



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 07:31 AM UTC

PDB ID : 4HEL / pdb_00004hel
Title : Crystal structure analysis of apo-GroEL structure
Authors : Saxena, A.K.; Meena, S.R.
Deposited on : 2012-10-04
Resolution : 3.20 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:

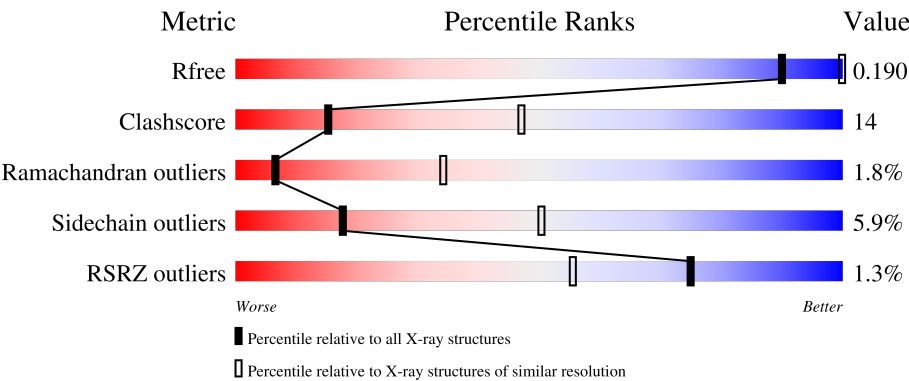
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 3.20 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	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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	525	% 72% 25% .
1	B	525	73% 24% .
1	C	525	% 75% 22% .
1	D	525	2% 67% 29% .
1	E	525	2% 74% 23% ..

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Mol	Chain	Length	Quality of chain
1	F	525	
1	G	525	
1	H	525	
1	I	525	
1	J	525	
1	K	525	
1	L	525	
1	M	525	
1	N	525	

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 54997 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 60 kDa chaperonin 4.

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			

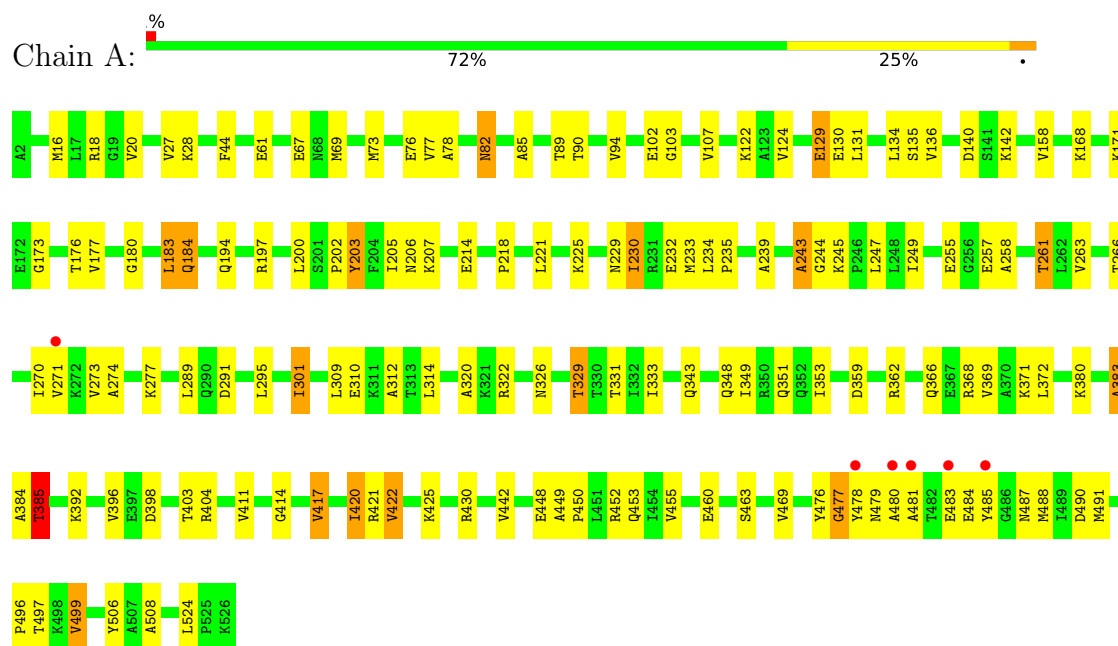
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	60	Total 60	O 60	0	0
2	B	83	Total 83	O 83	0	0
2	C	65	Total 65	O 65	0	0
2	D	62	Total 62	O 62	0	0
2	E	79	Total 79	O 79	0	0
2	F	53	Total 53	O 53	0	0
2	G	74	Total 74	O 74	0	0
2	H	52	Total 52	O 52	0	0
2	I	64	Total 64	O 64	0	0
2	J	75	Total 75	O 75	0	0
2	K	55	Total 55	O 55	0	0
2	L	64	Total 64	O 64	0	0
2	M	57	Total 57	O 57	0	0
2	N	58	Total 58	O 58	0	0

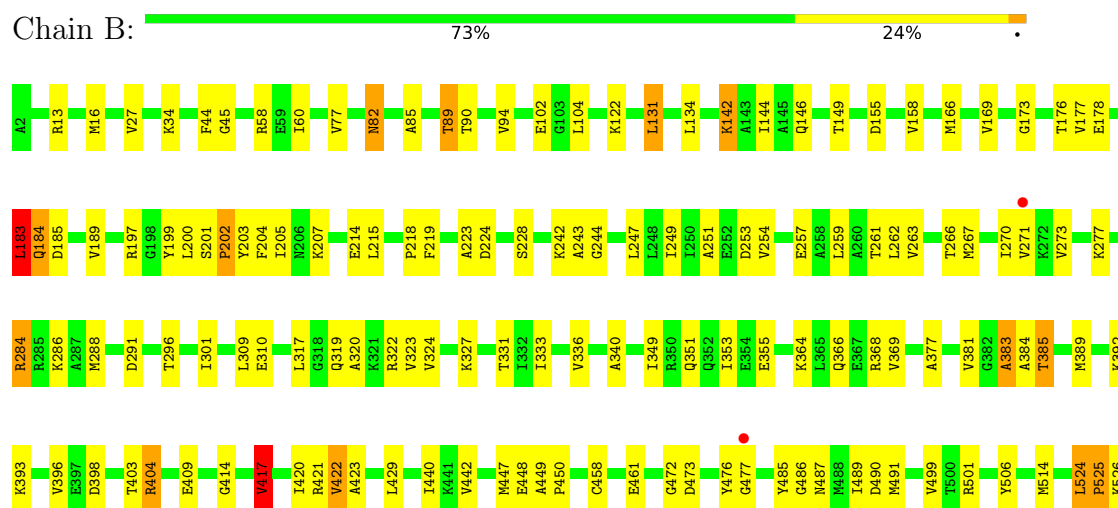
3 Residue-property plots

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.

