47	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:69:MET:O	1:E:73:MET:HG3	2.07	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: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:A:213:VAL:HB	1:A:325:ILE:HB	1.89	0.54
1:G:193:MET:CE	1:G:292:ILE:HG12	2.25	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:A:486:GLY:C	1:A:491:MET:HE2	2.32	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:607:TRP:H	2:Q:607:TRP:CD1	2.25	0.54
1:G:349:ILE:HA	1:G:352:GLN:HG3	1.89	0.54
1:I:193:MET:CE	1:I:292:ILE:HG12	2.25	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
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
2:T:607:TRP:H	2:T:607:TRP:CD1	2.25	0.54
1:A:215:LEU:HB2	1:A:323:VAL:HG22	1.89	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:E:486:GLY:C	1:E:491:MET:HE2	2.32	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:J:252:GLU:O	1:J:253:ASP:HB2	2.08	0.54
1:K:202:PRO:C	1:K:204:PHE:H	2.16	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: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:M:265:ASN:ND2	2:1:610:LEU:H	2.01	0.53
1:C:120:ILE:O	1:C:124:VAL:HG23	2.08	0.53
1:C:486:GLY:C	1:C:491:MET:HE2	2.32	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:166:MET:HE2	1:M:171:LYS:HA	1.90	0.53
1:M:270:ILE:HA	1:N:229:ASN:HD22	1.73	0.53
1:N:265:ASN:ND2	2:2:610:LEU:H	2.04	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
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:414:GLY:H	1:L:494:LEU:HA	1.74	0.53
1:L:455:VAL:HG13	1:L:460:GLU:HB2	1.90	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:K:271:VAL:HG21	2:Y:607:TRP:HZ3	1.72	0.53
1:L:202:PRO:C	1:L:204:PHE:H	2.17	0.53
1:M:13:ARG:HD2	1:M:104:LEU:HD22	1.90	0.53
1:E:7:LYS:HG3	1:E:66:PHE:CZ	2.43	0.53
1:E:193:MET:CE	1:E:292:ILE:HG12	2.23	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:G:16:MET:HB3	1:G:514:MET:HE3	1.91	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:27:VAL:CG1	1:B:90:THR:HG23	2.39	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:C:271:VAL:HG21	2:Q:607:TRP:HZ3	1.72	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:G:202:PRO:C	1:G:204:PHE:H	2.16	0.53
1:I:265:ASN:ND2	2:W:610:LEU:H	2.05	0.53
1:K:37:ASN:ND2	1:K:51:LYS:HG3	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:5:ASP:HB2	1:A:524:LEU:HD12	1.91	0.53
1:A:349:ILE:HA	1:A:352:GLN:HG3	1.90	0.53
1:D:383:ALA:CB	1:E:281:PHE:CZ	2.89	0.53
1:B:5:ASP:HB2	1:B:524:LEU:HD12	1.91	0.53
1:B:349:ILE:HA	1:B:352:GLN:HG3	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:F:69:MET:O	1:F:73:MET:HG3	2.09	0.53
1:F:160:LYS:O	1:F:164:GLU:HG3	2.09	0.53
1:J:271:VAL:HG21	2:X:607:TRP:HZ3	1.73	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
2:2:607:TRP:CD1	2:2:607:TRP:H	2.26	0.53
1:F:166:MET:HE2	1:F:171:LYS:HA	1.91	0.52
1:F:271:VAL:HG21	2:T:607:TRP:HZ3	1.73	0.52
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:D:291:ASP:OD2	1:D:368:ARG:HD2	2.10	0.52
1:D:384:ALA:C	1:D:385:THR:HG23	2.34	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:266:THR:CG2	1:G:273:VAL:H	2.21	0.52
1:G:271:VAL:HG12	1:G:273:VAL:HG23	1.90	0.52
1:I:71:ALA:O	1:I:75:LYS:HB2	2.09	0.52
1:I:166:MET:HE2	1:I:171:LYS:HA	1.91	0.52
1:K:166:MET:HE2	1:K:171:LYS:HA	1.92	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:N:202:PRO:C	1:N:204:PHE:H	2.17	0.52
1:A:166:MET:HE2	1:A:171:LYS:HA	1.90	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:202:PRO:C	1:F:204:PHE:H	2.17	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:27:VAL:CG1	1:A:90:THR:HG23	2.39	0.52
1:A:263:VAL:O	1:A:267:MET:HB2	2.09	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:H:166:MET:HE2	1:H:171:LYS:HA	1.92	0.52
2:W:607:TRP:CD1	2:W:607:TRP:H	2.27	0.52
1:K:266:THR:HA	1:K:271:VAL:O	2.10	0.52
1:A:252:GLU:O	1:A:253:ASP:HB2	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:37:ASN:ND2	1:D:51:LYS:HG3	2.25	0.52
1:D:215:LEU:HB2	1:D:323:VAL:HG22	1.92	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
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:B:166:MET:HE2	1:B:171:LYS:HA	1.92	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:D:166:MET:HE2	1:D:171:LYS:HA	1.92	0.52
1:D:202:PRO:C	1:D:204:PHE:H	2.17	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:202:PRO:C	1:J:204:PHE:H	2.17	0.52
1:J:5:ASP:HB2	1:J:524:LEU:HD12	1.92	0.52
1:J:413:ALA:HB2	1:J:475:ASN:HD22	1.74	0.52
1:A:183:LEU:CD1	1:A:184:GLN:HG3	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:607:TRP:CD1	2:O:607:TRP:H	2.27	0.51
1:C:271:VAL:HG12	1:C:273:VAL:HG23	1.92	0.51
1:H:76:GLU:CG	1:N:46:ALA:HB2	2.38	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: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:37:ASN:ND2	1:G:51:LYS:HG3	2.26	0.51
1:G:200:LEU:O	1:G:201:SER:HB3	2.10	0.51
1:H:230:ILE:HD13	1:H:261:THR:HB	1.93	0.51
1:H:384:ALA:C	1:H:385:THR:HG23	2.36	0.51
1:H:496:PRO:HD2	1:H:499:VAL:HG11	1.91	0.51
1:J:166:MET:HE2	1:J:171:LYS:HA	1.92	0.51
1:J:266:THR:CG2	1:J:273:VAL:H	2.22	0.51
2:Z:607:TRP:CD1	2:Z:607:TRP:H	2.28	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
2:V:607:TRP:CD1	2:V:607:TRP:H	2.27	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:M:384:ALA:C	1:M:385:THR:HG23	2.36	0.51
1:N:193:MET:CE	1:N:292:ILE:HG12	2.25	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
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:L:384:ALA:C	1:L:385:THR:HG23	2.36	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:A:271:VAL:HG21	2:O:607:TRP:HZ3	1.76	0.51
1:B:384:ALA:C	1:B:385:THR:HG23	2.35	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:425:LYS:HD3	3:B:1203:HOH:O	2.10	0.51
1:E:202:PRO:C	1:E:204:PHE:H	2.18	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:B:5:ASP:HB2	1:B:524:LEU:CD1	2.41	0.51
1:B:200:LEU:HG	1:B:276:VAL:HA	1.92	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:202:PRO:C	1:C:204:PHE:H	2.18	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:M:193:MET:CE	1:M:292:ILE:HG12	2.23	0.51
1:N:201:SER:C	1:N:202:PRO:O	2.54	0.51
1:A:265:ASN:ND2	2:O:610:LEU:H	2.06	0.50
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
2:U:607:TRP:CD1	2:U:607:TRP:H	2.29	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:J:384:ALA:C	1:J:385:THR:HG23	2.36	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:271:VAL:HG12	1:A:273:VAL:HG23	1.91	0.50
1:A:384:ALA:C	1:A:385:THR:HG23	2.36	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:7:LYS:HG3	1:H:66:PHE:CZ	2.46	0.50
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:G:166:MET:HE2	1:G:171:LYS:HA	1.93	0.50
1:G:384:ALA:C	1:G:385:THR:HG23	2.36	0.50
1:H:27:VAL:CG1	1:H:90:THR:HG23	2.41	0.50
1:I:37:ASN:ND2	1:I:51:LYS:HG3	2.26	0.50
1:I:414:GLY:H	1:I:494:LEU:HA	1.77	0.50