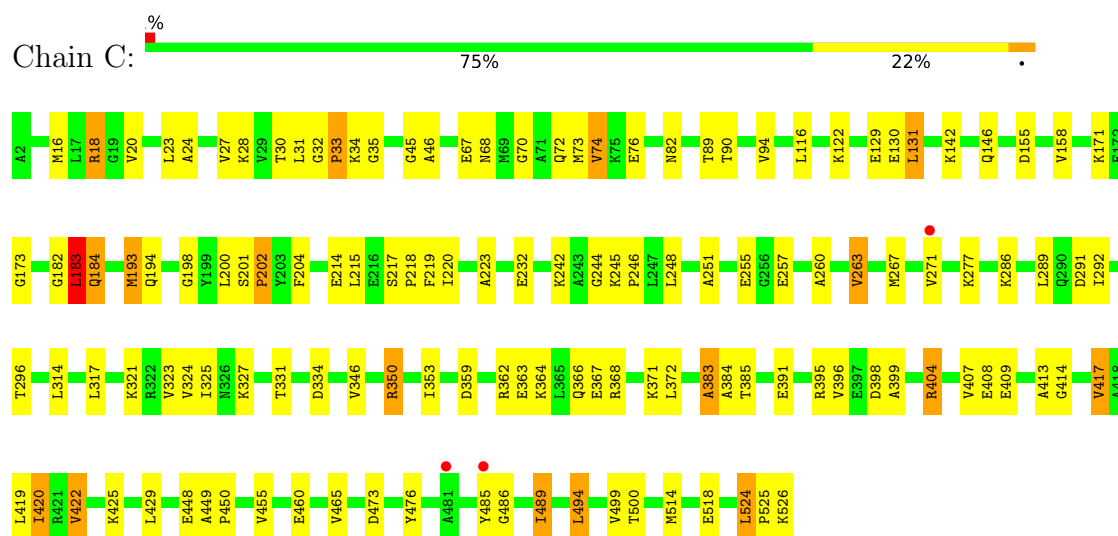
- Molecule 1: 60 kDa chaperonin 4



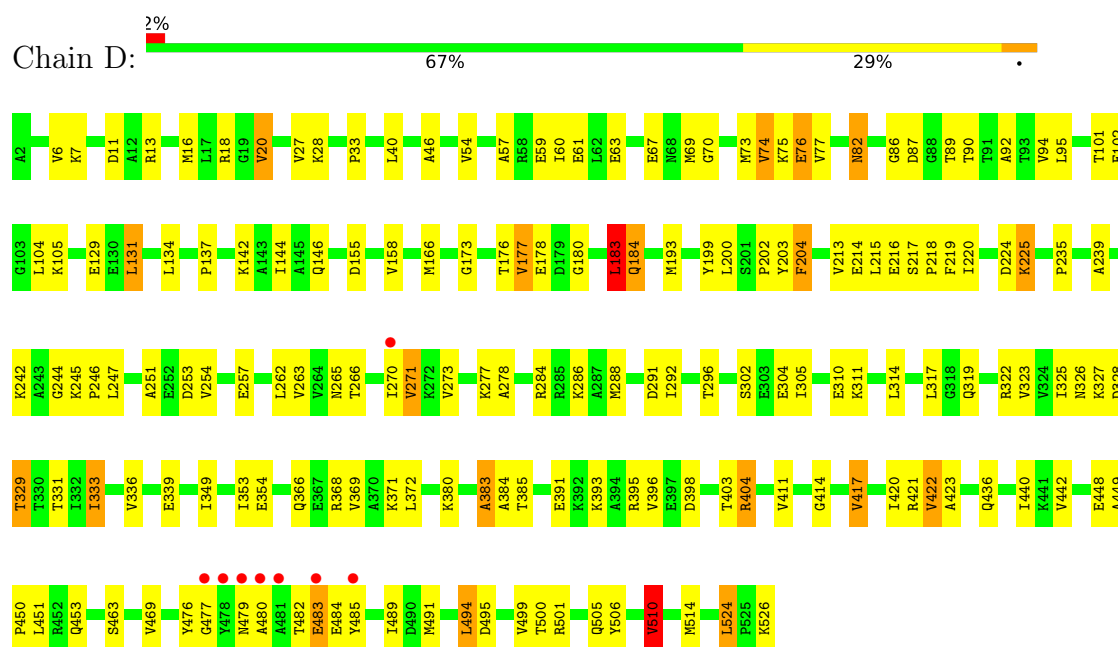
- Molecule 1: 60 kDa chaperonin 4



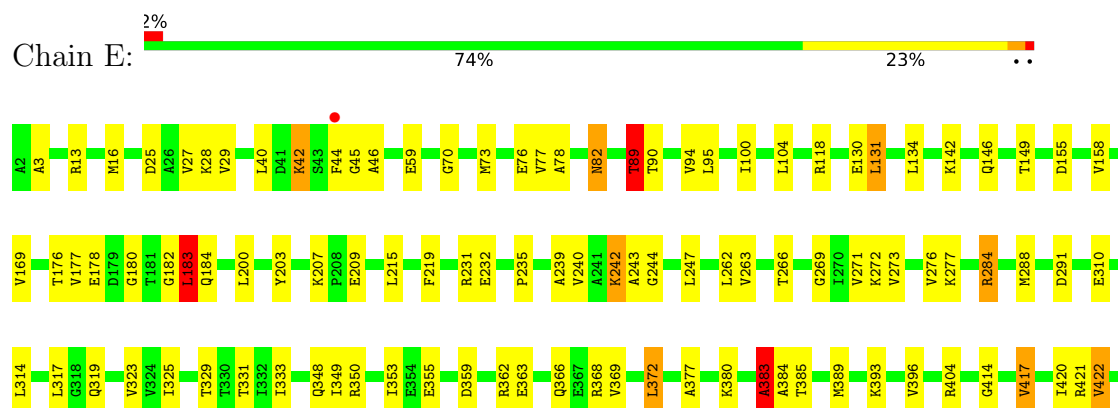
- Molecule 1: 60 kDa chaperonin 4

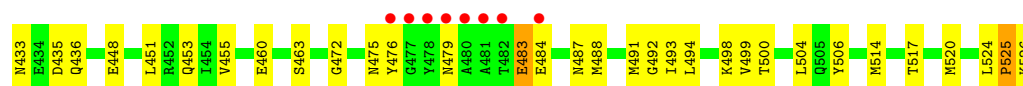


• Molecule 1: 60 kDa chaperonin 4

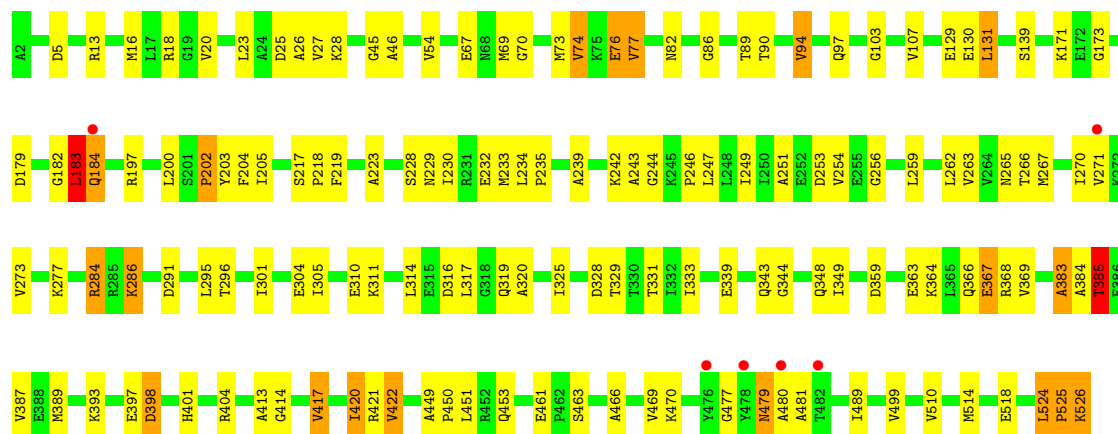


• Molecule 1: 60 kDa chaperonin 4

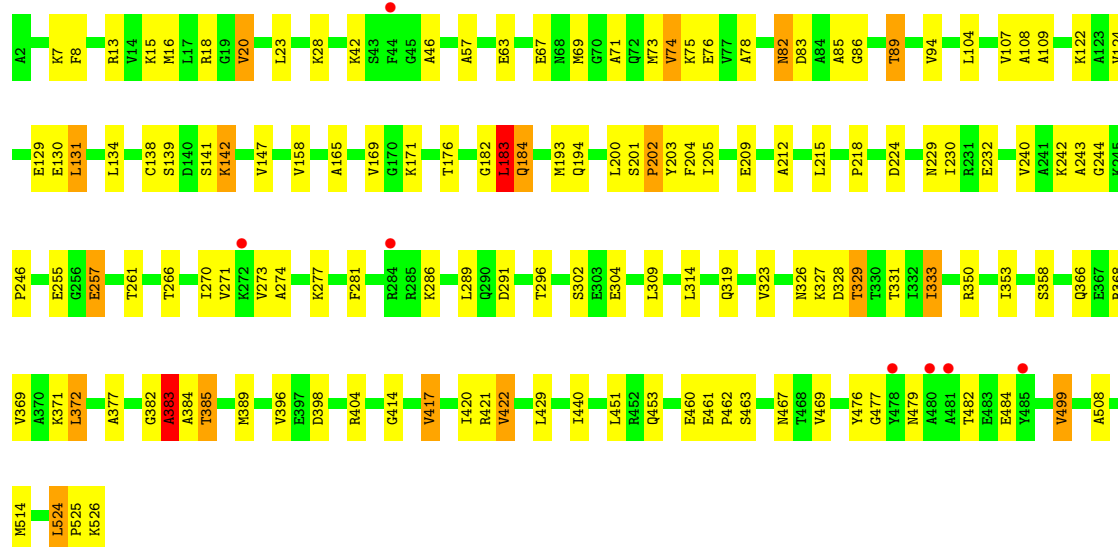
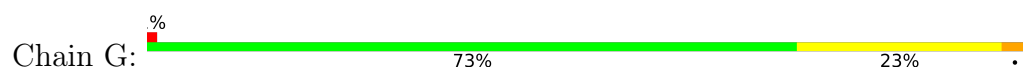




- Molecule 1: 60 kDa chaperonin 4

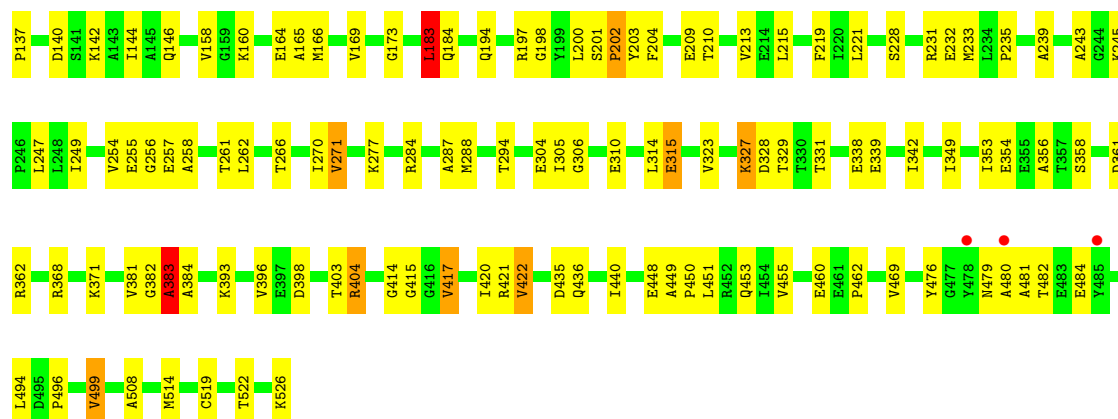


- Molecule 1: 60 kDa chaperonin 4

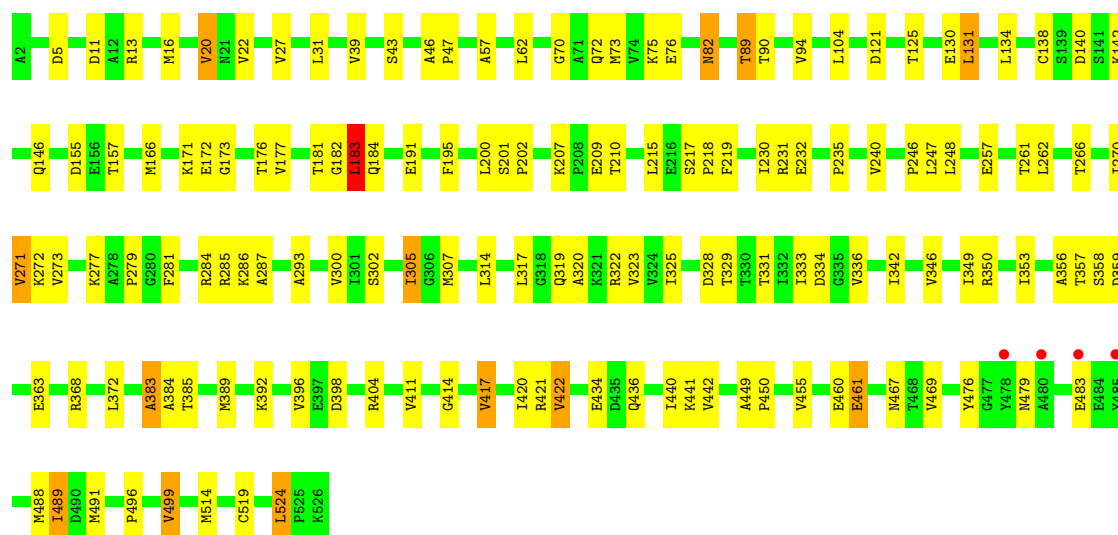


- Molecule 1: 60 kDa chaperonin 4

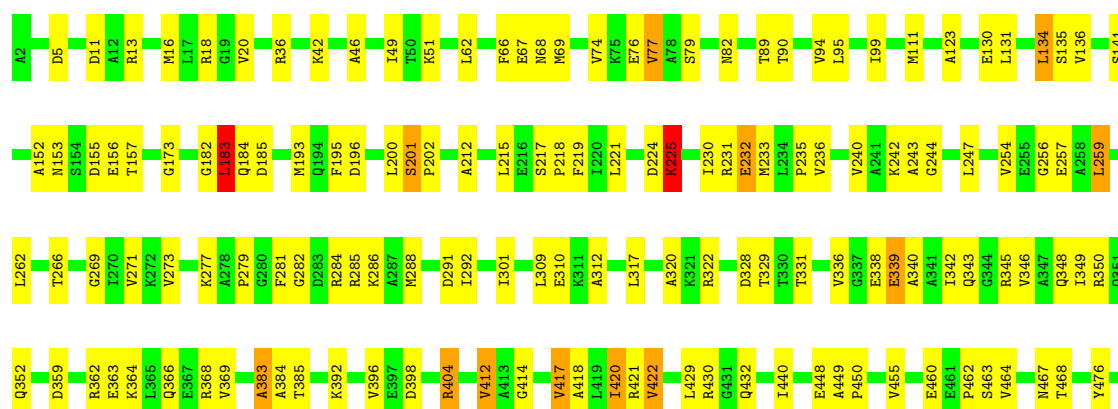




• Molecule 1: 60 kDa chaperonin 4

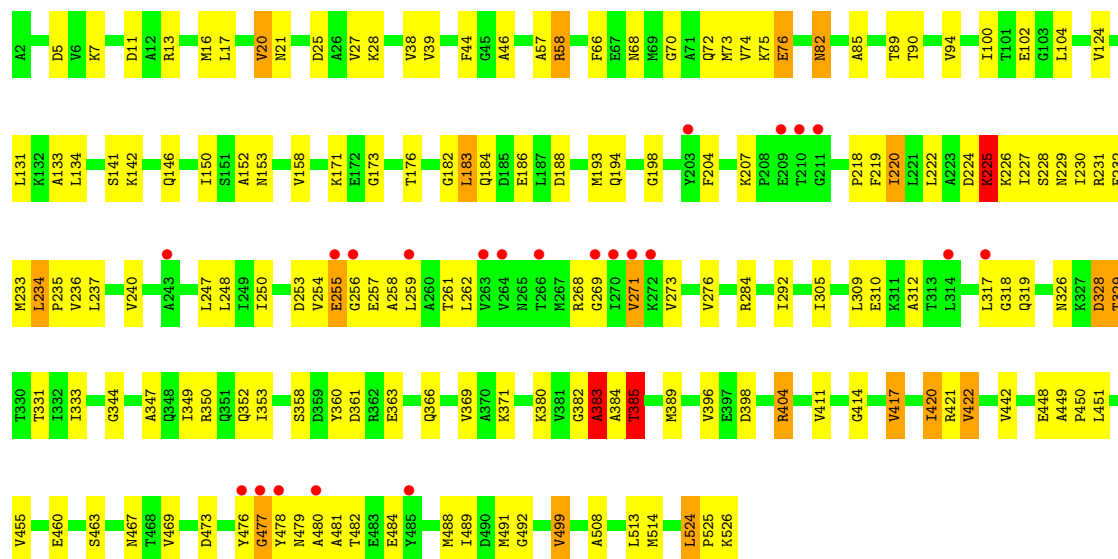


• Molecule 1: 60 kDa chaperonin 4

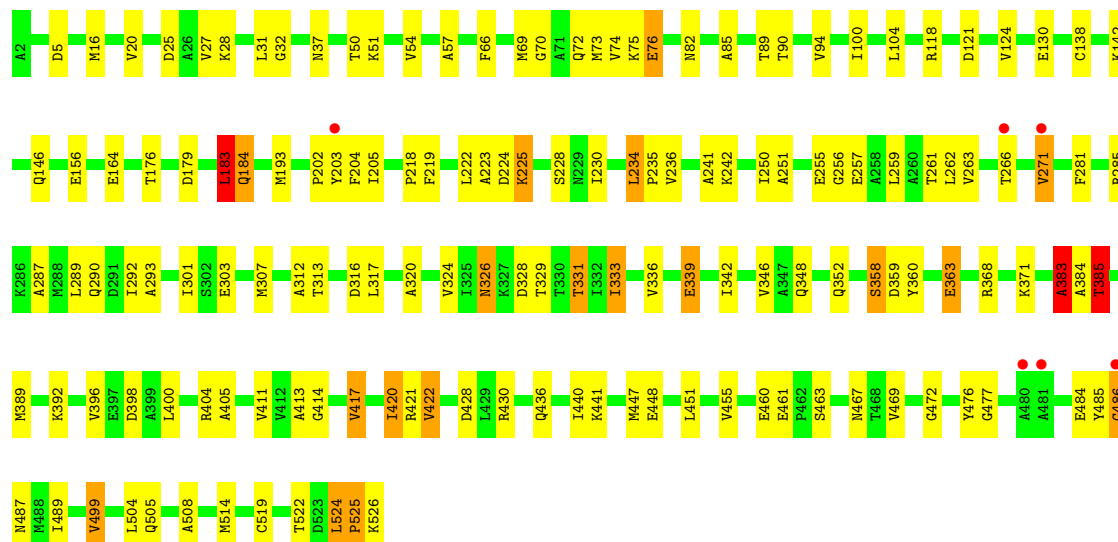




- Molecule 1: 60 kDa chaperonin 4

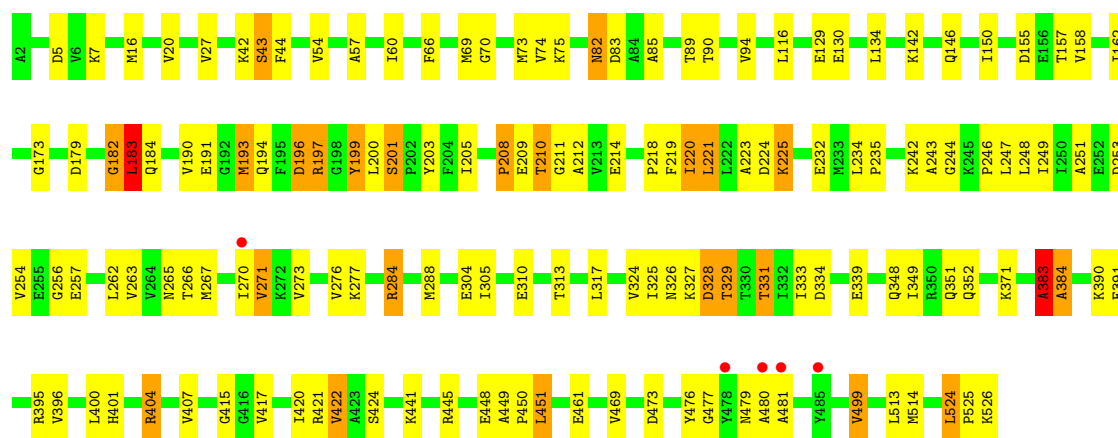


- Molecule 1: 60 kDa chaperonin 4

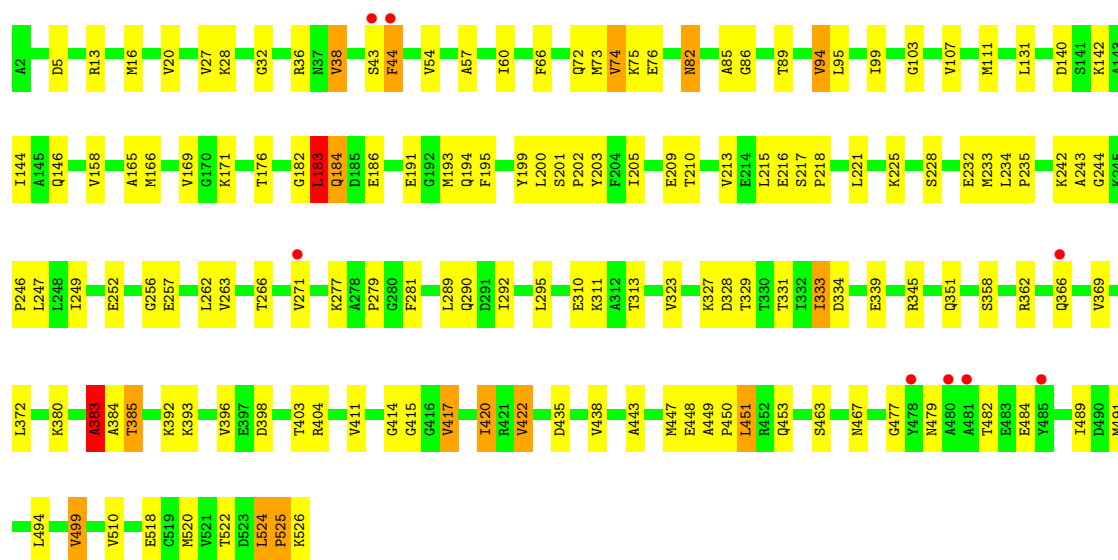
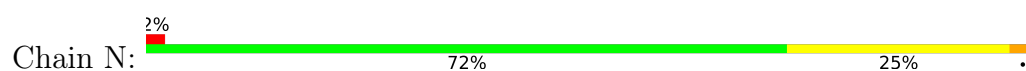