1:M:202:PRO:C	1:M:204:PHE:H	2.18	0.50
1:M:230:ILE:HD13	1:M:261:THR:HG21	1.93	0.50
1:A:202:PRO:C	1:A:204:PHE:H	2.18	0.50
1:C:37:ASN:ND2	1:C:51:LYS:HG3	2.27	0.50
1:C:200:LEU:HG	1:C:276:VAL:HA	1.93	0.50
1:E:245:LYS:HZ2	1:E:319:GLN:NE2	2.10	0.50
1:F:71:ALA:O	1:F:75:LYS: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: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:46:ALA:HB2	1:C:76:GLU:CG	2.40	0.50
1:B:198:GLY:HA3	1:B:328:ASP:HA	1.92	0.50
1:B:266:THR:HA	1:B:271:VAL:O	2.12	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:37:ASN:ND2	1:H:51:LYS:HG3	2.26	0.50
1:H:183:LEU:CD1	1:H:184:GLN:HG3	2.42	0.50
1:I:384:ALA:C	1:I:385:THR:HG23	2.35	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:200:LEU:HG	1:N:276:VAL:HA	1.92	0.50
1:C:166:MET:HE2	1:C:171:LYS:HA	1.94	0.50
1:C:463:SER:O	1:C:467:ASN:HB2	2.12	0.50
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:270:ILE:HA	1:K:229:ASN:ND2	2.26	0.50
1:J:525:PRO:HG2	3:J:1175:HOH:O	2.11	0.50
2:Y:607:TRP:H	2:Y:607:TRP:CD1	2.28	0.50
1:L:37:ASN:ND2	1:L:51:LYS:HG3	2.26	0.50
1:L:414:GLY:O	1:L:417:VAL:HG13	2.12	0.50
1:F:270:ILE:HG12	1:G:229:ASN:ND2	2.27	0.50
1:I:202:PRO:C	1:I:204:PHE:H	2.20	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:N:270:ILE:HD13	2:2:608:GLY:HA3	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:E:252:GLU:O	1:E:253:ASP:HB2	2.11	0.50
2:S:607:TRP:CD1	2:S:607:TRP:H	2.29	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:E:166:MET:HE2	1:E:171:LYS:HA	1.94	0.49
1:K:241:ALA:HA	1:K:271:VAL:HG22	1.94	0.49
1:K:384:ALA:C	1:K:385:THR:HG23	2.37	0.49
1:L:218:PRO:HB3	1:L:246:PRO:HG2	1.94	0.49
1:A:291:ASP:OD2	1:A:368:ARG:HD2	2.12	0.49
1:C:384:ALA:C	1:C:385:THR:HG23	2.37	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
2:1:602:TRP:NE1	2:1:612:PRO:HG3	2.27	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:384:ALA:O	1:D:385:THR:HG23	2.11	0.49
1:E:38:VAL:HG22	1:F:519:CYS:HB3	1.94	0.49
1:F:384:ALA:C	1:F:385:THR:HG23	2.37	0.49
1:F:414:GLY:H	1:F:494:LEU:HA	1.77	0.49
1:H:305:ILE:HG22	1:H:305:ILE:O	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
1:E:291:ASP:OD2	1:E:368:ARG:HD2	2.13	0.49
1:E:384:ALA:C	1:E:385:THR:HG23	2.37	0.49
1:F:200:LEU:HG	1:F:276:VAL:HA	1.93	0.49
2:X:602:TRP:CE2	2:X:612:PRO:HG3	2.47	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
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: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:N:384:ALA:C	1:N:385:THR:HG23	2.37	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
2:T:602:TRP:NE1	2:T:612:PRO:HG3	2.27	0.49
1:G:235:PRO:HG3	1:G:310:GLU:HA	1.93	0.49
1:G:252:GLU:O	1:G:253:ASP:HB2	2.12	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
1:D:238:GLU:O	1:D:241:ALA:HB3	2.12	0.49
1:G:245:LYS:HZ2	1:G:319:GLN:NE2	2.10	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:201:SER:C	1:C:202:PRO:O	2.56	0.49
1:F:336:VAL:O	1:F:337:GLY:C	2.56	0.49
1:H:5:ASP:HB2	1:H:524:LEU:HD12	1.95	0.49
1:J:71:ALA:O	1:J:75:LYS:HB2	2.13	0.49
1:L:166:MET:HE2	1:L:171:LYS:HA	1.95	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:M:231:ARG:NH1	2:1:612:PRO:O	2.46	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:5:ASP:HB2	1:E:524:LEU:CD1	2.42	0.49
1:E:240:VAL:HG11	1:E:247:LEU:HB2	1.94	0.49
1:F:305:ILE:O	1:F:305:ILE:HG22	2.13	0.49
1:G:231:ARG:NH1	2:U:612:PRO:O	2.46	0.49
1:H:201:SER:C	1:H:202:PRO:O	2.56	0.49
1:I:235:PRO:HG3	1:I:310:GLU:HA	1.95	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:A:245:LYS:HZ2	1:A:319:GLN:NE2	2.11	0.48
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:27:VAL:CG1	1:M:90:THR:HG23	2.43	0.48
1:M:241:ALA:HA	1:M:271:VAL:HG22	1.94	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:C:245:LYS:HZ2	1:C:319:GLN:NE2	2.11	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:16:MET:HB3	1:I:514:MET:HE3	1.94	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:252:GLU:O	1:L:253:ASP:HB2	2.14	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:27:VAL:HG12	1:E:90:THR:HG23	1.95	0.48
1:E:271:VAL:HG21	2:S:607:TRP:HZ3	1.78	0.48
1:J:5:ASP:HB2	1:J:524:LEU:CD1	2.44	0.48
1:J:349:ILE:HA	1:J:352:GLN:HG3	1.95	0.48
2:X:602:TRP:NE1	2:X:612:PRO:HG3	2.28	0.48
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
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:N:185:ASP:OD1	1:N:382:GLY:N	2.47	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
2:1:602:TRP:CE2	2:1:612:PRO:HG3	2.49	0.48
1:N:305:ILE:HG22	1:N:305:ILE:O	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:230:ILE:HD13	1:J:261:THR:HG21	1.95	0.48
1:J:247:LEU:HD21	1:J:249:ILE:HD11	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HG22	1:K:305:ILE:O	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: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
1:J:265:ASN:ND2	2:X:610:LEU:H	2.10	0.48
1:K:185:ASP:OD1	1:K:382:GLY:N	2.47	0.48
1:N:16:MET:O	1:N:20:VAL:HG13	2.14	0.48
1:A:201:SER:C	1:A:202:PRO:O	2.55	0.47
1:C:240:VAL:HG11	1:C:247:LEU:HB2	1.96	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
2:1:607:TRP:H	2:1:607:TRP:CD1	2.29	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:79:SER:HA	1:H:89:THR:CG2	2.44	0.47
1:H:155:ASP:OD1	1:H:157:THR:HB	2.14	0.47
1:I:63:GLU:HB3	3:I:1204:HOH:O	2.14	0.47
1:I:202:PRO:O	1:I:204:PHE:N	2.45	0.47
1:J:201:SER:C	1:J:202:PRO:O	2.56	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:M:201:SER:C	1:M:202:PRO:O	2.57	0.47
1:N:193:MET:HG3	1:N:371:LYS:HB3	1.96	0.47
1:D:214:GLU:CD	1:D:322:ARG:HH21	2.22	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:H:229:ASN:HD22	1:N:270:ILE:HA	1.78	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:5:ASP:HB2	1:M:524:LEU:CD1	2.43	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:N:245:LYS:HZ2	1:N:319:GLN:NE2	2.12	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
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
2:P:602:TRP:NE1	2:P:612:PRO:HG3	2.29	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:O	1:I:305:ILE:HG22	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:O	1:L:305:ILE:HG22	2.14	0.47
1:A:199:TYR:HA	1:A:276:VAL:HG12	1.97	0.47
1:A:270:ILE:HG12	1:B:229:ASN:HD21	1.80	0.47
1:A:336:VAL:O	1:A:337:GLY:C	2.56	0.47
1:B:382:GLY:O	1:B:389:MET:HG2	2.14	0.47
1:C:214:GLU:CD	1:C:322:ARG:HH21	2.23	0.47
1:D:247:LEU:HD21	1:D:249:ILE:HD11	1.95	0.47
1:E:336:VAL:O	1:E:337:GLY:C	2.58	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:G:414:GLY:H	1:G:494:LEU:HA	1.80	0.47
1:H:5:ASP:HB2	1:H:524:LEU:CD1	2.45	0.47
1:H:384:ALA:O	1:H:385:THR:HG23	2.14	0.47
2:V:602:TRP:NE1	2:V:612:PRO:HG3	2.29	0.47
1:I:214:GLU:CD	1:I:322:ARG:HH21	2.22	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:M:193:MET:HG2	1:M:194:GLN:N	2.29	0.47