- Molecule 1: 60 kDa chaperonin 4





● Molecule 1: 60 kDa chaperonin 4



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	136.24Å 261.83Å 282.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	59.38 – 3.20 59.38 – 3.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (59.38-3.20) 100.0 (59.38-3.20)	Depositor EDS
R_{merge}	0.32	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.36 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.198 , 0.223 0.189 , 0.190	Depositor DCC
R_{free} test set	8373 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	48.3	Xtriage
Anisotropy	0.273	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 36.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	54997	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.50% 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	0.79	0/3892	1.05	7/5254 (0.1%)
1	B	0.78	0/3892	1.04	8/5254 (0.2%)
1	C	0.76	0/3892	1.01	2/5254 (0.0%)
1	D	0.75	0/3892	1.05	7/5254 (0.1%)
1	E	0.81	0/3892	1.08	7/5254 (0.1%)
1	F	0.78	0/3892	1.06	8/5254 (0.2%)
1	G	0.80	0/3892	1.04	7/5254 (0.1%)
1	H	0.77	0/3892	1.02	5/5254 (0.1%)
1	I	0.74	0/3892	1.01	2/5254 (0.0%)
1	J	0.76	0/3892	1.02	6/5254 (0.1%)
1	K	0.70	0/3892	1.03	9/5254 (0.2%)
1	L	0.74	0/3892	1.05	6/5254 (0.1%)
1	M	0.80	0/3892	1.07	6/5254 (0.1%)
1	N	0.76	0/3892	1.03	8/5254 (0.2%)
All	All	0.77	0/54488	1.04	88/73556 (0.1%)

There are no bond length outliers.

All (88) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	477	GLY	N-CA-C	11.55	130.42	111.59
1	A	477	GLY	N-CA-C	10.90	128.73	111.08
1	D	477	GLY	N-CA-C	10.71	124.93	110.69
1	F	477	GLY	N-CA-C	10.38	127.58	110.55
1	M	477	GLY	N-CA-C	9.08	126.43	111.27
1	K	204	PHE	N-CA-C	-7.98	104.69	114.75
1	K	207	LYS	CA-C-N	7.44	127.15	119.56
1	K	207	LYS	C-N-CA	7.44	127.15	119.56
1	A	136	VAL	CA-C-N	7.17	127.09	119.85
1	A	136	VAL	C-N-CA	7.17	127.09	119.85
1	B	461	GLU	CA-C-N	6.97	126.22	118.97
1	B	461	GLU	C-N-CA	6.97	126.22	118.97
1	N	477	GLY	N-CA-C	6.80	129.29	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	259	LEU	N-CA-C	6.63	118.30	111.14
1	E	45	GLY	N-CA-C	-6.47	101.84	110.58
1	J	201	SER	CA-C-N	6.44	127.89	119.84
1	J	201	SER	C-N-CA	6.44	127.89	119.84
1	E	207	LYS	CA-C-N	6.40	126.90	119.47
1	E	207	LYS	C-N-CA	6.40	126.90	119.47
1	B	60	ILE	N-CA-C	6.37	117.59	107.98
1	G	333	ILE	N-CA-C	6.22	116.83	107.75
1	M	383	ALA	N-CA-C	6.15	123.89	110.80
1	M	333	ILE	N-CA-C	6.06	116.58	107.80
1	C	494	LEU	N-CA-C	6.02	118.11	109.14
1	G	383	ALA	N-CA-C	5.93	123.43	110.80
1	F	265	ASN	N-CA-C	5.88	118.16	111.11
1	L	255	GLU	N-CA-C	5.79	118.98	109.72
1	N	32	GLY	CA-C-N	5.78	125.40	119.56
1	N	32	GLY	C-N-CA	5.78	125.40	119.56
1	F	461	GLU	CA-C-N	5.77	125.25	119.24
1	F	461	GLU	C-N-CA	5.77	125.25	119.24
1	N	383	ALA	N-CA-C	5.77	123.09	110.80
1	B	207	LYS	CA-C-N	5.75	126.15	119.47
1	B	207	LYS	C-N-CA	5.75	126.15	119.47
1	I	461	GLU	CA-C-N	5.71	125.18	119.24
1	I	461	GLU	C-N-CA	5.71	125.18	119.24
1	H	383	ALA	N-CA-C	5.67	122.87	110.80
1	E	383	ALA	N-CA-C	5.66	122.86	110.80
1	J	383	ALA	N-CA-C	5.65	122.84	110.80
1	K	220	ILE	N-CA-C	5.64	115.99	107.75
1	L	333	ILE	N-CA-C	5.63	115.97	107.80
1	G	477	GLY	N-CA-C	5.63	119.35	111.19
1	G	385	THR	N-CA-CB	5.58	119.92	110.49
1	L	32	GLY	CA-C-N	5.54	125.90	119.47
1	L	32	GLY	C-N-CA	5.54	125.90	119.47
1	F	333	ILE	N-CA-C	5.48	115.75	107.80
1	G	461	GLU	CA-C-N	5.45	124.91	119.24
1	G	461	GLU	C-N-CA	5.45	124.91	119.24
1	A	477	GLY	CA-C-N	5.45	130.24	122.72
1	A	477	GLY	C-N-CA	5.45	130.24	122.72
1	D	204	PHE	N-CA-C	-5.42	107.31	114.31
1	A	385	THR	N-CA-CB	5.42	119.65	110.49
1	G	142	LYS	N-CA-C	-5.41	105.30	111.14
1	J	212	ALA	N-CA-C	5.39	117.87	109.52
1	E	325	ILE	N-CA-C	5.39	115.61	107.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	383	ALA	N-CA-C	5.37	122.23	110.80
1	M	60	ILE	N-CA-C	5.35	116.45	108.54
1	M	116	LEU	N-CA-C	-5.35	105.45	111.28
1	H	136	VAL	CA-C-N	5.33	125.31	120.03
1	H	136	VAL	C-N-CA	5.33	125.31	120.03
1	F	325	ILE	N-CA-C	5.32	115.52	107.75
1	K	383	ALA	N-CA-C	5.32	122.13	110.80
1	N	60	ILE	N-CA-C	5.30	116.38	108.54
1	K	385	THR	N-CA-CB	5.25	119.37	110.49
1	E	242	LYS	N-CA-C	-5.24	103.97	110.41
1	B	417	VAL	N-CA-C	5.21	115.99	110.72
1	K	255	GLU	N-CA-C	5.21	118.05	109.72
1	B	142	LYS	N-CA-C	-5.17	105.56	111.14
1	J	136	VAL	CA-C-N	5.17	125.07	119.85
1	J	136	VAL	C-N-CA	5.17	125.07	119.85
1	C	383	ALA	N-CA-C	5.16	121.78	110.80
1	D	60	ILE	N-CA-C	5.16	116.17	108.54
1	F	385	THR	N-CA-CB	5.15	119.20	110.49
1	H	494	LEU	N-CA-C	5.14	116.80	109.14
1	B	383	ALA	N-CA-C	5.13	121.73	110.80
1	N	27	VAL	N-CA-C	5.13	117.02	111.58
1	D	494	LEU	N-CA-C	5.12	117.19	109.41
1	D	333	ILE	N-CA-C	5.09	115.18	107.80
1	E	89	THR	N-CA-C	5.09	116.51	111.07
1	D	305	ILE	N-CA-C	-5.08	108.18	113.10
1	D	510	VAL	CB-CA-C	-5.06	105.31	112.14
1	M	220	ILE	N-CA-C	5.05	119.84	109.34
1	A	483	GLU	N-CA-C	5.03	118.72	112.58
1	F	286	LYS	N-CA-C	-5.03	105.99	111.82
1	N	333	ILE	N-CA-C	5.03	114.81	107.37
1	N	252	GLU	N-CA-C	-5.02	105.81	111.28
1	L	385	THR	N-CA-CB	5.01	118.97	110.49
1	H	315	GLU	CB-CG-CD	5.01	121.11	112.60

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	100	0
1	B	3864	0	3989	108	0
1	C	3864	0	3989	96	0
1	D	3864	0	3989	135	0
1	E	3864	0	3989	115	0
1	F	3864	0	3989	99	0
1	G	3864	0	3989	94	0
1	H	3864	0	3989	104	0
1	I	3864	0	3989	106	0
1	J	3864	0	3989	119	0
1	K	3864	0	3989	149	0
1	L	3864	0	3989	113	0
1	M	3864	0	3989	102	0
1	N	3864	0	3989	90	0
2	A	60	0	0	18	0
2	B	83	0	0	33	0
2	C	65	0	0	14	0
2	D	62	0	0	32	0
2	E	79	0	0	32	0
2	F	53	0	0	5	0
2	G	74	0	0	9	0
2	H	52	0	0	20	0
2	I	64	0	0	24	0
2	J	75	0	0	43	0
2	K	55	0	0	33	0
2	L	64	0	0	28	0
2	M	57	0	0	13	0
2	N	58	0	0	13	0
All	All	54997	0	55846	1494	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

All (1494) 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:K:234:LEU:HA	2:K:630:HOH:O	1.37	1.24
1:K:234:LEU:HD23	2:K:630:HOH:O	1.35	1.24
1:K:384:ALA:HA	2:L:635:HOH:O	1.36	1.22

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:219:PHE:HA	2:K:636:HOH:O	1.39	1.18
1:H:261:THR:HB	2:H:647:HOH:O	1.47	1.12
1:M:421:ARG:HD3	2:M:656:HOH:O	1.52	1.10
1:D:95:LEU:HB2	2:D:661:HOH:O	1.50	1.09
1:B:491:MET:SD	2:B:680:HOH:O	2.10	1.08
1:J:193:MET:HE1	1:J:292:ILE:HG12	1.30	1.07
1:J:18:ARG:HB2	2:J:650:HOH:O	1.53	1.06
1:E:526:LYS:HG3	2:E:649:HOH:O	1.53	1.06
1:L:486:GLY:CA	2:L:660:HOH:O	2.04	1.05
1:D:95:LEU:N	2:D:661:HOH:O	1.87	1.04
1:D:173:GLY:O	1:D:404:ARG:NH2	1.90	1.04
1:B:203:TYR:N	2:B:661:HOH:O	1.91	1.03
1:J:82:ASN:HB2	2:J:628:HOH:O	1.57	1.02
1:H:261:THR:CA	2:H:647:HOH:O	2.08	1.00
1:G:514:MET:SD	2:G:666:HOH:O	2.21	0.98
1:M:265:ASN:HB3	1:M:271:VAL:HG21	1.46	0.98
1:B:45:GLY:N	2:B:667:HOH:O	1.96	0.97
1:D:11:ASP:HB3	2:D:637:HOH:O	1.63	0.97
1:F:46:ALA:HB2	1:G:76:GLU:HG3	1.45	0.96
1:B:223:ALA:HA	2:B:658:HOH:O	1.67	0.95
1:A:385:THR:N	2:A:632:HOH:O	1.98	0.94
1:J:184:GLN:HB2	2:J:645:HOH:O	1.67	0.94
1:D:137:PRO:HD2	2:D:644:HOH:O	1.67	0.93
1:L:487:ASN:N	2:L:660:HOH:O	2.01	0.93
1:J:385:THR:N	2:J:644:HOH:O	2.00	0.93
1:K:254:VAL:HB	2:K:629:HOH:O	1.69	0.93
1:L:313:THR:N	2:L:643:HOH:O	1.98	0.93
1:L:234:LEU:H	1:L:235:PRO:HD2	1.33	0.92
1:M:288:MET:HE3	2:M:653:HOH:O	1.68	0.92
1:I:271:VAL:N	2:I:645:HOH:O	2.02	0.92
1:D:484:GLU:HG2	2:D:656:HOH:O	1.69	0.91
1:B:224:ASP:N	2:B:658:HOH:O	2.04	0.90
1:B:366:GLN:NE2	2:B:651:HOH:O	2.03	0.90
1:B:301:ILE:O	2:B:658:HOH:O	1.89	0.90
1:C:30:THR:C	2:C:651:HOH:O	2.14	0.90
1:H:258:ALA:O	2:H:647:HOH:O	1.89	0.89
1:D:137:PRO:CD	2:D:644:HOH:O	2.20	0.89
1:F:54:VAL:HG22	1:F:89:THR:HG21	1.53	0.89
1:D:489:ILE:HG23	1:D:494:LEU:HD21	1.54	0.89
1:H:173:GLY:O	1:H:404:ARG:NH2	2.06	0.89
1:I:285:ARG:NE	2:I:643:HOH:O	2.06	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:200:LEU:HD21	1:H:277:LYS:HG3	1.56	0.88
1:B:173:GLY:O	1:B:404:ARG:NH2	2.06	0.87
1:H:262:LEU:N	2:H:647:HOH:O	2.07	0.87
1:E:420:ILE:HD12	1:E:451:LEU:HD13	1.55	0.87
1:G:78:ALA:O	1:G:89:THR:HG22	1.75	0.87
1:H:261:THR:CB	2:H:647:HOH:O	2.08	0.87
1:N:247:LEU:HD21	1:N:249:ILE:HD11	1.57	0.87
1:K:233:MET:O	2:K:630:HOH:O	1.93	0.86
1:G:421:ARG:NH1	1:G:469:VAL:O	2.08	0.86
1:J:235:PRO:HG3	1:J:310:GLU:HA	1.55	0.86
1:A:417:VAL:HG11	1:A:488:MET:HE1	1.55	0.86
1:J:67:GLU:OE1	2:J:657:HOH:O	1.93	0.86
1:J:173:GLY:O	1:J:404:ARG:NH2	2.08	0.86
1:A:168:LYS:C	2:A:640:HOH:O	2.19	0.86
1:C:32:GLY:N	2:C:643:HOH:O	2.06	0.86
1:D:92:ALA:O	2:D:661:HOH:O	1.92	0.86
1:E:76:GLU:CG	2:E:657:HOH:O	2.23	0.86
1:K:417:VAL:HG11	1:K:488:MET:HE1	1.57	0.86
1:K:230:ILE:HG21	2:K:644:HOH:O	1.77	0.85
1:K:421:ARG:NH1	1:K:469:VAL:O	2.09	0.85
1:A:235:PRO:HG3	1:A:310:GLU:HA	1.58	0.85
1:L:54:VAL:HG22	1:L:89:THR:HG21	1.55	0.85
1:N:327:LYS:NZ	2:N:640:HOH:O	2.08	0.85
1:J:269:GLY:HA3	1:K:257:GLU:HG3	1.59	0.85
1:C:31:LEU:C	2:C:651:HOH:O	2.18	0.85
1:H:142:LYS:O	2:H:633:HOH:O	1.95	0.84
1:I:350:ARG:O	2:I:637:HOH:O	1.93	0.84
1:L:348:GLN:HB3	2:L:647:HOH:O	1.75	0.84
1:A:384:ALA:C	2:A:632:HOH:O	2.19	0.84
1:C:31:LEU:N	2:C:651:HOH:O	2.11	0.83
1:H:421:ARG:NH1	1:H:469:VAL:O	2.12	0.83
1:K:218:PRO:O	2:K:649:HOH:O	1.95	0.83
1:M:401:HIS:HB3	2:M:647:HOH:O	1.77	0.83
1:A:82:ASN:HB2	1:A:89:THR:HG23	1.57	0.83
1:F:463:SER:HB3	2:N:650:HOH:O	1.78	0.83
1:K:58:ARG:HH11	1:K:58:ARG:HB3	1.43	0.82
1:H:339:GLU:N	2:H:637:HOH:O	2.11	0.82
1:I:353:ILE:O	2:I:653:HOH:O	1.97	0.82
1:K:236:VAL:HG23	2:K:638:HOH:O	1.78	0.82
1:M:324:VAL:HG23	1:M:331:THR:HG23	1.62	0.82
1:F:45:GLY:O	2:F:644:HOH:O	1.99	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:232:GLU:OE1	2:J:629:HOH:O	1.97	0.81
1:D:421:ARG:NH1	1:D:469:VAL:O	2.14	0.81
1:A:421:ARG:NH1	1:A:469:VAL:O	2.13	0.81
1:K:420:ILE:HD12	1:K:451:LEU:HD13	1.64	0.80
1:F:398:ASP:OD1	2:F:635:HOH:O	2.00	0.80
1:K:193:MET:HE1	1:K:292:ILE:HG12	1.63	0.80
1:I:421:ARG:NH2	1:I:476:TYR:O	2.14	0.80
1:E:76:GLU:HB3	2:E:657:HOH:O	1.81	0.80
1:N:76:GLU:OE1	2:N:633:HOH:O	2.00	0.80
1:C:131:LEU:HD13	1:C:422:VAL:HG21	1.63	0.80
1:D:421:ARG:NH2	1:D:476:TYR:O	2.13	0.80
1:H:42:LYS:O	1:H:44:PHE:N	2.14	0.80
1:J:18:ARG:CB	2:J:650:HOH:O	2.18	0.80
1:L:202:PRO:O	1:L:205:ILE:HG13	1.83	0.79
1:C:404:ARG:HG2	1:C:404:ARG:HH11	1.46	0.79
1:J:156:GLU:OE2	2:J:667:HOH:O	2.00	0.79
1:N:193:MET:HE1	1:N:292:ILE:HG12	1.62	0.79
1:C:518:GLU:OE2	2:C:653:HOH:O	1.99	0.79
1:F:131:LEU:HD13	1:F:422:VAL:HG21	1.65	0.79
1:C:31:LEU:CA	2:C:651:HOH:O	2.29	0.79
1:K:232:GLU:HA	1:K:310:GLU:CD	2.08	0.79
1:G:158:VAL:HG13	1:G:396:VAL:HG22	1.65	0.78
1:L:316:ASP:OD2	2:L:643:HOH:O	2.01	0.78
1:B:85:ALA:O	2:B:673:HOH:O	2.01	0.78
1:L:485:TYR:CD1	2:L:646:HOH:O	2.36	0.78
1:M:421:ARG:NH2	1:M:476:TYR:O	2.15	0.78
1:J:350:ARG:NE	2:J:643:HOH:O	2.13	0.78
1:A:359:ASP:N	2:A:620:HOH:O	2.16	0.78
1:D:420:ILE:HD12	1:D:451:LEU:HD13	1.66	0.78
1:E:362:ARG:HD2	2:E:674:HOH:O	1.82	0.78
1:C:350:ARG:HH11	1:C:350:ARG:CG	1.98	0.77
1:E:272:LYS:NZ	2:E:665:HOH:O	2.10	0.77
1:D:101:THR:O	2:D:640:HOH:O	2.01	0.77
1:E:209:GLU:O	2:E:679:HOH:O	2.02	0.77
1:F:5:ASP:HB2	1:F:524:LEU:HD23	1.67	0.77
1:K:227:ILE:O	1:K:254:VAL:HA	1.83	0.77
1:D:183:LEU:O	1:D:184:GLN:HB2	1.81	0.77
1:E:130:GLU:HB3	1:E:422:VAL:HG22	1.65	0.77
2:E:665:HOH:O	1:F:256:GLY:HA3	1.82	0.77
1:I:284:ARG:NH2	2:I:601:HOH:O	2.17	0.77
1:A:44:PHE:HB2	2:A:660:HOH:O	1.85	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:130:GLU:HB3	1:F:422:VAL:HG22	1.67	0.76
1:I:353:ILE:N	2:I:637:HOH:O	2.17	0.76
1:K:58:ARG:HH11	1:K:58:ARG:CB	1.97	0.76
1:F:420:ILE:HD12	1:F:451:LEU:HD13	1.66	0.76
1:B:183:LEU:O	1:B:184:GLN:HB2	1.84	0.76
1:G:484:GLU:O	2:G:653:HOH:O	2.02	0.76
1:D:61:GLU:OE1	2:D:652:HOH:O	2.04	0.76
1:F:262:LEU:HD22	1:F:273:VAL:HG21	1.66	0.76
1:K:318:GLY:O	2:K:636:HOH:O	2.04	0.76
1:F:173:GLY:O	1:F:404:ARG:NH2	2.19	0.76
1:G:169:VAL:HG11	1:G:377:ALA:HB2	1.68	0.76
1:M:54:VAL:HG22	1:M:89:THR:HG21	1.68	0.76
1:G:171:LYS:O	1:G:404:ARG:NH2	2.19	0.75
1:L:486:GLY:C	2:L:660:HOH:O	2.23	0.75
1:E:183:LEU:HD22	2:E:670:HOH:O	1.87	0.74
1:I:166:MET:HE2	1:I:171:LYS:HA	1.67	0.74
1:F:286:LYS:NZ	1:F:304:GLU:OE1	2.19	0.74
1:M:44:PHE:CD2	2:M:651:HOH:O	2.39	0.74
1:K:232:GLU:HB3	1:K:309:LEU:HB2	1.69	0.74
1:K:254:VAL:N	2:K:629:HOH:O	2.20	0.74
1:M:208:PRO:O	1:M:210:THR:N	2.20	0.74
1:B:185:ASP:O	2:B:665:HOH:O	2.06	0.74
1:F:218:PRO:HB3	1:F:246:PRO:HG2	1.70	0.74
1:K:44:PHE:O	2:K:632:HOH:O	2.06	0.74
1:I:270:ILE:HA	2:I:645:HOH:O	1.86	0.74
1:K:235:PRO:C	2:K:638:HOH:O	2.30	0.74
1:B:44:PHE:CA	2:B:667:HOH:O	2.35	0.74
1:E:3:ALA:O	2:E:677:HOH:O	2.04	0.74
1:A:44:PHE:O	2:A:660:HOH:O	2.05	0.74
1:D:95:LEU:CA	2:D:661:HOH:O	2.26	0.74
1:D:271:VAL:HB	2:D:651:HOH:O	1.86	0.74
1:E:235:PRO:HG3	1:E:310:GLU:HA	1.69	0.74
1:C:46:ALA:N	2:C:658:HOH:O	2.14	0.73
1:C:173:GLY:O	1:C:404:ARG:NH2	2.20	0.73
1:L:428:ASP:OD2	2:L:663:HOH:O	2.04	0.73
1:D:54:VAL:HG22	1:D:89:THR:HG21	1.68	0.73
1:G:18:ARG:NH2	2:G:654:HOH:O	2.19	0.73
1:G:326:ASN:ND2	1:G:329:THR:OG1	2.21	0.73
1:E:463:SER:OG	2:E:643:HOH:O	2.06	0.73
1:M:421:ARG:NH1	1:M:469:VAL:O	2.22	0.73
1:G:398:ASP:OD2	2:G:648:HOH:O	2.05	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:27:VAL:HG12	1:F:90:THR:HG23	1.70	0.73
1:I:207:LYS:NZ	2:I:646:HOH:O	2.22	0.73
1:H:78:ALA:O	1:H:89:THR:HG22	1.89	0.73
1:N:327:LYS:O	2:N:648:HOH:O	2.06	0.73
1:M:158:VAL:HG13	1:M:396:VAL:HG22	1.70	0.73
1:L:505:GLN:O	2:L:662:HOH:O	2.07	0.72
1:I:270:ILE:C	2:I:645:HOH:O	2.31	0.72
1:M:66:PHE:HA	1:M:69:MET:HE3	1.72	0.72
1:B:205:ILE:HG13	2:B:661:HOH:O	1.89	0.72
1:K:414:GLY:O	1:K:417:VAL:HG13	1.90	0.72
1:A:168:LYS:O	2:A:640:HOH:O	2.07	0.72
1:K:131:LEU:HD13	1:K:422:VAL:HG21	1.70	0.72
1:K:360:TYR:HB3	2:K:633:HOH:O	1.89	0.72
1:K:228:SER:O	1:K:257:GLU:HB3	1.90	0.72
1:F:171:LYS:O	1:F:404:ARG:NH1	2.22	0.72
1:K:228:SER:N	2:K:631:HOH:O	2.09	0.72
1:K:319:GLN:HG3	2:K:649:HOH:O	1.90	0.72
1:C:257:GLU:OE1	2:C:656:HOH:O	2.07	0.71
1:E:78:ALA:O	1:E:89:THR:HG22	1.89	0.71
1:H:339:GLU:HG2	2:H:634:HOH:O	1.89	0.71
1:K:358:SER:OG	2:K:633:HOH:O	2.07	0.71
1:L:485:TYR:OH	2:L:652:HOH:O	2.06	0.71
1:B:223:ALA:CA	2:B:658:HOH:O	2.30	0.71