1:N:336:VAL:O	1:N:337:GLY:C	2.58	0.47
1:A:238:GLU:O	1:A:241:ALA:HB3	2.15	0.47
1:B:202:PRO:C	1:B:204:PHE:N	2.73	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: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
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:I:266:THR:CG2	1:I:273:VAL:H	2.27	0.47
1:J:214:GLU:CD	1:J:322:ARG:HH21	2.22	0.47
1:K:240:VAL:HG11	1:K:247:LEU:HB2	1.96	0.47
1:A:37:ASN:ND2	1:A:51:LYS:HG3	2.30	0.47
1:A:245:LYS:NZ	1:A:319:GLN:NE2	2.62	0.47
1:A:319:GLN:HB3	1:A:336:VAL:HG21	1.96	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:L:201:SER:C	1:L:202:PRO:O	2.55	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:F:245:LYS:HZ2	1:F:319:GLN:NE2	2.12	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:I:200:LEU:O	1:I:201:SER:HB3	2.13	0.46
1:K:155:ASP:OD1	1:K:157:THR:HB	2.15	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:L:130:GLU:HG3	3:L:1115:HOH:O	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:199:TYR:HA	1:L:276:VAL:HG12	1.97	0.46
1:L:369:VAL:HG23	1:L:370:ALA:N	2.29	0.46
1:M:199:TYR:HA	1:M:276:VAL:HG12	1.98	0.46
1:B:193:MET:HG3	1:B:371:LYS:HB3	1.96	0.46
1:D:27:VAL:CG1	1:D:90:THR:HG23	2.45	0.46
1:D:463:SER:O	1:D:467:ASN:HB2	2.15	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:I:270:ILE:CD1	2:W:608:GLY:HA3	2.45	0.46
1:J:27:VAL:CG1	1:J:90:THR:HG23	2.45	0.46
1:J:185:ASP:OD1	1:J:382:GLY:N	2.48	0.46
1:A:230:ILE:CD1	1:A:261:THR:HB	2.46	0.46
1:D:90:THR:O	1:D:94:VAL:HG13	2.15	0.46
1:D:199:TYR:CZ	1:D:327:LYS:HA	2.51	0.46
1:E:131:LEU:HD13	1:E:422:VAL:HG21	1.97	0.46
1:E:231:ARG:NH1	2:S:612:PRO:O	2.48	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:H:38:VAL:HG22	1:I:519:CYS:HB3	1.96	0.46
1:I:95:LEU:O	1:I:99:ILE:HG13	2.16	0.46
1:I:384:ALA:O	1:I:385:THR:HG23	2.15	0.46
1:J:384:ALA:O	1:J:385:THR:HG23	2.15	0.46
1:L:193:MET:CE	1:L:292:ILE:HG12	2.26	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:79:SER:HA	1:G:89:THR:HG22	1.97	0.46
1:G:131:LEU:HD13	1:G:422:VAL:HG21	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:K:242:LYS:C	1:K:244:GLY:N	2.73	0.46
1:A:321:LYS:HD2	1:A:334:ASP:OD2	2.15	0.46
1:D:201:SER:C	1:D:202:PRO:O	2.59	0.46
1:E:193:MET:HG2	1:E:194:GLN:N	2.31	0.46
2:V:605:THR:HG1	2:V:607:TRP:CD1	2.33	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:79:SER:HA	1:K:89:THR:CG2	2.46	0.46
2:Y:604:THR:HG22	2:Y:605:THR:O	2.16	0.46
1:L:79:SER:HA	1:L:89:THR:HG22	1.98	0.46
1:L:265:ASN:HD21	2:Z:610:LEU:N	2.00	0.46
1:M:247:LEU:HD21	1:M:249:ILE:HD11	1.96	0.46
1:M:336:VAL:O	1:M:337:GLY:C	2.59	0.46
1:M:384:ALA:O	1:M:385:THR:HG23	2.14	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:D:242:LYS:C	1:D:244:GLY:N	2.74	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:K:270:ILE:CD1	2:Y:608:GLY:HA3	2.45	0.46
1:L:242:LYS:C	1:L:244:GLY:N	2.73	0.46
1:M:230:ILE:HD13	1:M:261:THR:HB	1.96	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:G:201:SER:C	1:G:202:PRO:O	2.59	0.46
1:H:79:SER:HA	1:H:89:THR:HG22	1.97	0.46
2:V:602:TRP:CE2	2:V:612:PRO:HG3	2.51	0.46
1:I:241:ALA:HA	1:I:271:VAL:HG22	1.98	0.46
1:K:336:VAL:O	1:K:337:GLY:C	2.58	0.46
1:M:240:VAL:HG11	1:M:247:LEU:HB2	1.96	0.46
1:A:90:THR:O	1:A:94:VAL:HG13	2.14	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:B:199:TYR:CZ	1:B:327:LYS:HA	2.51	0.46
2:P:602:TRP:CE2	2:P:612:PRO:HG3	2.50	0.46
1:C:90:THR:O	1:C:94:VAL:HG13	2.15	0.46
1:C:270:ILE:CD1	2:Q:608:GLY:HA3	2.45	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:J:242:LYS:C	1:J:244:GLY:N	2.74	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:270:ILE:HA	1:G:229:ASN:HD22	1.81	0.46
1:G:202:PRO:C	1:G:204:PHE:N	2.74	0.46
1:H:198:GLY:HA3	1:H:328:ASP:HA	1.97	0.46
1:J:131:LEU:HD13	1:J:422:VAL:HG21	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:N:5:ASP:HB2	1:N:524:LEU:CD1	2.46	0.46
1:N:199:TYR:HA	1:N:276:VAL:HG12	1.98	0.46
1:B:199:TYR:HA	1:B:276:VAL:HG12	1.98	0.46
1:B:245:LYS:HZ2	1:B:319:GLN:NE2	2.13	0.46
1:B:270:ILE:HD13	2:P:608:GLY:HA3	1.97	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
2:R:602:TRP:CE2	2:R:612:PRO:HG3	2.51	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:D:265:ASN:HD21	2:R:610:LEU:N	2.03	0.45
2:T:602:TRP:CE2	2:T:612:PRO:HG3	2.52	0.45
1:G:90:THR:O	1:G:94:VAL:HG13	2.15	0.45
1:G:336:VAL:O	1:G:337:GLY:C	2.59	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
1:K:214:GLU:CD	1:K:322:ARG:HH21	2.24	0.45
1:B:201:SER:C	1:B:202:PRO:O	2.58	0.45
1:C:245:LYS:NZ	1:C:319:GLN:NE2	2.64	0.45
2:Q:602:TRP:NE1	2:Q:612:PRO:HG3	2.31	0.45
1:D:16:MET:HB3	1:D:514:MET:HE3	1.97	0.45
1:D:270:ILE:CD1	2:R:608:GLY:HA3	2.46	0.45
1:E:201:SER:C	1:E:202:PRO:O	2.59	0.45
1:E:242:LYS:C	1:E:244:GLY:N	2.74	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:87:ASP:O	1:H:499:VAL:HG23	2.16	0.45
1:H:185:ASP:OD1	1:H:382:GLY:N	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:349:ILE:O	1:H:353:ILE:HG13	2.16	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: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
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:95:LEU:O	1:J:99:ILE:HG13	2.17	0.45
1:J:263:VAL:O	1:J:267:MET:HB2	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:M:238:GLU:O	1:M:241:ALA:HB3	2.16	0.45
1:M:242:LYS:C	1:M:244:GLY:N	2.74	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
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:199:TYR:CZ	1:I:327:LYS:HA	2.51	0.45
1:I:222:LEU:HD23	1:I:250:ILE:HB	1.98	0.45
2:W:604:THR:HG22	2:W:605:THR:O	2.16	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
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:D:336:VAL:O	1:D:337:GLY:C	2.58	0.45
1:F:7:LYS:HG3	1:F:66:PHE:CZ	2.51	0.45
1:F:16:MET:HB3	1:F:514:MET:HE3	1.98	0.45
1:F:241:ALA:HA	1:F:271:VAL:HG22	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:231:ARG:NH1	2:V:612:PRO:O	2.50	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:218:PRO:HD2	1:D:320:ALA:O	2.16	0.45
1:D:240:VAL:HG11	1:D:247:LEU:HB2	1.97	0.45
1:H:217:SER:N	1:H:218:PRO:CD	2.80	0.45
1:I:336:VAL:O	1:I:337:GLY:C	2.58	0.45
1:J:193:MET:HG2	1:J:194:GLN:N	2.31	0.45
1:J:336:VAL:O	1:J:337:GLY:C	2.58	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:L:202:PRO:C	1:L:204:PHE:N	2.75	0.45
1:N:176:THR:HG22	1:N:177:VAL:N	2.32	0.45
1:B:214:GLU:CD	1:B:322:ARG:HH21	2.25	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:F:214:GLU:CD	1:F:322:ARG:HH21	2.24	0.45
1:F:273:VAL:HG12	1:F:274:ALA:N	2.30	0.45
2:U:602:TRP:NE1	2:U:612:PRO:HG3	2.31	0.45
1:H:202:PRO:C	1:H:204:PHE:N	2.74	0.45
1:K:106:ALA:HA	1:K:111:MET:HE3	1.97	0.45
1:L:146:GLN:O	1:L:150:ILE:HG13	2.17	0.45
1:M:409:GLU:OE2	1:M:498:LYS:HG3	2.15	0.45
1:D:16:MET:O	1:D:20:VAL:HG13	2.17	0.45