1:M:235:PRO:HG3	1:M:310:GLU:HA	1.72	0.71
1:K:236:VAL:N	2:K:638:HOH:O	2.23	0.71
1:D:354:GLU:OE2	2:D:654:HOH:O	2.08	0.71
1:N:327:LYS:HD3	2:N:640:HOH:O	1.91	0.71
1:D:46:ALA:HB2	1:E:76:GLU:HG3	1.73	0.71
1:J:185:ASP:OD2	2:J:646:HOH:O	2.07	0.71
1:B:259:LEU:O	1:B:263:VAL:HG23	1.91	0.71
1:H:42:LYS:C	1:H:44:PHE:H	1.99	0.71
1:J:384:ALA:C	2:J:644:HOH:O	2.32	0.71
1:E:525:PRO:O	2:E:649:HOH:O	2.08	0.70
1:H:371:LYS:O	2:H:643:HOH:O	2.09	0.70
1:A:129:GLU:OE1	2:A:658:HOH:O	2.08	0.70
1:C:413:ALA:O	2:C:605:HOH:O	2.07	0.70
1:H:146:GLN:HG3	2:H:633:HOH:O	1.90	0.70
1:J:266:THR:O	2:J:647:HOH:O	2.08	0.70
1:L:285:ARG:HD2	2:L:651:HOH:O	1.92	0.70
1:K:229:ASN:O	2:K:640:HOH:O	2.10	0.70
1:I:479:ASN:O	1:I:483:GLU:N	2.24	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:423:ALA:O	2:B:664:HOH:O	2.10	0.69
1:K:44:PHE:HB3	2:K:632:HOH:O	1.90	0.69
1:K:482:THR:OG1	1:K:484:GLU:HG2	1.92	0.69
1:M:328:ASP:N	1:M:328:ASP:OD2	2.21	0.69
1:E:76:GLU:OE1	2:E:657:HOH:O	2.10	0.69
1:K:420:ILE:HG12	1:K:448:GLU:HG2	1.74	0.69
1:M:247:LEU:HB3	1:M:273:VAL:HG22	1.73	0.69
1:L:485:TYR:HD1	2:L:646:HOH:O	1.70	0.69
1:A:173:GLY:O	1:A:404:ARG:NH2	2.26	0.69
1:E:359:ASP:O	1:E:363:GLU:HG3	1.93	0.69
1:I:173:GLY:O	1:I:404:ARG:NH2	2.25	0.69
1:I:421:ARG:NH1	1:I:469:VAL:O	2.26	0.69
1:A:488:MET:HA	1:A:491:MET:HE3	1.75	0.69
1:J:288:MET:HE1	2:J:639:HOH:O	1.92	0.69
1:M:288:MET:CE	2:M:649:HOH:O	2.41	0.69
1:B:487:ASN:CB	2:B:652:HOH:O	2.41	0.68
1:E:16:MET:SD	1:E:73:MET:HE1	2.34	0.68
1:G:514:MET:CG	2:G:666:HOH:O	2.40	0.68
1:B:490:ASP:OD1	2:B:679:HOH:O	2.11	0.68
1:L:193:MET:HE1	1:L:292:ILE:HG12	1.72	0.68
1:N:194:GLN:NE2	2:N:643:HOH:O	2.25	0.68
1:A:27:VAL:HG12	1:A:90:THR:HG23	1.74	0.68
1:D:16:MET:HB3	1:D:514:MET:HE3	1.75	0.68
1:E:27:VAL:HG12	1:E:90:THR:HG23	1.74	0.68
1:E:239:ALA:HB1	1:E:314:LEU:HG	1.75	0.68
1:E:348:GLN:OE1	2:E:663:HOH:O	2.10	0.68
1:H:27:VAL:HG12	1:H:90:THR:HG23	1.76	0.68
1:K:173:GLY:O	1:K:404:ARG:NH2	2.27	0.68
1:A:477:GLY:HA3	1:A:488:MET:HE2	1.74	0.68
1:B:27:VAL:HG12	1:B:90:THR:HG23	1.75	0.68
1:B:44:PHE:HA	2:B:667:HOH:O	1.92	0.68
1:C:183:LEU:O	1:C:184:GLN:HB2	1.92	0.68
1:C:408:GLU:OE1	2:C:642:HOH:O	2.10	0.68
1:I:302:SER:H	1:I:307:MET:HE3	1.59	0.68
1:L:228:SER:O	1:L:257:GLU:HB3	1.94	0.68
1:H:219:PHE:CE2	1:H:245:LYS:HD2	2.29	0.68
1:N:411:VAL:HG23	1:N:489:ILE:HD13	1.76	0.68
1:A:183:LEU:O	1:A:184:GLN:HB2	1.94	0.68
1:B:27:VAL:CG1	1:B:90:THR:HG23	2.24	0.68
1:M:173:GLY:O	1:M:404:ARG:NH2	2.26	0.68
1:B:44:PHE:C	2:B:667:HOH:O	2.33	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:254:VAL:O	2:H:632:HOH:O	2.10	0.67
1:D:28:LYS:HD2	1:D:453:GLN:OE1	1.94	0.67
1:B:202:PRO:C	2:B:661:HOH:O	2.31	0.67
1:D:420:ILE:HG12	1:D:448:GLU:HG2	1.77	0.67
1:E:420:ILE:HG12	1:E:448:GLU:HG2	1.74	0.67
1:B:340:ALA:N	2:B:655:HOH:O	2.09	0.67
1:L:411:VAL:HG23	1:L:489:ILE:HD13	1.77	0.67
1:M:43:SER:OG	2:M:651:HOH:O	2.13	0.67
1:N:13:ARG:NH2	1:N:518:GLU:OE2	2.25	0.67
1:C:346:VAL:HG12	1:C:350:ARG:HD2	1.76	0.67
1:D:6:VAL:O	2:D:660:HOH:O	2.13	0.67
1:K:254:VAL:CA	2:K:629:HOH:O	2.43	0.67
1:D:391:GLU:OE1	1:D:395:ARG:NH1	2.28	0.67
1:C:419:LEU:HD11	1:C:500:THR:HG23	1.77	0.66
1:K:46:ALA:HB2	1:L:76:GLU:HG3	1.76	0.66
1:L:384:ALA:O	1:L:385:THR:HG23	1.93	0.66
1:E:284:ARG:NH2	2:E:602:HOH:O	2.18	0.66
1:G:414:GLY:O	1:G:417:VAL:HG13	1.95	0.66
1:A:421:ARG:NH2	1:A:476:TYR:O	2.28	0.66
1:N:86:GLY:O	2:N:630:HOH:O	2.12	0.66
1:A:78:ALA:O	1:A:89:THR:HG22	1.95	0.66
1:K:358:SER:HB3	2:K:645:HOH:O	1.95	0.66
1:A:359:ASP:HA	1:A:362:ARG:NH1	2.11	0.66
1:I:460:GLU:OE2	2:I:659:HOH:O	2.13	0.66
1:J:339:GLU:C	2:J:656:HOH:O	2.38	0.66
1:N:94:VAL:O	2:N:632:HOH:O	2.14	0.66
1:C:30:THR:O	2:C:651:HOH:O	2.13	0.65
1:D:354:GLU:O	2:D:650:HOH:O	2.14	0.65
1:I:27:VAL:HG12	1:I:90:THR:HG23	1.79	0.65
1:B:286:LYS:NZ	2:B:683:HOH:O	2.29	0.65
1:K:247:LEU:HB3	1:K:273:VAL:HG22	1.77	0.65
1:D:95:LEU:CB	2:D:661:HOH:O	2.16	0.65
1:G:319:GLN:OE1	2:G:670:HOH:O	2.15	0.65
1:K:227:ILE:HB	1:K:254:VAL:HG22	1.77	0.65
1:C:404:ARG:HG2	1:C:404:ARG:NH1	2.07	0.65
1:I:270:ILE:CA	2:I:645:HOH:O	2.43	0.65
1:K:232:GLU:HG3	2:K:640:HOH:O	1.97	0.65
1:E:76:GLU:CD	2:E:657:HOH:O	2.40	0.65
1:G:82:ASN:H	1:G:89:THR:HG23	1.61	0.65
1:B:200:LEU:HD21	1:B:277:LYS:HG3	1.79	0.65
1:M:158:VAL:O	1:M:162:ILE:HG12	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:82:ASN:HB2	1:G:89:THR:CG2	2.27	0.64
1:H:338:GLU:OE1	2:H:634:HOH:O	2.15	0.64
1:J:183:LEU:O	2:J:645:HOH:O	2.15	0.64
1:L:312:ALA:HA	2:L:643:HOH:O	1.96	0.64
1:B:262:LEU:O	1:B:266:THR:HG23	1.98	0.64
1:B:447:MET:O	2:B:649:HOH:O	2.14	0.64
1:G:224:ASP:HB3	1:G:302:SER:HA	1.79	0.64
1:F:13:ARG:NH2	1:F:518:GLU:OE2	2.30	0.64
1:H:261:THR:N	2:H:647:HOH:O	2.26	0.64
1:J:262:LEU:O	1:J:266:THR:HG23	1.98	0.64
1:J:479:ASN:HD22	1:J:493:ILE:HG13	1.63	0.64
1:J:480:ALA:CB	2:J:661:HOH:O	2.45	0.64
1:J:18:ARG:CG	2:J:650:HOH:O	2.40	0.64
1:D:137:PRO:O	2:D:644:HOH:O	2.15	0.64
1:E:525:PRO:C	2:E:649:HOH:O	2.40	0.64
1:H:239:ALA:HB1	1:H:314:LEU:HD11	1.78	0.64
1:I:231:ARG:NE	2:I:639:HOH:O	2.29	0.64
1:J:183:LEU:HD22	1:J:184:GLN:H	1.63	0.64
1:G:122:LYS:HE2	1:G:429:LEU:HD11	1.79	0.63
1:I:414:GLY:O	1:I:417:VAL:HG13	1.98	0.63
1:M:208:PRO:O	1:M:211:GLY:N	2.24	0.63
1:L:54:VAL:HG22	1:L:89:THR:CG2	2.28	0.63
1:B:253:ASP:OD2	1:B:254:VAL:N	2.29	0.63
1:K:319:GLN:OE1	2:K:652:HOH:O	2.15	0.63
1:G:86:GLY:O	2:G:648:HOH:O	2.16	0.63
1:M:42:LYS:O	1:M:44:PHE:N	2.24	0.63
1:M:129:GLU:OE2	2:M:648:HOH:O	2.15	0.63
1:C:130:GLU:HB3	1:C:422:VAL:HG22	1.80	0.63
1:D:224:ASP:HB3	1:D:302:SER:HA	1.80	0.63
1:F:202:PRO:O	1:F:205:ILE:HG13	1.99	0.63
1:H:11:ASP:OD2	2:H:645:HOH:O	2.16	0.63
1:K:349:ILE:O	1:K:353:ILE:HG13	1.98	0.63
1:L:219:PHE:HB3	1:L:317:LEU:HD23	1.80	0.63
1:E:231:ARG:NH1	2:E:671:HOH:O	2.23	0.63
1:M:404:ARG:HG2	1:M:404:ARG:HH11	1.64	0.63
1:A:171:LYS:O	1:A:404:ARG:NH1	2.32	0.63
1:B:176:THR:HG21	1:B:333:ILE:HD11	1.80	0.63
1:I:166:MET:CE	1:I:171:LYS:HA	2.27	0.63
1:L:358:SER:OG	1:L:359:ASP:N	2.30	0.63
1:D:137:PRO:CB	2:D:644:HOH:O	2.46	0.63
1:E:493:ILE:HA	2:E:644:HOH:O	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:27:VAL:CG1	1:F:90:THR:HG23	2.29	0.63
1:K:236:VAL:HG12	1:K:236:VAL:O	1.98	0.63
1:L:360:TYR:OH	2:L:635:HOH:O	2.15	0.63
1:A:142:LYS:NZ	2:A:637:HOH:O	2.29	0.62
1:E:433:ASN:HD21	1:E:435:ASP:HB2	1.64	0.62
1:F:183:LEU:O	1:F:184:GLN:HB2	1.97	0.62
1:K:236:VAL:CG2	2:K:638:HOH:O	2.39	0.62
1:H:261:THR:C	2:H:647:HOH:O	2.25	0.62
1:G:420:ILE:HD12	1:G:451:LEU:HD13	1.81	0.62
1:K:194:GLN:O	1:K:371:LYS:HE3	1.99	0.62
1:B:404:ARG:HH11	1:B:404:ARG:HG2	1.63	0.62
1:J:184:GLN:OE1	2:J:645:HOH:O	2.16	0.62
1:M:199:TYR:HB3	1:M:201:SER:H	1.65	0.62
1:B:218:PRO:HD2	1:B:320:ALA:O	2.00	0.62
1:E:76:GLU:CB	2:E:657:HOH:O	2.38	0.62
1:K:477:GLY:HA3	1:K:488:MET:HE2	1.81	0.62
1:L:234:LEU:H	1:L:235:PRO:CD	2.11	0.62
1:I:207:LYS:CE	2:I:646:HOH:O	2.48	0.62
1:M:415:GLY:O	1:M:451:LEU:HD12	2.00	0.62
1:K:310:GLU:N	1:K:310:GLU:OE1	2.32	0.62
1:L:463:SER:O	1:L:467:ASN:HB2	1.99	0.62
1:J:185:ASP:CG	2:J:646:HOH:O	2.43	0.61
1:J:342:ILE:O	1:J:346:VAL:HG23	2.00	0.61
1:D:155:ASP:OD2	1:D:395:ARG:NH2	2.32	0.61
1:E:433:ASN:ND2	1:E:435:ASP:HB2	2.15	0.61
1:E:494:LEU:N	2:E:644:HOH:O	2.09	0.61
1:A:243:ALA:O	1:A:245:LYS:N	2.33	0.61
1:B:242:LYS:C	1:B:244:GLY:H	2.08	0.61
1:J:349:ILE:HA	1:J:352:GLN:HG3	1.83	0.61
1:D:92:ALA:C	2:D:661:HOH:O	2.38	0.61
1:J:266:THR:HA	2:J:647:HOH:O	2.01	0.61
1:J:285:ARG:NH1	2:J:649:HOH:O	2.05	0.61
1:D:137:PRO:CA	2:D:644:HOH:O	2.49	0.61
1:E:414:GLY:O	1:E:417:VAL:HG13	2.01	0.61
1:B:404:ARG:HG2	1:B:404:ARG:NH1	2.14	0.61
1:I:131:LEU:HD13	1:I:422:VAL:HG21	1.81	0.61
1:G:183:LEU:O	1:G:382:GLY:HA3	2.00	0.61
1:H:197:ARG:NH1	2:H:607:HOH:O	2.29	0.61
1:N:158:VAL:HG13	1:N:396:VAL:HG22	1.81	0.61
1:I:183:LEU:HD22	1:I:184:GLN:H	1.65	0.61
1:J:340:ALA:N	2:J:656:HOH:O	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:131:LEU:HD13	1:N:422:VAL:HG21	1.83	0.61
1:D:383:ALA:O	1:D:384:ALA:HB3	2.01	0.61
1:F:54:VAL:CG2	1:F:89:THR:HG21	2.30	0.61
1:H:130:GLU:HB3	1:H:422:VAL:HG22	1.82	0.61