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: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:16:MET:HB3	1:M:514:MET:HE3	1.98	0.45
1:M:270:ILE:HD13	2:1:608:GLY:HA3	1.99	0.45
1:A:242:LYS:C	1:A:244:GLY:N	2.75	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:139:SER:O	1:E:171:LYS:HE2	2.17	0.45
1:H:245:LYS:HZ2	1:H:319:GLN:NE2	2.15	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:E:16:MET:HB3	1:E:514:MET:HE3	1.98	0.45
1:F:70:GLY:HA2	1:F:73:MET:HE3	1.99	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:G:214:GLU:CD	1:G:322:ARG:HH21	2.25	0.45
1:H:218:PRO:HD2	1:H:320:ALA:O	2.17	0.45
1:J:219:PHE:HB3	1:J:317:LEU:HD23	1.99	0.45
1:J:273:VAL:HG12	1:J:274:ALA:N	2.31	0.45
1:L:217:SER:N	1:L:218:PRO:CD	2.80	0.45
1:L:270:ILE:O	1:L:271:VAL:HB	2.16	0.45
1:M:155:ASP:OD1	1:M:157:THR:HB	2.17	0.45
1:N:79:SER:HA	1:N:89:THR:CG2	2.46	0.45
1:N:384:ALA:O	1:N:385:THR:HG23	2.16	0.45
1:A:240:VAL:HG11	1:A:247:LEU:HB2	1.98	0.44
1:C:202:PRO:C	1:C:204:PHE:N	2.76	0.44
1:C:264:VAL:O	1:C:268:ARG:HG3	2.17	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
1:D:245:LYS:HZ2	1:D:319:GLN:NE2	2.16	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:F:201:SER:C	1:F:202:PRO:O	2.60	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:222:LEU:HD23	1:J:250:ILE:HB	1.99	0.44
1:J:240:VAL:HG11	1:J:247:LEU:HB2	1.98	0.44
1:K:202:PRO:C	1:K:204:PHE:N	2.75	0.44
1:M:25:ASP:HA	1:M:28:LYS:HE2	2.00	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:E:106:ALA:HA	1:E:111:MET:HE3	1.99	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: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:C:242:LYS:C	1:C:244:GLY:N	2.75	0.44
1:E:100:ILE:HD13	1:E:514:MET:CE	2.47	0.44
2:S:602:TRP:CE2	2:S:612:PRO:HG3	2.52	0.44
1:F:230:ILE:HD13	1:F:261:THR:HG21	2.00	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:H:336:VAL:O	1:H:337:GLY:C	2.59	0.44
1:I:79:SER:HA	1:I:89:THR:HG22	1.99	0.44
1:I:201:SER:C	1:I:202:PRO:O	2.58	0.44
2:W:602:TRP:NE1	2:W:612:PRO:HG3	2.32	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
1:A:217:SER:N	1:A:218:PRO:CD	2.81	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
1:E:198:GLY:HA3	1:E:328:ASP:HA	2.00	0.44
1:E:214:GLU:CD	1:E:322:ARG:HH21	2.26	0.44
2:S:602:TRP:NE1	2:S:612:PRO:HG3	2.33	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:95:LEU:O	1:K:99:ILE:HG13	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:B:242:LYS:C	1:B:244:GLY:N	2.76	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
2:S:604:THR:HG22	2:S:605:THR:O	2.17	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:87:ASP:O	1:K:499:VAL:HG23	2.17	0.44
1:K:202:PRO:O	1:K:204:PHE:N	2.48	0.44
2:Y:602:TRP:NE1	2:Y:612:PRO:HG3	2.33	0.44
1:L:214:GLU:CD	1:L:322:ARG:HH21	2.24	0.44
1:M:87:ASP:O	1:M:499:VAL:HG23	2.18	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:N:87:ASP:O	1:N:499:VAL:HG23	2.17	0.44
1:N:349:ILE:O	1:N:353:ILE:HG13	2.18	0.44
1:C:305:ILE:HG22	1:C:305:ILE:O	2.18	0.44
2:Q:604:THR:HG22	2:Q:605:THR:O	2.18	0.44
1:D:241:ALA:HA	1:D:271:VAL:HG22	1.99	0.44
2:R:602:TRP:NE1	2:R:612:PRO:HG3	2.33	0.44
1:F:68:ASN:O	1:F:72:GLN:HG2	2.17	0.44
1:F:231:ARG:NH1	2:T:612:PRO:O	2.51	0.44
2:U:602:TRP:CE2	2:U:612:PRO:HG3	2.52	0.44
1:J:139:SER:O	1:J:171:LYS:HE2	2.18	0.44
1:K:201:SER:C	1:K:202:PRO:O	2.58	0.44
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
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:J:369:VAL:HG23	1:J:370:ALA:N	2.32	0.44
1:K:16:MET:HB3	1:K:514:MET:HE3	1.99	0.44
1:M:106:ALA:HA	1:M:111:MET:HE3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:79:SER:HA	1:B:89:THR:HG22	2.00	0.44
1:B:217:SER:N	1:B:218:PRO:HD3	2.33	0.44
1:C:106:ALA:HA	1:C:111:MET:HE3	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: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
2:W:602:TRP:CE2	2:W:612:PRO:HG3	2.53	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:90:THR:O	1:N:94:VAL:HG13	2.17	0.43
1:A:16:MET:HB3	1:A:514:MET:HE3	2.00	0.43
2:O:604:THR:HG22	2:O:605:THR:O	2.18	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
1:N:214:GLU:CD	1:N:322:ARG:HH21	2.25	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
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:I:369:VAL:HG23	1:I:370:ALA:N	2.32	0.43
1:J:176:THR:HG22	1:J:177:VAL:N	2.34	0.43
2:X:604:THR:HG22	2:X:605:THR:O	2.18	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:N:202:PRO:C	1:N:204:PHE:N	2.74	0.43
1:A:270:ILE:HG12	1:B:229:ASN:ND2	2.32	0.43
1:B:200:LEU:O	1:B:201:SER:HB3	2.18	0.43
1:B:336:VAL:O	1:B:337:GLY:C	2.60	0.43
1:B:381:VAL:O	1:B:382:GLY:O	2.37	0.43
1:C:16:MET:HB3	1:C:514:MET:HE3	1.99	0.43
1:C:42:LYS:HE3	1:C:48:THR:OG1	2.18	0.43
1:C:193:MET:HG3	1:C:371:LYS:HB3	2.00	0.43
2:Q:602:TRP:CE2	2:Q:612:PRO:HG3	2.53	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:42:LYS:HE3	1:E:48:THR:OG1	2.19	0.43
1:E:230:ILE:CD1	1:E:261:THR:HB	2.47	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:HD13	1:K:295:LEU:O	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
1:A:199:TYR:CZ	1:A:327:LYS:HA	2.53	0.43
1:A:247:LEU:HD21	1:A:249:ILE:HD11	2.00	0.43
1:B:186:GLU:HB2	1:B:380:LYS:HB2	2.00	0.43
1:F:79:SER:HA	1:F:89:THR:CG2	2.48	0.43
1:F:186:GLU:HB2	1:F:380:LYS:HB2	1.99	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: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:34:LYS:HG3	1:E:458:CYS:SG	2.59	0.43
1:E:171:LYS:H	1:E:171:LYS:HG2	1.68	0.43
1:E:193:MET:HG3	1:E:371:LYS:HB3	2.01	0.43
1:E:200:LEU:HD13	1:E:254:VAL:HB	2.00	0.43
1:F:106:ALA:HA	1:F:111:MET:HE3	2.01	0.43
1:F:139:SER:O	1:F:171:LYS:HE2	2.18	0.43
1:G:106:ALA:HA	1:G:111:MET:HE3	2.00	0.43
1:I:202:PRO:O	1:I:203:TYR:CB	2.66	0.43
1:I:202:PRO:C	1:I:204:PHE:N	2.76	0.43
1:M:200:LEU:HD12	1:M:275:ALA:CB	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:209:GLU:H	1:E:209:GLU:CD	2.24	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:H:214:GLU:CD	1:H:322:ARG:HH21	2.27	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
2:Y:602:TRP:CE2	2:Y:612:PRO:HG3	2.53	0.43
1:L:16:MET:HB3	1:L:514:MET:HE3	1.99	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:M:202:PRO:C	1:M:204:PHE:N	2.76	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
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:242:LYS:C	1:H:244:GLY:N	2.75	0.43
1:H:291:ASP:OD2	1:H:368:ARG:HD2	2.19	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:H	1:N:171:LYS:HG2	1.68	0.43
1:A:230:ILE:HD13	1:A:261:THR:CB	2.48	0.43
2:P:604:THR:HG22	2:P:605:THR:O	2.18	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:H:354:GLU:C	1:H:356:ALA:H	2.27	0.43
1:I:200:LEU:HG	1:I:276:VAL:HA	2.00	0.43
1:K:295:LEU:HD13	1:K:295:LEU:C	2.44	0.43
1:M:201:SER:O	1:M:202:PRO:O	2.37	0.43
1:N:25:ASP:HA	1:N:28:LYS:HE2	2.00	0.43
1:N:242:LYS:C	1:N:244:GLY:N	2.75	0.43
1:N:438:VAL:O	1:N:442:VAL:HG23	2.18	0.43
1:A:369:VAL:HG23	1:A:370:ALA:N	2.33	0.43
1:C:201:SER:O	1:C:202:PRO:O	2.36	0.43
1:E:27:VAL:CG1	1:E:90:THR:HG23	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:J:202:PRO:C	1:J:204:PHE:N	2.77	0.43
1:L:321:LYS:HD2	1:L:334:ASP:OD2	2.18	0.43
1:L:326:ASN:HB2	1:L:329:THR:HG22	2.01	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
2:2:602:TRP:NE1	2:2:612:PRO:HG3	2.34	0.43
1:A:202:PRO:C	1:A:204:PHE:N	2.76	0.42
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: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:M:95:LEU:O	1:M:99:ILE:HG13	2.19	0.42
1:A:42:LYS:HE3	1:A:48:THR:OG1	2.19	0.42
1:A:264:VAL:O	1:A:268:ARG:HG3	2.18	0.42
1:B:231:ARG:NH1	2:P:612:PRO:O	2.52	0.42
1:B:283:ASP:C	1:B:285:ARG:N	2.78	0.42
1:B:345:ARG:HG2	1:B:372:LEU:HD21	2.02	0.42
1:D:202:PRO:C	1:D:204:PHE:N	2.76	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:G:261:THR:HG23	2:U:610:LEU:O	2.19	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:I:242:LYS:C	1:I:244:GLY:N	2.76	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:J:245:LYS:NZ	1:J:319:GLN:NE2	2.66	0.42
1:J:264:VAL:O	1:J:268:ARG:HG3	2.19	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:604:THR:HG22	2:2:605:THR:O	2.19	0.42
1:A:186:GLU:HB2	1:A:380:LYS:HB2	2.01	0.42
1:A:221:LEU:HD23	1:A:249:ILE:CD1	2.47	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:22:VAL:HG11	1:D:62:LEU:HD21	2.00	0.42
1:D:42:LYS:HE3	1:D:48:THR:OG1	2.19	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: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:F:202:PRO:C	1:F:204:PHE:N	2.75	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:27:VAL:CG1	1:K:90:THR:HG23	2.49	0.42
1:K:524:LEU:HD12	1:K:524:LEU:HA	1.87	0.42
1:L:171:LYS:H	1:L:171:LYS:HG2	1.68	0.42
1:L:524:LEU:HD12	1:L:524:LEU:HA	1.88	0.42
1:N:95:LEU:O	1:N:99:ILE:HG13	2.20	0.42
1:N:266:THR:HG22	1:N:271:VAL:O	2.19	0.42
1:A:221:LEU:CD2	1:A:233:MET:HE1	2.49	0.42
1:B:230:ILE:HD13	1:B:261:THR:HB	2.00	0.42
1:C:524:LEU:HD12	1:C:524:LEU:HA	1.89	0.42
1:D:245:LYS:NZ	1:D:319:GLN:NE2	2.67	0.42
1:G:271:VAL:HG21	2:U:607:TRP:HZ3	1.83	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:K:193:MET:CE	1:K:292:ILE:HG12	2.26	0.42
1:L:336:VAL:O	1:L:337:GLY:C	2.62	0.42
1:M:193:MET:HG3	1:M:371:LYS:HB3	2.01	0.42
1:M:218:PRO:CB	1:M:246:PRO:HG2	2.46	0.42
1:N:372:LEU:HD12	1:N:372:LEU:HA	1.87	0.42
1:B:139:SER:O	1:B:171:LYS:HE2	2.20	0.42
1:E:201:SER:O	1:E:202:PRO:O	2.38	0.42
1:E:202:PRO:C	1:E:204:PHE:N	2.76	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:242:LYS:C	1:F:244:GLY:N	2.77	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:N:218:PRO:HD2	1:N:320:ALA:O	2.19	0.42
1:A:111:MET:SD	1:A:438:VAL:HG21	2.60	0.42
1:B:79:SER:HA	1:B:89:THR:CG2	2.49	0.42
1:B:106:ALA:HA	1:B:111:MET:HE3	2.01	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:C:369:VAL:HG23	1:C:370:ALA:N	2.35	0.42
1:D:79:SER:HA	1:D:89:THR:HG22	2.01	0.42
1:D:171:LYS:H	1:D:171:LYS:HG2	1.68	0.42
1:E:79:SER:HA	1:E:89:THR:CG2	2.48	0.42
1:E:199:TYR:CZ	1:E:327:LYS:HA	2.55	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:42:LYS:HE3	1:L:48:THR:OG1	2.20	0.42
1:L:349:ILE:O	1:L:353:ILE:HG13	2.20	0.42
1:M:185:ASP:OD1	1:M:382:GLY:N	2.47	0.42
1:M:524:LEU:HD12	1:M:524:LEU:HA	1.86	0.42
1:N:230:ILE:CD1	1:N:261:THR:HB	2.50	0.42
1:A:106:ALA:HA	1:A:111:MET:HE3	2.01	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:28:LYS:HB2	1:C:453:GLN:HG2	2.02	0.42
1:C:146:GLN:O	1:C:150:ILE:HG13	2.20	0.42
1:E:354:GLU:C	1:E:356:ALA:H	2.28	0.42
1:E:369:VAL:HG23	1:E:370:ALA:N	2.35	0.42
1:G:42:LYS:HE3	1:G:48:THR:OG1	2.19	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:16:MET:HB3	1:J:514:MET:HE3	2.02	0.42
1:J:111:MET:SD	1:J:438:VAL:HG21	2.60	0.42
1:J:382:GLY:O	1:J:389:MET:HG2	2.18	0.42
1:M:131:LEU:HD13	1:M:422:VAL:HG21	2.01	0.42
2:1:604:THR:HG22	2:1:605:THR:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:SER:N	1:A:218:PRO:HD3	2.35	0.42
1:D:494:LEU:C	1:D:494:LEU:HD12	2.45	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
1:G:283:ASP:C	1:G:285:ARG:N	2.77	0.42
1:H:176:THR:HG22	1:H:177:VAL:N	2.35	0.42
1:H:446:ALA:C	1:H:448:GLU:H	2.27	0.42
1:I:414:GLY:N	1:I:494:LEU:HA	2.35	0.42
1:J:245:LYS:HZ2	1:J:319:GLN:NE2	2.17	0.42
1:K:42:LYS:HE3	1:K:48:THR:OG1	2.20	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:L:186:GLU:HB2	1:L:380:LYS:HB2	2.01	0.42
1:L:296:THR:HB	1:L:319:GLN:H	1.84	0.42
1:N:34:LYS:HG3	1:N:458:CYS:SG	2.59	0.42
1:N:186:GLU:HB2	1:N:380:LYS:HB2	2.01	0.42
1:N:199:TYR:CZ	1:N:327:LYS:HA	2.54	0.42
1:N:217:SER:N	1:N:218:PRO:HD3	2.35	0.42
1:B:500:THR:HB	3:B:1206:HOH:O	2.20	0.42
1:D:95:LEU:O	1:D:99:ILE:HG13	2.20	0.42
1:D:271:VAL:CG2	2:R:607:TRP:HZ3	2.30	0.42
1:D:349:ILE:O	1:D:353:ILE:HG13	2.20	0.42
1:G:350:ARG:O	1:G:354:GLU:HG2	2.19	0.42
1:H:42:LYS:HE3	1:H:48:THR:OG1	2.20	0.42
1:L:90:THR:O	1:L:94:VAL:HG13	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:N:202:PRO:O	1:N:204:PHE:N	2.42	0.42
1:B:230:ILE:CD1	1:B:261:THR:HB	2.50	0.42
1:C:79:SER:HA	1:C:89:THR:HG22	2.02	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:D:106:ALA:HA	1:D:111:MET:HE3	2.01	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:G:218:PRO:HD2	1:G:320:ALA:O	2.20	0.42
1:H:106:ALA:HA	1:H:111:MET:HE3	2.02	0.42
1:H:139:SER:O	1:H:171:LYS:HE2	2.20	0.42
1:I:144:ILE:HG23	1:I:403:THR:CG2	2.50	0.42
1:I:200:LEU:HD13	1:I:254:VAL:HB	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:245:LYS:NZ	1:I:319:GLN:NE2	2.68	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:J:358:SER:O	1:J:362:ARG:HB2	2.20	0.42
1:M:42:LYS:HE3	1:M:48:THR:OG1	2.20	0.42
1:M:183:LEU:O	1:M:184:GLN:CB	2.67	0.42
1:M:270:ILE:HG12	1:N:229:ASN:ND2	2.34	0.42
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:D:496:PRO:O	1:D:497:THR:C	2.62	0.41
1:E:270:ILE:CD1	2:S:608:GLY:HA3	2.50	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:524:LEU:HD12	1:I:524:LEU:HA	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:214:GLU:CD	1:M:322:ARG:HH21	2.28	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
2:2:602:TRP:CE2	2:2:612:PRO:HG3	2.55	0.41
2:O:602:TRP:NE1	2:O:612:PRO:HG3	2.35	0.41
1:C:336:VAL:O	1:C:337:GLY:C	2.62	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
2:R:604:THR:HG22	2:R:605:THR:O	2.21	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:HD12	1:H:524:LEU:HA	1.84	0.41
1:J:270:ILE:HD13	2:X:608:GLY:HA3	2.02	0.41
1:K:25:ASP:HA	1:K:28:LYS:HE2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:N:106:ALA:HA	1:N:111:MET:HE3	2.02	0.41
1:A:4:LYS:HG3	1:G:59:GLU:O	2.21	0.41
1:A:193:MET:HG3	1:A:371:LYS:HB3	2.01	0.41