1:J:414:GLY:O	1:J:417:VAL:HG13	2.00	0.61
1:A:131:LEU:HD13	1:A:422:VAL:HG21	1.82	0.60
1:D:366:GLN:HA	1:D:369:VAL:HG22	1.82	0.60
1:E:349:ILE:O	1:E:353:ILE:HG13	2.00	0.60
1:G:16:MET:SD	1:G:73:MET:HE1	2.41	0.60
1:H:247:LEU:HD21	1:H:249:ILE:HD11	1.83	0.60
1:B:102:GLU:HB2	1:B:442:VAL:HG13	1.83	0.60
1:K:58:ARG:HB3	1:K:58:ARG:NH1	2.15	0.60
1:L:421:ARG:NH2	1:L:476:TYR:O	2.23	0.60
1:B:420:ILE:HG13	1:B:448:GLU:HG2	1.82	0.60
1:H:215:LEU:HB2	1:H:323:VAL:HG22	1.83	0.60
1:N:235:PRO:HG3	1:N:310:GLU:HA	1.83	0.60
1:B:524:LEU:O	1:B:526:LYS:N	2.34	0.60
1:N:200:LEU:HD21	1:N:277:LYS:HG3	1.81	0.60
1:L:525:PRO:HD3	2:L:632:HOH:O	2.01	0.60
1:B:228:SER:N	2:B:672:HOH:O	2.07	0.60
1:G:169:VAL:CG1	1:G:377:ALA:HB2	2.32	0.60
1:A:82:ASN:HB2	1:A:89:THR:CG2	2.30	0.60
1:C:350:ARG:HH11	1:C:350:ARG:HG2	1.66	0.60
1:F:202:PRO:O	1:F:204:PHE:N	2.34	0.60
1:M:262:LEU:O	1:M:266:THR:HG23	2.01	0.60
1:M:404:ARG:HG2	1:M:404:ARG:NH1	2.17	0.60
1:C:45:GLY:HA3	2:C:658:HOH:O	2.00	0.59
1:K:328:ASP:OD1	1:K:328:ASP:N	2.34	0.59
1:B:131:LEU:HD13	1:B:422:VAL:HG21	1.83	0.59
1:H:314:LEU:HD12	1:H:314:LEU:H	1.67	0.59
1:I:353:ILE:HB	2:I:637:HOH:O	2.00	0.59
1:J:224:ASP:O	1:J:225:LYS:HB3	2.01	0.59
1:C:200:LEU:HD21	1:C:277:LYS:HG3	1.83	0.59
1:D:495:ASP:OD2	2:D:636:HOH:O	2.16	0.59
1:G:286:LYS:NZ	1:G:304:GLU:OE2	2.32	0.59
1:K:384:ALA:O	1:K:385:THR:HG23	2.02	0.59
1:A:479:ASN:C	1:A:481:ALA:H	2.11	0.59
1:L:121:ASP:OD1	2:L:630:HOH:O	2.16	0.59
1:N:85:ALA:HB1	1:N:499:VAL:HG12	1.84	0.59
1:E:158:VAL:HG13	1:E:396:VAL:HG22	1.83	0.59
1:H:479:ASN:HB2	1:H:484:GLU:O	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:420:ILE:HG12	1:H:448:GLU:HG2	1.85	0.59
1:I:322:ARG:HD2	2:I:658:HOH:O	2.01	0.59
1:C:524:LEU:O	1:C:526:LYS:N	2.36	0.59
1:H:287:ALA:HB1	1:H:368:ARG:NH1	2.18	0.59
1:M:218:PRO:HB3	1:M:246:PRO:HG2	1.85	0.59
1:D:291:ASP:OD2	1:D:368:ARG:HD2	2.03	0.59
1:N:111:MET:HE1	1:N:438:VAL:HG21	1.85	0.59
1:N:166:MET:HE2	1:N:171:LYS:HA	1.85	0.59
1:E:183:LEU:HD13	1:E:184:GLN:HG3	1.83	0.59
1:E:524:LEU:O	1:E:526:LYS:N	2.36	0.59
1:H:448:GLU:OE2	2:H:625:HOH:O	2.17	0.59
1:A:16:MET:SD	1:A:73:MET:HE1	2.43	0.58
1:D:16:MET:SD	1:D:73:MET:HE1	2.43	0.58
1:G:429:LEU:HG	1:G:440:ILE:HD13	1.83	0.58
1:K:225:LYS:HD3	1:K:226:LYS:O	2.03	0.58
1:B:82:ASN:HB2	1:B:89:THR:OG1	2.03	0.58
1:B:202:PRO:O	1:B:204:PHE:N	2.33	0.58
1:B:215:LEU:HB2	1:B:323:VAL:HG22	1.85	0.58
1:G:131:LEU:HD13	1:G:422:VAL:HG21	1.85	0.58
1:K:182:GLY:HA2	1:L:281:PHE:CZ	2.38	0.58
1:G:200:LEU:HD21	1:G:277:LYS:HG3	1.86	0.58
1:H:414:GLY:O	1:H:417:VAL:HG13	2.03	0.58
1:J:155:ASP:OD1	1:J:157:THR:OG1	2.15	0.58
1:D:213:VAL:HB	1:D:325:ILE:HB	1.84	0.58
1:F:291:ASP:OD2	1:F:368:ARG:HD2	2.04	0.58
1:I:130:GLU:HB3	1:I:422:VAL:HG22	1.85	0.58
1:J:134:LEU:HD12	1:J:412:VAL:HG22	1.85	0.58
1:K:27:VAL:HG12	1:K:90:THR:HG23	1.84	0.58
1:E:76:GLU:HG3	2:E:657:HOH:O	1.97	0.58
1:K:44:PHE:C	2:K:632:HOH:O	2.45	0.58
1:H:202:PRO:O	1:H:203:TYR:HB2	2.04	0.58
1:H:421:ARG:NH2	1:H:476:TYR:O	2.35	0.58
1:J:285:ARG:HD2	2:J:649:HOH:O	2.03	0.58
1:K:326:ASN:OD1	1:K:329:THR:N	2.36	0.58
1:N:449:ALA:HB3	1:N:450:PRO:HD3	1.86	0.58
1:D:411:VAL:HB	1:D:494:LEU:HD22	1.85	0.58
1:H:131:LEU:HD13	1:H:422:VAL:HG21	1.86	0.58
1:J:11:ASP:OD2	2:J:633:HOH:O	2.17	0.58
1:L:85:ALA:HB1	1:L:499:VAL:HG12	1.86	0.58
1:C:449:ALA:HB3	1:C:450:PRO:HD3	1.86	0.58
1:N:111:MET:HE2	1:N:435:ASP:OD1	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:215:LEU:HB2	1:N:323:VAL:HG22	1.86	0.58
1:E:479:ASN:HD22	1:E:491:MET:HE3	1.69	0.57
1:K:133:ALA:O	2:K:625:HOH:O	2.17	0.57
1:N:16:MET:SD	1:N:73:MET:HE1	2.44	0.57
1:D:46:ALA:CB	1:E:76:GLU:HG3	2.33	0.57
1:J:77:VAL:HG21	1:J:510:VAL:HB	1.86	0.57
1:K:13:ARG:HD2	1:K:104:LEU:HD22	1.85	0.57
1:M:248:LEU:HD13	1:M:325:ILE:HD11	1.86	0.57
1:H:16:MET:SD	1:H:73:MET:HE1	2.45	0.57
1:B:491:MET:CE	2:B:680:HOH:O	2.47	0.57
1:C:142:LYS:O	1:C:146:GLN:HG3	2.05	0.57
1:E:13:ARG:HD2	1:E:104:LEU:HD22	1.86	0.57
1:K:361:ASP:OD2	2:K:645:HOH:O	2.17	0.57
1:H:194:GLN:O	1:H:371:LYS:HE3	2.04	0.57
1:L:486:GLY:HA2	2:L:660:HOH:O	1.83	0.57
1:N:247:LEU:CD2	1:N:249:ILE:HD11	2.33	0.57
1:D:414:GLY:O	1:D:417:VAL:HG13	2.04	0.57
1:H:435:ASP:OD2	2:H:624:HOH:O	2.18	0.57
1:J:131:LEU:HD13	1:J:422:VAL:HG21	1.86	0.57
1:K:85:ALA:HB1	1:K:499:VAL:HG12	1.85	0.57
1:I:262:LEU:O	1:I:266:THR:HG23	2.05	0.57
1:K:478:TYR:N	1:K:488:MET:HE2	2.20	0.57
1:L:25:ASP:HA	1:L:28:LYS:HE2	1.85	0.57
1:N:414:GLY:O	1:N:417:VAL:HG13	2.04	0.57
1:D:239:ALA:HB1	1:D:314:LEU:HG	1.87	0.57
1:L:225:LYS:HE3	1:L:303:GLU:HB2	1.85	0.57
1:M:421:ARG:CD	2:M:656:HOH:O	2.25	0.57
1:B:449:ALA:HB3	1:B:450:PRO:HD3	1.85	0.56
1:D:203:TYR:HB2	1:D:263:VAL:HG13	1.87	0.56
1:N:262:LEU:O	1:N:266:THR:HG23	2.05	0.56
1:C:194:GLN:O	1:C:371:LYS:HE3	2.05	0.56
1:D:57:ALA:O	1:D:75:LYS:HE3	2.05	0.56
1:E:27:VAL:CG1	1:E:90:THR:HG23	2.35	0.56
1:G:291:ASP:OD2	1:G:368:ARG:HD2	2.05	0.56
1:J:141:SER:CB	2:J:635:HOH:O	2.53	0.56
1:K:46:ALA:CB	1:L:76:GLU:HG3	2.34	0.56
1:K:268:ARG:NH2	2:K:637:HOH:O	2.37	0.56
1:K:358:SER:CB	2:K:645:HOH:O	2.51	0.56
1:L:312:ALA:CA	2:L:643:HOH:O	2.52	0.56
1:M:421:ARG:NH1	2:M:656:HOH:O	2.11	0.56
1:A:257:GLU:O	1:A:261:THR:OG1	2.23	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:472:GLY:HA3	1:B:476:TYR:CD2	2.40	0.56
1:D:423:ALA:O	2:D:657:HOH:O	2.17	0.56
1:F:200:LEU:HD21	1:F:277:LYS:HG3	1.86	0.56
1:I:411:VAL:HG23	1:I:489:ILE:HD13	1.86	0.56
1:A:420:ILE:CG1	1:A:448:GLU:HG2	2.35	0.56
1:D:82:ASN:HB2	1:D:89:THR:HB	1.86	0.56
1:I:305:ILE:HD12	1:I:307:MET:HE2	1.87	0.56
1:F:70:GLY:HA2	1:F:73:MET:HE3	1.87	0.56
1:D:214:GLU:OE2	1:D:322:ARG:NH2	2.39	0.56
1:F:94:VAL:O	2:F:645:HOH:O	2.18	0.56
1:J:62:LEU:HD13	1:J:68:ASN:HA	1.87	0.56
1:L:193:MET:HE1	1:L:292:ILE:CG1	2.35	0.56
1:M:70:GLY:HA2	1:M:73:MET:HE3	1.87	0.56
1:D:235:PRO:HG3	1:D:310:GLU:HA	1.88	0.56
1:E:231:ARG:HD2	2:E:671:HOH:O	2.06	0.56
1:K:39:VAL:HG12	1:L:69:MET:HE2	1.88	0.56
1:N:327:LYS:CD	2:N:640:HOH:O	2.51	0.56
1:C:33:PRO:C	1:C:35:GLY:H	2.14	0.56
1:G:57:ALA:O	1:G:75:LYS:HE3	2.06	0.56
1:H:381:VAL:HG21	1:H:393:LYS:HB2	1.88	0.56
1:J:18:ARG:HG2	2:J:650:HOH:O	2.05	0.56
1:K:7:LYS:HG3	1:K:66:PHE:CZ	2.40	0.56
1:L:100:ILE:O	1:L:104:LEU:HG	2.06	0.56
1:M:179:ASP:OD1	1:M:390:LYS:NZ	2.39	0.56
1:I:16:MET:HB3	1:I:514:MET:HE3	1.87	0.55
1:J:82:ASN:CB	2:J:628:HOH:O	2.31	0.55
1:D:326:ASN:HD22	1:D:329:THR:HB	1.72	0.55
1:G:383:ALA:HB3	1:G:389:MET:HB2	1.88	0.55
1:K:421:ARG:NH2	1:K:476:TYR:O	2.39	0.55
1:A:122:LYS:NZ	2:A:653:HOH:O	2.40	0.55
1:C:155:ASP:OD2	1:C:395:ARG:NH2	2.40	0.55
1:D:451:LEU:HD11	1:D:469:VAL:HG21	1.89	0.55
1:I:479:ASN:HB2	1:I:491:MET:SD	2.46	0.55
1:K:235:PRO:CG	1:K:310:GLU:HA	2.36	0.55
1:A:449:ALA:HB3	1:A:450:PRO:HD3	1.89	0.55
1:A:452:ARG:NH1	2:A:604:HOH:O	2.36	0.55
1:D:266:THR:HG22	1:D:273:VAL:H	1.71	0.55
1:N:95:LEU:O	1:N:99:ILE:HG13	2.06	0.55
1:B:34:LYS:HD2	1:B:458:CYS:HA	1.89	0.55
1:E:200:LEU:HD21	1:E:277:LYS:HG3	1.87	0.55
1:F:366:GLN:HA	1:F:369:VAL:HG22	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:358:SER:HB3	1:H:361:ASP:OD2	2.05	0.55
1:K:70:GLY:HA2	1:K:73:MET:HE3	1.88	0.55
1:L:5:ASP:OD2	2:L:632:HOH:O	2.18	0.55
1:M:253:ASP:OD2	1:M:254:VAL:N	2.39	0.55
1:N:221:LEU:HD23	1:N:249:ILE:HD12	1.87	0.55
1:D:158:VAL:HG13	1:D:396:VAL:HG22	1.89	0.55
1:D:193:MET:HE1	1:D:292:ILE:HG12	1.89	0.55
1:H:144:ILE:HG23	1:H:403:THR:HG21	1.87	0.55
1:N:193:MET:HE1	1:N:292:ILE:CG1	2.34	0.55
1:C:214:GLU:HG3	1:C:324:VAL:HG22	1.88	0.55
1:J:16:MET:HB3	1:J:514:MET:HE3	1.88	0.55
1:A:353:ILE:HG23	1:A:362:ARG:HG3	1.88	0.55
1:C:242:LYS:C	1:C:244:GLY:H	2.15	0.55
1:D:54:VAL:CG2	1:D:89:THR:HG21	2.36	0.55
1:H:70:GLY:HA2	1:H:73:MET:HE3	1.89	0.55
1:I:183:LEU:O	1:I:184:GLN:HB2	2.06	0.55
1:A:27:VAL:CG1	1:A:90:THR:HG23	2.37	0.55
1:A:239:ALA:HB1	1:A:314:LEU:HG	1.88	0.55
1:G:366:GLN:HA	1:G:369:VAL:HG22	1.88	0.55
1:N:415:GLY:O	1:N:451:LEU:HD12	2.06	0.55
1:B:487:ASN:N	2:B:652:HOH:O	1.99	0.54
1:F:259:LEU:O	1:F:263:VAL:HG23	2.07	0.54
1:I:287:ALA:HB1	1:I:368:ARG:NH1	2.22	0.54
1:J:359:ASP:OD1	1:J:362:ARG:NH1	2.39	0.54
1:K:44:PHE:CB	2:K:632:HOH:O	2.52	0.54
1:A:69:MET:O	1:A:73:MET:HG3	2.07	0.54
1:L:352:GLN:HA	2:L:638:HOH:O	2.07	0.54
1:L:421:ARG:NH1	1:L:469:VAL:O	2.40	0.54
1:M:473:ASP:O	1:M:476:TYR:HB3	2.07	0.54
1:G:524:LEU:O	1:G:526:LYS:N	2.37	0.54
1:A:202:PRO:O	1:A:205:ILE:HG13	2.07	0.54
1:C:33:PRO:O	1:C:35:GLY:N	2.40	0.54
1:C:353:ILE:HD13	1:C:366:GLN:HG3	1.89	0.54
1:D:105:LYS:HG3	2:D:640:HOH:O	2.07	0.54
1:E:142:LYS:O	1:E:146:GLN:HG3	2.07	0.54
1:J:5:ASP:OD1	2:J:671:HOH:O	2.18	0.54
1:M:449:ALA:HB3	1:M:450:PRO:HD3	1.90	0.54
1:N:186:GLU:HB2	1:N:380:LYS:HB2	1.90	0.54
1:F:69:MET:O	1:F:73:MET:HG3	2.06	0.54
1:A:479:ASN:O	1:A:481:ALA:N	2.41	0.54
1:B:349:ILE:O	1:B:353:ILE:HG13	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:23:LEU:HD23	1:G:74:VAL:HG22	1.88	0.54
1:G:479:ASN:ND2	1:G:482:THR:OG1	2.41	0.54
1:J:364:LYS:NZ	2:J:639:HOH:O	2.39	0.54
1:N:242:LYS:C	1:N:244:GLY:H	2.15	0.54
1:D:218:PRO:HB3	1:D:246:PRO:HG2	1.89	0.54
1:D:242:LYS:C	1:D:244:GLY:H	2.15	0.54
1:E:76:GLU:OE2	2:E:668:HOH:O	2.18	0.54
1:M:193:MET:HE1	2:M:646:HOH:O	2.08	0.54
1:C:414:GLY:O	1:C:417:VAL:HG13	2.08	0.54
1:E:242:LYS:C	1:E:244:GLY:H	2.15	0.54
1:F:242:LYS:C	1:F:244:GLY:H	2.16	0.54
1:F:524:LEU:O	1:F:526:LYS:N	2.40	0.54
1:G:82:ASN:HB2	1:G:89:THR:HG23	1.88	0.54
1:K:102:GLU:HB2	1:K:442:VAL:HG13	1.90	0.54
1:K:411:VAL:HG23	1:K:489:ILE:HD13	1.89	0.54
1:C:23:LEU:HD23	1:C:74:VAL:HG22	1.90	0.54
1:G:242:LYS:C	1:G:244:GLY:H	2.15	0.54
1:I:181:THR:O	1:J:282:GLY:HA3	2.08	0.54
1:K:142:LYS:HE3	1:K:146:GLN:NE2	2.23	0.54
1:M:27:VAL:HG12	1:M:90:THR:HG23	1.88	0.54
1:A:353:ILE:HD13	1:A:366:GLN:HG3	1.89	0.53
1:G:82:ASN:HB2	1:G:89:THR:HG21	1.89	0.53
1:I:455:VAL:HG13	1:I:460:GLU:HB2	1.90	0.53
1:K:349:ILE:HA	1:K:352:GLN:HG3	1.89	0.53
1:I:350:ARG:C	2:I:637:HOH:O	2.45	0.53
1:K:183:LEU:O	1:K:382:GLY:HA3	2.08	0.53
1:K:350:ARG:HG3	1:K:353:ILE:HD12	1.89	0.53
1:N:28:LYS:HD2	1:N:453:GLN:OE1	2.08	0.53
1:B:491:MET:HE1	2:B:680:HOH:O	2.06	0.53
1:C:202:PRO:O	1:C:204:PHE:N	2.39	0.53
1:I:215:LEU:HB2	1:I:323:VAL:HG22	1.91	0.53
1:K:38:VAL:HG13	1:L:519:CYS:HB3	1.88	0.53
1:M:479:ASN:C	1:M:481:ALA:H	2.15	0.53
1:A:366:GLN:HA	1:A:369:VAL:HG22	1.90	0.53
1:H:258:ALA:O	1:H:262:LEU:HG	2.08	0.53
1:I:27:VAL:CG1	1:I:90:THR:HG23	2.38	0.53
1:L:5:ASP:HB2	1:L:524:LEU:HD12	1.90	0.53
1:L:420:ILE:HG12	1:L:448:GLU:HG2	1.90	0.53
1:M:199:TYR:CZ	1:M:205:ILE:HD11	2.44	0.53
1:A:168:LYS:HB3	2:A:640:HOH:O	2.09	0.53
1:A:257:GLU:OE1	2:A:652:HOH:O	2.19	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:455:VAL:HG13	1:E:460:GLU:HB2	1.89	0.53
1:I:207:LYS:HE3	2:I:646:HOH:O	2.08	0.53
1:A:194:GLN:O	1:A:371:LYS:HE3	2.09	0.53
1:E:492:GLY:O	2:E:644:HOH:O	2.19	0.53
1:I:496:PRO:HB2	1:I:499:VAL:HG13	1.91	0.53
1:A:206:ASN:O	1:A:207:LYS:HD2	2.09	0.53
1:B:414:GLY:O	1:B:417:VAL:HG13	2.09	0.53
1:F:314:LEU:HD23	1:F:317:LEU:HD12	1.91	0.53
1:K:344:GLY:O	1:K:347:ALA:HB3	2.09	0.53
1:F:86:GLY:O	2:F:635:HOH:O	2.19	0.53
1:H:183:LEU:O	1:H:382:GLY:HA3	2.08	0.53
1:H:354:GLU:C	1:H:356:ALA:H	2.17	0.53
1:J:480:ALA:HB2	2:J:661:HOH:O	2.06	0.53
1:B:487:ASN:HB3	2:B:652:HOH:O	2.07	0.53
1:I:140:ASP:OD2	1:I:142:LYS:HB3	2.09	0.53
1:K:82:ASN:HB2	1:K:89:THR:OG1	2.08	0.53
1:K:420:ILE:HD12	1:K:451:LEU:CD1	2.38	0.53
1:D:137:PRO:C	2:D:644:HOH:O	2.52	0.52
1:J:464:VAL:O	1:J:468:THR:HG23	2.09	0.52
1:M:420:ILE:HG12	1:M:448:GLU:HG2	1.92	0.52
1:F:247:LEU:HD21	1:F:249:ILE:HD11	1.90	0.52
1:E:493:ILE:CA	2:E:644:HOH:O	2.57	0.52
1:M:5:ASP:HB2	1:M:524:LEU:HD12	1.92	0.52
1:M:16:MET:HB3	1:M:514:MET:HE3	1.90	0.52
1:N:383:ALA:O	1:N:384:ALA:HB3	2.09	0.52
1:C:18:ARG:HG2	1:C:67:GLU:CD	2.35	0.52
1:J:82:ASN:ND2	2:J:628:HOH:O	2.20	0.52
1:L:236:VAL:HG22	1:L:312:ALA:O	2.10	0.52
1:N:82:ASN:HB2	1:N:89:THR:HB	1.90	0.52
1:M:220:ILE:HG22	1:M:220:ILE:O	2.09	0.52
1:D:131:LEU:HD13	1:D:422:VAL:HG21	1.91	0.52
1:D:219:PHE:CE2	1:D:245:LYS:HD2	2.45	0.52
1:I:176:THR:HG21	1:I:333:ILE:HD13	1.92	0.52
1:N:176:THR:HG21	1:N:333:ILE:HD13	1.91	0.52
1:C:409:GLU:OE1	2:C:649:HOH:O	2.19	0.52
1:D:137:PRO:N	2:D:644:HOH:O	2.36	0.52
1:I:72:GLN:HE22	1:I:75:LYS:HE3	1.74	0.52
1:B:266:THR:HG21	1:B:273:VAL:HB	1.91	0.52
1:C:248:LEU:HD13	1:C:325:ILE:HD11	1.91	0.52
1:E:262:LEU:O	1:E:266:THR:HG23	2.10	0.52
1:H:140:ASP:OD2	1:H:142:LYS:HB3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:218:PRO:HB3	1:I:246:PRO:HG2	1.91	0.52
1:I:350:ARG:HA	1:I:353:ILE:HD12	1.91	0.52
1:J:449:ALA:HB3	1:J:450:PRO:HD3	1.92	0.52
1:K:158:VAL:HG13	1:K:396:VAL:HG22	1.92	0.52
1:K:420:ILE:CD1	1:K:451:LEU:HD13	2.38	0.52
1:F:219:PHE:HB3	1:F:317:LEU:HD13	1.92	0.52
1:I:200:LEU:HD21	1:I:277:LYS:HG3	1.91	0.52
1:N:479:ASN:HB3	1:N:484:GLU:H	1.75	0.52
1:B:142:LYS:O	1:B:146:GLN:HG3	2.10	0.51
1:C:217:SER:O	1:C:245:LYS:HD3	2.10	0.51
1:D:451:LEU:C	1:D:451:LEU:HD23	2.35	0.51
1:F:16:MET:SD	1:F:73:MET:HE1	2.50	0.51
1:G:296:THR:HB	1:G:319:GLN:H	1.75	0.51
1:M:476:TYR:HB2	2:M:632:HOH:O	2.09	0.51
1:D:200:LEU:HD21	1:D:277:LYS:HG3	1.91	0.51
1:F:301:ILE:HD11	1:F:316:ASP:HB3	1.91	0.51
1:H:23:LEU:CD2	1:H:74:VAL:HG22	2.41	0.51
1:I:11:ASP:OD2	2:I:640:HOH:O	2.18	0.51
1:C:291:ASP:OD2	1:C:368:ARG:HD2	2.10	0.51
1:D:69:MET:O	1:D:73:MET:HG3	2.09	0.51
1:D:178:GLU:HA	1:D:393:LYS:HE3	1.92	0.51
1:D:411:VAL:HG23	1:D:489:ILE:HD13	1.90	0.51
1:K:176:THR:HG21	1:K:333:ILE:HD13	1.92	0.51
1:L:72:GLN:OE1	1:L:75:LYS:HE2	2.11	0.51
1:A:76:GLU:HG3	1:G:46:ALA:HB2	1.93	0.51
1:A:229:ASN:HB3	2:A:652:HOH:O	2.11	0.51
1:D:339:GLU:H	1:D:339:GLU:CD	2.18	0.51
1:G:202:PRO:O	1:G:204:PHE:N	2.41	0.51
1:M:184:GLN:OE1	1:M:184:GLN:HA	2.09	0.51
1:A:28:LYS:HD2	1:A:453:GLN:OE1	2.10	0.51
1:A:348:GLN:NE2	2:A:606:HOH:O	2.37	0.51
1:E:288:MET:HG2	1:E:368:ARG:HD3	1.93	0.51
1:E:291:ASP:OD2	1:E:368:ARG:HD2	2.11	0.51
1:I:314:LEU:HA	1:I:317:LEU:HD22	1.93	0.51
1:J:141:SER:HB3	2:J:635:HOH:O	2.10	0.51
1:B:291:ASP:OD2	1:B:368:ARG:HD2	2.11	0.51
1:B:421:ARG:NH2	1:B:476:TYR:O	2.43	0.51
1:C:383:ALA:O	1:C:384:ALA:HB3	2.09	0.51
1:E:149:THR:HG23	1:E:155:ASP:C	2.36	0.51
1:H:202:PRO:C	1:H:204:PHE:H	2.19	0.51
1:I:217:SER:HA	1:I:320:ALA:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:27:VAL:CG1	1:K:90:THR:HG23	2.40	0.51
1:L:486:GLY:HA3	2:L:660:HOH:O	1.85	0.51
1:K:193:MET:HG3	1:K:371:LYS:HB3	1.92	0.51
1:A:247:LEU:HD21	1:A:249:ILE:HD11	1.91	0.51
1:B:247:LEU:HD21	1:B:249:ILE:HD11	1.92	0.51
1:C:215:LEU:HB2	1:C:323:VAL:HG22	1.92	0.51
1:C:420:ILE:HG13	1:C:448:GLU:HG2	1.93	0.51
1:E:355:GLU:HB3	2:E:648:HOH:O	2.10	0.51
1:M:57:ALA:O	1:M:75:LYS:HD2	2.11	0.51
1:E:215:LEU:HB2	1:E:323:VAL:HG22	1.91	0.51
1:E:455:VAL:CG1	1:E:460:GLU:HB2	2.41	0.51
1:G:353:ILE:HD13	1:G:366:GLN:HG3	1.92	0.51
1:G:383:ALA:O	1:G:384:ALA:HB3	2.10	0.51
1:L:16:MET:HB3	1:L:514:MET:HE3	1.93	0.51
1:M:85:ALA:HB1	1:M:499:VAL:HG12	1.93	0.51
1:C:31:LEU:HD13	1:C:90:THR:HG21	1.92	0.51
1:E:28:LYS:HD2	1:E:453:GLN:OE1	2.11	0.51
1:F:284:ARG:NH1	1:F:367:GLU:OE1	2.40	0.51
1:M:221:LEU:HD23	1:M:249:ILE:HG12	1.92	0.51
1:G:202:PRO:C	1:G:204:PHE:H	2.18	0.50
1:N:165:ALA:O	1:N:169:VAL:HG22	2.12	0.50
1:N:183:LEU:O	1:N:184:GLN:HB2	2.10	0.50
1:C:350:ARG:HH11	1:C:350:ARG:HG3	1.76	0.50
1:E:82:ASN:HB2	1:E:89:THR:HG23	1.93	0.50
1:E:176:THR:HG21	1:E:333:ILE:HD13	1.92	0.50
1:L:202:PRO:O	1:L:204:PHE:N	2.44	0.50
1:B:266:THR:CG2	1:B:273:VAL:HB	2.41	0.50
1:B:384:ALA:O	1:B:385:THR:HG23	2.11	0.50
1:D:500:THR:HG22	2:D:638:HOH:O	2.10	0.50
1:F:23:LEU:HD23	1:F:74:VAL:HG22	1.93	0.50
1:G:130:GLU:HB3	1:G:422:VAL:HG22	1.92	0.50
1:H:496:PRO:HB2	1:H:499:VAL:HG13	1.94	0.50
1:I:70:GLY:HA2	1:I:73:MET:HE3	1.94	0.50
1:L:218:PRO:HD2	1:L:320:ALA:O	2.12	0.50
1:A:372:LEU:O	2:A:633:HOH:O	2.20	0.50
1:F:479:ASN:O	1:F:481:ALA:N	2.43	0.50
1:I:342:ILE:O	1:I:346:VAL:HG23	2.11	0.50
1:J:111:MET:O	2:J:651:HOH:O	2.19	0.50
1:K:240:VAL:HG21	1:K:247:LEU:HB2	1.93	0.50
1:G:16:MET:HB3	1:G:514:MET:HE3	1.93	0.50
1:L:336:VAL:HG12	1:L:336:VAL:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:7:LYS:HG3	1:M:66:PHE:CZ	2.47	0.50
1:D:137:PRO:HB2	2:D:644:HOH:O	2.10	0.50