1:A:270:ILE:O	1:A:271:VAL:HB	2.20	0.41
1:C:230:ILE:CD1	1:C:261:THR:HB	2.51	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:283:ASP:C	1:G:285:ARG:H	2.27	0.41
1:G:382:GLY:O	1:G:389:MET:HG2	2.20	0.41
1:H:16:MET:HB3	1:H:514:MET:HE3	2.01	0.41
1:H:201:SER:O	1:H:202:PRO:O	2.37	0.41
1:H:268:ARG:O	1:I:257:GLU:HG2	2.20	0.41
1:I:176:THR:HG22	1:I:177:VAL:N	2.35	0.41
1:J:22:VAL:HG11	1:J:62:LEU:HD21	2.02	0.41
1:L:25:ASP:HA	1:L:28:LYS:HE2	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:B:70:GLY:HA2	1:B:73:MET:HE3	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: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:270:ILE:CD1	2:V:608:GLY:HA3	2.49	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: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:296:THR:HB	1:N:319:GLN:H	1.84	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: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
1:K:358:SER:O	1:K:362:ARG:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:524:LEU:C	1:M:526:LYS:H	2.29	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:16:MET:O	1:C:20:VAL:HG13	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: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:F:349:ILE:O	1:F:353:ILE:HG13	2.21	0.41
1:G:87:ASP:O	1:G:499:VAL:HG23	2.20	0.41
1:G:218:PRO:HG3	1:G:323:VAL:HG13	2.02	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:K:123:ALA:HA	1:K:429:LEU:CD2	2.50	0.41
1:K:270:ILE:O	1:K:271:VAL:HB	2.20	0.41
1:M:199:TYR:CZ	1:M:327:LYS:HA	2.55	0.41
1:M:354:GLU:C	1:M:356:ALA:H	2.28	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:19:GLY:HA3	1:D:67:GLU:O	2.20	0.41
1:D:25:ASP:HA	1:D:28:LYS:HE2	2.03	0.41
1:D:38:VAL:HG22	1:E:519:CYS:HB3	2.03	0.41
1:D:202:PRO:O	1:D:203:TYR:CB	2.66	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:F:19:GLY:HA3	1:F:67:GLU:O	2.20	0.41
1:F:70:GLY:HA2	1:F:73:MET:CE	2.51	0.41
1:F:233:MET:O	1:F:234:LEU:C	2.63	0.41
1:G:242:LYS:C	1:G:244:GLY:N	2.76	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:I:186:GLU:HB2	1:I:380:LYS:HB2	2.02	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
2:O:602:TRP:CE2	2:O:612:PRO:HG3	2.55	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:I:354:GLU:C	1:I:356:ALA:H	2.28	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
1:A:95:LEU:O	1:A:99:ILE:HG13	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:A:451:LEU:HD22	1:A:455:VAL:HG23	2.02	0.41
1:B:271:VAL:HG21	2:P:607:TRP:HZ3	1.86	0.41
1:B:283:ASP:C	1:B:285:ARG:H	2.27	0.41
1:B:369:VAL:HG23	1:B:370:ALA:N	2.35	0.41
1:C:87:ASP:O	1:C:499: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:455:VAL:CG1	1:C:460:GLU:HB2	2.50	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:D:524:LEU:HD12	1:D:524:LEU:HA	1.88	0.41
1:F:200:LEU:HD13	1:F:254:VAL:HB	2.02	0.41
1:F:201:SER:HB3	1:F:259:LEU:HD21	2.02	0.41
2:T:604:THR:HG22	2:T:605:THR:O	2.20	0.41
1:H:100:ILE:HD13	1:H:514:MET:CE	2.51	0.41
2:V:604:THR:HG22	2:V:605:THR:O	2.21	0.41
1:I:350:ARG:O	1:I:354:GLU:HG2	2.21	0.41
1:J:38:VAL:HG22	1:K:519:CYS:HB3	2.03	0.41
1:J:176:THR:HG21	1:J:333:ILE:CD1	2.51	0.41
1:J:350:ARG:O	1:J:354:GLU:HG2	2.21	0.41
1:K:100:ILE:HD13	1:K:514:MET:CE	2.51	0.41
1:K:193:MET:HG3	1:K:371:LYS:HB3	2.02	0.41
1:L:16:MET:O	1:L:20:VAL:HG13	2.21	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
1:N:482:THR:O	1:N:484:GLU:HG2	2.21	0.41
1:A:519:CYS:HB3	1:G:38:VAL:HG22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:229:ASN:C	1:I:231:ARG:H	2.29	0.41
1:I:372:LEU:HD12	1:I:372:LEU:HA	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:106:ALA:HA	1:L:111:MET:HE3	2.03	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:A:229:ASN:HD22	1:G:270:ILE:HA	1.83	0.40
1:B:16:MET:HB3	1:B:514:MET:HE3	2.02	0.40
1:B:270:ILE:CD1	2:P:608:GLY:HA3	2.51	0.40
1:B:496:PRO:O	1:B:497:THR:C	2.64	0.40
1:C:144:ILE:HG23	1:C:403:THR:CG2	2.51	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:200:LEU:HD13	1:H:254:VAL:HB	2.02	0.40
1:J:19:GLY:HA2	1:J:62:LEU:CD1	2.51	0.40
1:J:177:VAL:HG21	1:J:397:GLU:HG3	2.02	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:446:ALA:C	1:M:448:GLU:H	2.29	0.40
1:M:511:ALA:O	1:M:515:ILE:HG13	2.21	0.40
1:N:16:MET:HB3	1:N:514:MET:HE3	2.02	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:95:LEU:O	1:G:99:ILE:HG13	2.21	0.40
1:G:111:MET:SD	1:G:438:VAL:HG21	2.62	0.40
1:G:152:ALA:O	1:G:153:ASN:HB3	2.21	0.40
1:G:444:LEU:HD23	1:G:447:MET:CE	2.52	0.40
2:U:604:THR:HG22	2:U:605:THR:O	2.21	0.40
1:J:494:LEU:HD12	1:J:494:LEU:C	2.46	0.40
1:L:511:ALA:O	1:L:515:ILE:HG13	2.21	0.40
1:N:200:LEU:HD21	1:N:277:LYS:HG3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:ASN:O	1:A:154:SER:HB2	2.20	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:68:ASN:O	1:B:72:GLN:HG2	2.22	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:354:GLU:C	1:B:356:ALA:H	2.30	0.40
1:B:444:LEU:HD23	1:B:447:MET:CE	2.52	0.40
1:C:171:LYS:H	1:C:171:LYS:HG2	1.70	0.40
1:C:496:PRO:O	1:C:497:THR:C	2.64	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:D:193:MET:CE	1:D:292:ILE:HG12	2.22	0.40
1:D:222:LEU:HD23	1:D:250:ILE:HB	2.03	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:HD12	1:F:524:LEU:HA	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: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:L:524:LEU:C	1:L:526:LYS:H	2.29	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:N:354:GLU:C	1:N:356:ALA:H	2.30	0.40
1:N:524:LEU:C	1:N:526:LYS:H	2.29	0.40
1:A:511:ALA:O	1:A:515:ILE:HG13	2.22	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:123:ALA:HA	1:D:429:LEU:CD2	2.51	0.40
1:D:218:PRO:HG3	1:D:323:VAL:HG13	2.03	0.40
1:F:414:GLY:N	1:F:494:LEU:HA	2.37	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:123:ALA:HA	1:J:429:LEU:CD2	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:414:GLY:N	1:J:494:LEU:HA	2.37	0.40
1:K:383:ALA:O	1:K:384:ALA:CB	2.68	0.40
1:K:494:LEU:HD12	1:K:494:LEU:O	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:C:354:GLU:C	1:C:356:ALA:H	2.28	0.40
1:D:459:GLY:HA3	1:E:112:ASN:ND2	2.36	0.40
1:E:70:GLY:HA2	1:E:73:MET:CE	2.51	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:26:ALA:HA	1:I:8:PHE:HE1	1.85	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:J:345:ARG:HG2	1:J:372:LEU:HD21	2.03	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:K:131:LEU:HD12	1:K:131:LEU:HA	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:L:46:ALA:HB2	1:M:76:GLU:CG	2.49	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
1:N:366:GLN:O	1:N:369:VAL:HG22	2.22	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:C:316:ASP:OD1	1:J:311:LYS:NZ[1_554]	2.13	0.07
1:H:166:MET:O	1:L:359:ASP:OD2[1_455]	2.13	0.07

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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%)	5	25
1	B	523/547 (96%)	496 (95%)	15 (3%)	12 (2%)	5	25
1	C	523/547 (96%)	493 (94%)	18 (3%)	12 (2%)	5	25
1	D	523/547 (96%)	494 (94%)	17 (3%)	12 (2%)	5	25
1	E	523/547 (96%)	495 (95%)	16 (3%)	12 (2%)	5	25
1	F	523/547 (96%)	492 (94%)	19 (4%)	12 (2%)	5	25
1	G	523/547 (96%)	495 (95%)	17 (3%)	11 (2%)	5	27
1	H	523/547 (96%)	495 (95%)	17 (3%)	11 (2%)	5	27
1	I	523/547 (96%)	494 (94%)	17 (3%)	12 (2%)	5	25
1	J	523/547 (96%)	493 (94%)	18 (3%)	12 (2%)	5	25
1	K	523/547 (96%)	494 (94%)	17 (3%)	12 (2%)	5	25
1	L	523/547 (96%)	494 (94%)	17 (3%)	12 (2%)	5	25
1	M	523/547 (96%)	495 (95%)	16 (3%)	12 (2%)	5	25
1	N	523/547 (96%)	495 (95%)	16 (3%)	12 (2%)	5	25
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%)	5	26

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

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Mol	Chain	Res	Type
1	K	256	GLY
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

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Mol	Chain	Res	Type
1	C	385	THR
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

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Mol	Chain	Res	Type
1	C	384	ALA
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 ⓘ

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%)	388 (96%)	17 (4%)	26	61
1	B	405/414 (98%)	388 (96%)	17 (4%)	26	61
1	C	405/414 (98%)	388 (96%)	17 (4%)	26	61
1	D	405/414 (98%)	387 (96%)	18 (4%)	25	60
1	E	405/414 (98%)	388 (96%)	17 (4%)	26	61
1	F	405/414 (98%)	388 (96%)	17 (4%)	26	61
1	G	405/414 (98%)	387 (96%)	18 (4%)	25	60
1	H	405/414 (98%)	387 (96%)	18 (4%)	25	60
1	I	405/414 (98%)	387 (96%)	18 (4%)	25	60
1	J	405/414 (98%)	387 (96%)	18 (4%)	25	60
1	K	405/414 (98%)	388 (96%)	17 (4%)	26	61
1	L	405/414 (98%)	387 (96%)	18 (4%)	25	60
1	M	405/414 (98%)	387 (96%)	18 (4%)	25	60
1	N	405/414 (98%)	388 (96%)	17 (4%)	26	61
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%)	5579 (96%)	245 (4%)	26	61

All (245) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	VAL
1	A	74	VAL
1	A	82	ASN
1	A	94	VAL
1	A	134	LEU
1	A	160	LYS
1	A	171	LYS
1	A	183	LEU
1	A	201	SER
1	A	231	ARG
1	A	289	LEU
1	A	329	THR
1	A	331	THR
1	A	397	GLU
1	A	417	VAL
1	A	422	VAL
1	A	451	LEU
1	B	20	VAL
1	B	74	VAL
1	B	82	ASN
1	B	94	VAL
1	B	134	LEU
1	B	160	LYS
1	B	171	LYS
1	B	183	LEU
1	B	201	SER
1	B	231	ARG
1	B	289	LEU
1	B	329	THR
1	B	331	THR
1	B	397	GLU
1	B	417	VAL
1	B	422	VAL
1	B	451	LEU

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Mol	Chain	Res	Type
1	C	20	VAL
1	C	74	VAL
1	C	82	ASN
1	C	94	VAL
1	C	134	LEU
1	C	160	LYS
1	C	171	LYS
1	C	183	LEU
1	C	201	SER
1	C	231	ARG
1	C	289	LEU
1	C	329	THR
1	C	331	THR
1	C	397	GLU
1	C	417	VAL
1	C	422	VAL
1	C	451	LEU
1	D	20	VAL
1	D	74	VAL
1	D	76	GLU
1	D	82	ASN
1	D	94	VAL
1	D	134	LEU
1	D	160	LYS
1	D	171	LYS
1	D	183	LEU
1	D	201	SER
1	D	231	ARG
1	D	289	LEU
1	D	329	THR
1	D	331	THR
1	D	397	GLU
1	D	417	VAL
1	D	422	VAL
1	D	451	LEU
1	E	20	VAL
1	E	74	VAL
1	E	82	ASN
1	E	94	VAL
1	E	134	LEU
1	E	160	LYS
1	E	171	LYS

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Mol	Chain	Res	Type
1	E	183	LEU
1	E	201	SER
1	E	231	ARG
1	E	289	LEU
1	E	329	THR
1	E	331	THR
1	E	397	GLU
1	E	417	VAL
1	E	422	VAL
1	E	451	LEU
1	F	20	VAL
1	F	74	VAL
1	F	82	ASN
1	F	94	VAL
1	F	134	LEU
1	F	160	LYS
1	F	171	LYS
1	F	183	LEU
1	F	201	SER
1	F	231	ARG
1	F	289	LEU
1	F	329	THR
1	F	331	THR
1	F	397	GLU
1	F	417	VAL
1	F	422	VAL
1	F	451	LEU
1	G	20	VAL
1	G	74	VAL
1	G	76	GLU
1	G	82	ASN
1	G	94	VAL
1	G	134	LEU
1	G	160	LYS
1	G	171	LYS
1	G	183	LEU
1	G	201	SER
1	G	231	ARG
1	G	289	LEU
1	G	329	THR
1	G	331	THR
1	G	397	GLU

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Mol	Chain	Res	Type
1	G	417	VAL
1	G	422	VAL
1	G	451	LEU
1	H	20	VAL
1	H	74	VAL
1	H	76	GLU
1	H	82	ASN
1	H	94	VAL
1	H	134	LEU
1	H	160	LYS
1	H	171	LYS
1	H	183	LEU
1	H	201	SER
1	H	231	ARG
1	H	289	LEU
1	H	329	THR
1	H	331	THR
1	H	397	GLU
1	H	417	VAL
1	H	422	VAL
1	H	451	LEU
1	I	20	VAL
1	I	74	VAL
1	I	76	GLU
1	I	82	ASN
1	I	94	VAL
1	I	134	LEU
1	I	160	LYS
1	I	171	LYS
1	I	183	LEU
1	I	201	SER
1	I	231	ARG
1	I	289	LEU
1	I	329	THR
1	I	331	THR
1	I	397	GLU
1	I	417	VAL
1	I	422	VAL
1	I	451	LEU
1	J	20	VAL
1	J	74	VAL
1	J	76	GLU

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Mol	Chain	Res	Type
1	J	82	ASN
1	J	94	VAL
1	J	134	LEU
1	J	160	LYS
1	J	171	LYS
1	J	183	LEU
1	J	201	SER
1	J	231	ARG
1	J	289	LEU
1	J	329	THR
1	J	331	THR
1	J	397	GLU
1	J	417	VAL
1	J	422	VAL
1	J	451	LEU
1	K	20	VAL
1	K	74	VAL
1	K	82	ASN
1	K	94	VAL
1	K	134	LEU
1	K	160	LYS
1	K	171	LYS
1	K	183	LEU
1	K	201	SER
1	K	231	ARG
1	K	289	LEU
1	K	329	THR
1	K	331	THR
1	K	397	GLU
1	K	417	VAL
1	K	422	VAL
1	K	451	LEU
1	L	20	VAL
1	L	74	VAL
1	L	82	ASN
1	L	94	VAL
1	L	134	LEU
1	L	160	LYS
1	L	171	LYS
1	L	183	LEU
1	L	201	SER
1	L	231	ARG

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Mol	Chain	Res	Type
1	L	289	LEU
1	L	326	ASN
1	L	329	THR
1	L	331	THR
1	L	397	GLU
1	L	417	VAL
1	L	422	VAL
1	L	451	LEU
1	M	20	VAL
1	M	74	VAL
1	M	82	ASN
1	M	94	VAL
1	M	134	LEU
1	M	160	LYS
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	329	THR
1	M	331	THR
1	M	397	GLU
1	M	417	VAL
1	M	422	VAL
1	M	451	LEU
1	N	20	VAL
1	N	74	VAL
1	N	82	ASN
1	N	94	VAL
1	N	134	LEU
1	N	160	LYS
1	N	171	LYS
1	N	183	LEU
1	N	201	SER
1	N	231	ARG
1	N	289	LEU
1	N	329	THR
1	N	331	THR
1	N	397	GLU
1	N	417	VAL
1	N	422	VAL

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Mol	Chain	Res	Type
1	N	451	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (130) 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	432	GLN
1	A	436	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	432	GLN
1	B	436	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	453	GLN
1	C	475	ASN
1	D	37	ASN
1	D	146	GLN
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

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Mol	Chain	Res	Type
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	432	GLN
1	F	436	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	432	GLN
1	G	436	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	432	GLN
1	H	436	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
1	I	351	GLN

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Mol	Chain	Res	Type
1	I	366	GLN
1	I	432	GLN
1	I	436	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	432	GLN
1	L	436	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	432	GLN
1	M	436	GLN
1	M	453	GLN
1	M	475	ASN
1	N	37	ASN

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Mol	Chain	Res	Type
1	N	146	GLN
1	N	265	ASN
1	N	319	GLN
1	N	351	GLN
1	N	366	GLN
1	N	432	GLN
1	N	436	GLN
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 oligosaccharides 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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	525/547 (95%)	0.02	10 (1%) 66 43	12, 36, 70, 88	0
1	B	525/547 (95%)	0.12	14 (2%) 56 33	12, 36, 70, 88	0
1	C	525/547 (95%)	0.02	6 (1%) 78 57	12, 36, 69, 88	0
1	D	525/547 (95%)	0.09	11 (2%) 63 40	12, 36, 69, 88	0
1	E	525/547 (95%)	0.13	6 (1%) 78 57	12, 36, 69, 88	0
1	F	525/547 (95%)	0.06	10 (1%) 66 43	13, 36, 69, 88	0
1	G	525/547 (95%)	0.13	19 (3%) 46 26	11, 35, 69, 88	0
1	H	525/547 (95%)	0.04	12 (2%) 61 38	12, 36, 71, 88	0
1	I	525/547 (95%)	0.02	8 (1%) 72 49	12, 36, 71, 88	0
1	J	525/547 (95%)	-0.03	4 (0%) 82 64	13, 37, 69, 88	0
1	K	525/547 (95%)	0.09	7 (1%) 75 53	12, 36, 70, 88	0
1	L	525/547 (95%)	0.08	6 (1%) 78 57	12, 36, 69, 88	0
1	M	525/547 (95%)	-0.06	10 (1%) 66 43	12, 37, 70, 88	0
1	N	525/547 (95%)	0.04	13 (2%) 58 35	12, 36, 70, 88	0
2	1	12/12 (100%)	0.63	1 (8%) 17 9	42, 55, 70, 74	0
2	2	12/12 (100%)	0.57	0 100 100	43, 55, 71, 74	0
2	O	12/12 (100%)	0.41	1 (8%) 17 9	43, 55, 70, 74	0
2	P	12/12 (100%)	0.73	0 100 100	42, 55, 70, 74	0
2	Q	12/12 (100%)	0.54	1 (8%) 17 9	43, 55, 70, 74	0
2	R	12/12 (100%)	0.80	1 (8%) 17 9	43, 55, 70, 74	0
2	S	12/12 (100%)	0.65	0 100 100	43, 54, 70, 74	0
2	T	12/12 (100%)	0.34	0 100 100	43, 54, 70, 74	0
2	U	12/12 (100%)	0.73	2 (16%) 4 3	42, 54, 70, 74	0
2	V	12/12 (100%)	0.58	0 100 100	43, 54, 71, 74	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
2	W	12/12 (100%)	0.46	0 100 100	44, 55, 71, 74	0
2	X	12/12 (100%)	0.35	0 100 100	43, 55, 70, 74	0
2	Y	12/12 (100%)	0.58	1 (8%) 17 9	44, 55, 70, 74	0
2	Z	12/12 (100%)	0.48	0 100 100	43, 55, 70, 74	0
All	All	7518/7826 (96%)	0.07	143 (1%) 66 43	11, 37, 71, 88	0

All (143) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	382	GLY	5.9
1	G	358	SER	5.5
1	D	354	GLU	5.1
1	C	366	GLN	4.3
1	G	383	ALA	4.2
1	D	352	GLN	4.1
1	J	366	GLN	4.1
1	B	363	GLU	3.8
1	N	382	GLY	3.8
1	D	358	SER	3.8
1	M	382	GLY	3.8
1	N	44	PHE	3.8
1	H	343	GLN	3.6
1	N	358	SER	3.6
1	E	490	ASP	3.6
1	A	361	ASP	3.5
1	G	359	ASP	3.5
1	G	43	SER	3.5
1	I	366	GLN	3.2
1	H	366	GLN	3.2
1	B	359	ASP	3.1
1	E	384	ALA	3.1
1	L	44	PHE	3.1
1	D	362	ARG	3.0
1	D	356	ALA	3.0
2	1	601	SER	3.0
1	H	182	GLY	3.0
1	G	361	ASP	2.9
1	D	382	GLY	2.9
1	G	343	GLN	2.9
1	K	192	GLY	2.9
1	A	182	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	I	354	GLU	2.8
1	G	363	GLU	2.8
1	E	224	ASP	2.8
1	M	358	SER	2.8
1	K	44	PHE	2.7
1	B	266	THR	2.7
1	G	167	ASP	2.7
1	B	182	GLY	2.7
1	M	526	LYS	2.7
1	C	211	GLY	2.7
1	L	383	ALA	2.7
1	A	196	ASP	2.7
1	L	361	ASP	2.7
2	Y	601	SER	2.6
1	N	182	GLY	2.6
1	K	302	SER	2.6
1	N	259	LEU	2.6
1	N	181	THR	2.5
1	B	366	GLN	2.5
1	K	382	GLY	2.5
1	D	203	TYR	2.5
1	A	363	GLU	2.5
1	B	281	PHE	2.5
1	H	359	ASP	2.5
1	C	357	THR	2.4
1	I	180	GLY	2.4
1	F	270	ILE	2.4
1	D	43	SER	2.4
1	I	43	SER	2.4
1	L	43	SER	2.4
1	E	361	ASP	2.4
1	G	352	GLN	2.4
1	B	302	SER	2.4
2	Q	601	SER	2.4
1	N	306	GLY	2.4
1	E	354	GLU	2.4
1	G	257	GLU	2.4
1	M	354	GLU	2.4
1	H	302	SER	2.4
2	U	601	SER	2.4
1	A	306	GLY	2.3
1	I	361	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	H	355	GLU	2.3
1	F	284	ARG	2.3
1	G	284	ARG	2.3
1	M	360	TYR	2.3
1	H	361	ASP	2.3
1	I	359	ASP	2.3
1	F	44	PHE	2.3
1	M	43	SER	2.3
1	D	183	LEU	2.3
1	B	352	GLN	2.3
1	F	306	GLY	2.3
1	K	234	LEU	2.3
1	I	348	GLN	2.3
1	D	214	GLU	2.3
1	G	356	ALA	2.3
1	B	183	LEU	2.3
1	G	357	THR	2.3
1	H	44	PHE	2.3
1	L	358	SER	2.3
1	G	366	GLN	2.3
1	M	361	ASP	2.3
1	A	358	SER	2.2
1	C	360	TYR	2.2
1	G	308	GLU	2.2
1	J	43	SER	2.2
1	A	206	ASN	2.2
1	F	255	GLU	2.2
1	H	388	GLU	2.2
1	F	382	GLY	2.2
2	R	604	THR	2.2
1	M	203	TYR	2.2
1	M	153	ASN	2.2
1	K	284	ARG	2.2
1	A	366	GLN	2.2
1	F	358	SER	2.2
1	F	366	GLN	2.2
1	N	184	GLN	2.2
2	O	601	SER	2.2
1	C	257	GLU	2.2
1	G	354	GLU	2.2
2	U	603	MET	2.2
1	B	526	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	343	GLN	2.1
1	H	242	LYS	2.1
1	H	45	GLY	2.1
1	M	284	ARG	2.1
1	N	397	GLU	2.1
1	N	484	GLU	2.1
1	A	382	GLY	2.1
1	N	326	ASN	2.1
1	J	307	MET	2.1
1	D	363	GLU	2.1
1	N	304	GLU	2.1
1	H	284	ARG	2.1
1	C	343	GLN	2.1
1	J	382	GLY	2.1
1	B	361	ASP	2.1
1	F	203	TYR	2.1
1	N	343	GLN	2.1
1	E	336	VAL	2.1
1	L	387	VAL	2.1
1	B	206	ASN	2.1
1	K	385	THR	2.0
1	B	44	PHE	2.0
1	I	298	GLY	2.0
1	G	310	GLU	2.0
1	F	365	LEU	2.0
1	G	183	LEU	2.0
1	B	356	ALA	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 oligosaccharides 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.