1:D:216:GLU:C	1:D:218:PRO:HD3	2.37	0.50
1:G:85:ALA:HB1	1:G:499:VAL:HG12	1.92	0.50
1:J:257:GLU:C	2:J:670:HOH:O	2.54	0.50
1:D:63:GLU:HB2	1:E:524:LEU:HD11	1.94	0.50
1:J:359:ASP:O	1:J:363:GLU:HG3	2.12	0.50
1:L:414:GLY:O	1:L:417:VAL:HG13	2.11	0.50
1:M:155:ASP:OD1	1:M:157:THR:OG1	2.28	0.50
1:N:310:GLU:OE1	1:N:310:GLU:N	2.43	0.50
1:A:383:ALA:O	1:A:384:ALA:HB3	2.11	0.50
1:G:202:PRO:O	1:G:203:TYR:HB2	2.12	0.50
1:H:160:LYS:O	1:H:164:GLU:HG3	2.11	0.50
1:H:383:ALA:O	1:H:384:ALA:HB3	2.12	0.50
1:M:326:ASN:OD1	1:M:329:THR:N	2.45	0.50
1:I:449:ALA:HB3	1:I:450:PRO:HD3	1.94	0.50
1:J:42:LYS:NZ	1:J:46:ALA:O	2.45	0.50
1:J:141:SER:HB2	2:J:635:HOH:O	2.11	0.50
1:A:524:LEU:HD11	1:G:63:GLU:HB2	1.93	0.49
1:C:314:LEU:HD23	1:C:317:LEU:HD22	1.93	0.49
1:F:383:ALA:O	1:F:384:ALA:HB3	2.12	0.49
1:J:200:LEU:HD21	1:J:277:LYS:HG3	1.94	0.49
1:J:479:ASN:ND2	1:J:493:ILE:HG13	2.26	0.49
1:K:236:VAL:HG21	1:K:312:ALA:HB3	1.94	0.49
1:E:383:ALA:O	1:E:384:ALA:HB3	2.11	0.49
1:H:90:THR:O	1:H:94:VAL:HG13	2.11	0.49
1:K:68:ASN:O	1:K:72:GLN:HG2	2.12	0.49
1:K:198:GLY:O	1:K:276:VAL:HG12	2.12	0.49
1:M:348:GLN:O	1:M:351:GLN:HB3	2.11	0.49
1:C:420:ILE:CG1	1:C:448:GLU:HG2	2.43	0.49
1:C:476:TYR:HA	1:C:486:GLY:O	2.11	0.49
1:D:16:MET:HB3	1:D:514:MET:CE	2.41	0.49
1:J:495:ASP:OD1	2:J:660:HOH:O	2.20	0.49
1:M:220:ILE:O	1:M:220:ILE:CG2	2.60	0.49
1:A:359:ASP:HA	1:A:362:ARG:HH12	1.76	0.49
1:B:351:GLN:NE2	1:B:355:GLU:OE1	2.45	0.49
1:C:16:MET:SD	1:C:73:MET:HE1	2.52	0.49
1:C:158:VAL:HG13	1:C:396:VAL:HG22	1.94	0.49
1:E:266:THR:HG21	1:E:273:VAL:O	2.12	0.49
1:E:498:LYS:NZ	2:E:661:HOH:O	2.44	0.49
1:H:82:ASN:HB3	1:H:89:THR:HG23	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:229:ASN:C	1:K:231:ARG:H	2.21	0.49
1:A:76:GLU:HG3	1:G:46:ALA:CB	2.41	0.49
1:C:321:LYS:HB2	1:C:334:ASP:HB3	1.93	0.49
1:L:383:ALA:O	1:L:384:ALA:HB3	2.11	0.49
1:M:219:PHE:HB3	1:M:317:LEU:HD23	1.95	0.49
1:E:362:ARG:HG2	1:E:366:GLN:NE2	2.27	0.49
1:H:233:MET:HE1	1:H:249:ILE:CD1	2.42	0.49
1:J:266:THR:CA	2:J:647:HOH:O	2.60	0.49
1:J:338:GLU:C	1:J:340:ALA:H	2.20	0.49
1:M:183:LEU:O	1:M:184:GLN:HB2	2.12	0.49
1:N:525:PRO:HD3	2:N:645:HOH:O	2.11	0.49
1:B:409:GLU:OE2	1:B:501:ARG:NH2	2.33	0.49
1:F:421:ARG:NH1	1:F:469:VAL:O	2.46	0.49
1:K:193:MET:HE1	1:K:292:ILE:CG1	2.40	0.49
1:A:455:VAL:HG13	1:A:460:GLU:HB2	1.93	0.49
1:B:383:ALA:HB3	1:B:389:MET:HB2	1.94	0.49
1:C:260:ALA:O	1:C:263:VAL:HG12	2.12	0.49
1:G:82:ASN:N	1:G:89:THR:HG23	2.28	0.49
1:J:366:GLN:HA	1:J:369:VAL:HG22	1.95	0.49
1:K:524:LEU:O	1:K:526:LYS:N	2.45	0.49
1:F:25:ASP:OD1	1:F:28:LYS:HE2	2.12	0.49
1:H:85:ALA:HB1	1:H:499:VAL:HG12	1.95	0.49
1:I:436:GLN:O	1:I:440:ILE:HG13	2.13	0.49
1:J:134:LEU:CD1	1:J:412:VAL:HG22	2.42	0.49
1:C:70:GLY:HA2	1:C:73:MET:HE3	1.95	0.49
1:E:78:ALA:O	1:E:89:THR:CG2	2.60	0.49
1:K:57:ALA:O	1:K:75:LYS:HD2	2.13	0.49
1:K:449:ALA:HB3	1:K:450:PRO:HD3	1.94	0.49
1:M:130:GLU:HB3	1:M:422:VAL:HG22	1.95	0.49
1:H:262:LEU:O	1:H:266:THR:HG23	2.13	0.48
1:K:226:LYS:HG3	1:K:253:ASP:HB3	1.95	0.48
1:L:485:TYR:O	1:L:486:GLY:O	2.31	0.48
1:N:203:TYR:HB2	1:N:263:VAL:HG13	1.95	0.48
1:N:327:LYS:NZ	2:N:633:HOH:O	2.18	0.48
1:B:242:LYS:O	1:B:243:ALA:HB3	2.12	0.48
1:J:254:VAL:HG12	1:J:259:LEU:HB2	1.95	0.48
1:J:281:PHE:HD1	1:J:284:ARG:HH21	1.60	0.48
1:A:200:LEU:HD21	1:A:277:LYS:HG3	1.93	0.48
1:F:466:ALA:O	1:F:470:LYS:HG3	2.13	0.48
1:H:455:VAL:HG13	1:H:460:GLU:HB2	1.95	0.48
1:I:176:THR:HG22	1:I:177:VAL:N	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:288:MET:O	1:J:292:ILE:HG13	2.14	0.48
1:D:27:VAL:CG1	1:D:90:THR:HG23	2.43	0.48
1:F:524:LEU:HD22	1:F:525:PRO:HD2	1.96	0.48
1:H:353:ILE:HG23	1:H:362:ARG:HG3	1.94	0.48
1:I:353:ILE:CA	2:I:637:HOH:O	2.57	0.48
1:K:230:ILE:N	1:K:257:GLU:OE1	2.42	0.48
1:L:25:ASP:OD1	1:L:28:LYS:HE2	2.14	0.48
1:A:221:LEU:HD23	1:A:249:ILE:HD12	1.96	0.48
1:A:417:VAL:HG11	1:A:488:MET:CE	2.36	0.48
1:B:166:MET:HE3	1:B:404:ARG:NH1	2.29	0.48
1:E:16:MET:HB3	1:E:514:MET:HE3	1.96	0.48
1:G:83:ASP:OD2	1:G:327:LYS:HD3	2.14	0.48
1:J:219:PHE:HB3	1:J:317:LEU:HD23	1.96	0.48
1:D:265:ASN:ND2	2:D:612:HOH:O	2.46	0.48
1:G:242:LYS:O	1:G:243:ALA:HB3	2.14	0.48
1:A:102:GLU:HB2	1:A:442:VAL:HG13	1.96	0.48
1:F:18:ARG:HG2	1:F:67:GLU:CD	2.38	0.48
1:J:240:VAL:HG11	1:J:247:LEU:HB2	1.95	0.48
1:L:27:VAL:CG1	1:L:90:THR:HG23	2.44	0.48
1:N:66:PHE:CZ	1:N:522:THR:HG22	2.49	0.48
1:C:183:LEU:HA	1:C:383:ALA:N	2.29	0.48
1:D:46:ALA:HB2	1:E:76:GLU:CG	2.43	0.48
1:D:217:SER:N	1:D:218:PRO:CD	2.76	0.48
1:D:349:ILE:O	1:D:353:ILE:HG13	2.13	0.48
1:K:124:VAL:HG21	1:K:508:ALA:CB	2.44	0.48
1:C:476:TYR:HB3	1:C:485:TYR:OH	2.14	0.48
1:F:28:LYS:HD2	1:F:453:GLN:OE1	2.14	0.48
1:F:179:ASP:OD2	1:F:393:LYS:HE3	2.14	0.48
1:J:46:ALA:HB2	1:K:76:GLU:HG3	1.96	0.48
1:K:224:ASP:O	1:K:225:LYS:HB3	2.13	0.48
1:K:366:GLN:HA	1:K:369:VAL:HG22	1.96	0.48
1:C:218:PRO:HB3	1:C:246:PRO:HG2	1.94	0.48
1:G:18:ARG:HG2	1:G:67:GLU:CD	2.39	0.48
1:H:201:SER:C	1:H:202:PRO:O	2.56	0.48
1:I:142:LYS:O	1:I:146:GLN:HG3	2.14	0.48
1:I:392:LYS:O	1:I:396:VAL:HG23	2.14	0.48
1:K:326:ASN:HD21	1:K:329:THR:HB	1.79	0.48
1:K:358:SER:N	2:K:645:HOH:O	2.47	0.48
1:N:218:PRO:HB3	1:N:246:PRO:HG2	1.94	0.48
1:A:124:VAL:HG21	1:A:508:ALA:HB2	1.96	0.47
1:B:16:MET:HB3	1:B:514:MET:HE3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:349:ILE:CG2	1:F:369:VAL:HG13	2.44	0.47
1:F:451:LEU:HD11	1:F:469:VAL:HG21	1.95	0.47
1:I:359:ASP:O	1:I:363:GLU:HG2	2.14	0.47
1:I:383:ALA:HB3	1:I:389:MET:HA	1.96	0.47
1:J:412:VAL:HG13	1:J:418:ALA:HB2	1.96	0.47
1:K:219:PHE:O	1:K:247:LEU:HD12	2.15	0.47
1:L:118:ARG:HD2	1:L:436:GLN:HE22	1.78	0.47
1:L:477:GLY:O	1:L:485:TYR:HA	2.14	0.47
1:F:420:ILE:CD1	1:F:451:LEU:HD13	2.42	0.47
1:G:232:GLU:HB3	1:G:309:LEU:HB3	1.95	0.47
1:G:460:GLU:O	1:G:462:PRO:HD3	2.14	0.47
1:I:16:MET:O	1:I:20:VAL:HG13	2.14	0.47
1:I:235:PRO:HG2	2:I:634:HOH:O	2.12	0.47
1:J:524:LEU:O	1:J:526:LYS:N	2.47	0.47
1:K:183:LEU:HG	1:K:384:ALA:HB2	1.96	0.47
1:C:24:ALA:HA	1:C:27:VAL:HG12	1.97	0.47
1:D:33:PRO:HG3	1:D:480:ALA:HB1	1.96	0.47
1:F:139:SER:O	1:F:171:LYS:NZ	2.29	0.47
1:E:484:GLU:HG3	2:E:645:HOH:O	2.15	0.47
1:M:155:ASP:OD2	1:M:395:ARG:NH2	2.48	0.47
1:M:349:ILE:HA	1:M:352:GLN:HG3	1.96	0.47
1:D:319:GLN:O	1:D:336:VAL:HG23	2.14	0.47
1:H:449:ALA:HB3	1:H:450:PRO:HD3	1.95	0.47
1:M:205:ILE:HG23	1:M:212:ALA:O	2.14	0.47
1:M:271:VAL:HG12	1:M:273:VAL:HG23	1.97	0.47
1:B:201:SER:C	1:B:202:PRO:O	2.57	0.47
1:F:413:ALA:HB3	1:F:417:VAL:HG22	1.95	0.47
1:I:5:ASP:HB2	1:I:524:LEU:HD12	1.96	0.47
1:I:319:GLN:HB3	1:I:336:VAL:HG21	1.96	0.47
1:K:186:GLU:HB2	1:K:380:LYS:HB2	1.97	0.47
1:L:118:ARG:HD2	1:L:436:GLN:NE2	2.29	0.47
1:L:230:ILE:HG21	1:L:261:THR:HG21	1.96	0.47
1:B:263:VAL:O	1:B:267:MET:HB2	2.15	0.47
1:B:270:ILE:HD12	1:B:270:ILE:H	1.80	0.47
1:C:489:ILE:HG23	1:C:494:LEU:HD23	1.95	0.47
1:D:40:LEU:HD13	1:D:59:GLU:HG3	1.97	0.47
1:D:70:GLY:HA2	1:D:73:MET:HE3	1.96	0.47
1:D:484:GLU:CG	2:D:656:HOH:O	2.44	0.47
1:E:25:ASP:HA	1:E:28:LYS:HE2	1.95	0.47
1:K:360:TYR:CB	2:K:633:HOH:O	2.55	0.47
1:K:473:ASP:OD2	1:K:473:ASP:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:205:ILE:HA	1:N:213:VAL:HG22	1.97	0.47
1:B:197:ARG:HD2	1:B:277:LYS:HB2	1.96	0.47
1:B:219:PHE:HB3	1:B:317:LEU:HD23	1.96	0.47
1:C:122:LYS:HE2	1:C:429:LEU:HD11	1.96	0.47
1:H:526:LYS:HA	1:H:526:LYS:HD3	1.69	0.47
1:J:135:SER:HA	1:J:412:VAL:HG23	1.97	0.47
1:K:477:GLY:HA3	1:K:488:MET:CE	2.45	0.47
1:C:413:ALA:CB	1:C:417:VAL:HG22	2.43	0.47
1:C:473:ASP:O	1:C:476:TYR:HB2	2.15	0.47
1:E:421:ARG:NH2	1:E:476:TYR:O	2.48	0.47
1:L:392:LYS:O	1:L:396:VAL:HG23	2.15	0.47
1:M:441:LYS:O	1:M:445:ARG:HB2	2.15	0.47
1:B:524:LEU:HD12	1:B:525:PRO:HD2	1.97	0.47
1:D:20:VAL:HB	1:D:74:VAL:HG11	1.97	0.47
1:D:166:MET:HE2	1:D:404:ARG:NH1	2.29	0.47
2:H:652:HOH:O	1:N:36:ARG:NH2	2.48	0.47
1:K:7:LYS:HD3	1:K:11:ASP:OD1	2.15	0.47
1:K:16:MET:SD	1:K:73:MET:HE1	2.55	0.47
1:N:142:LYS:O	1:N:146:GLN:HG3	2.15	0.47
1:N:290:GLN:HB3	1:N:345:ARG:NH2	2.30	0.47
1:A:301:ILE:HD12	1:A:312:ALA:HB2	1.98	0.46
1:B:383:ALA:O	1:B:384:ALA:HB3	2.13	0.46
1:C:16:MET:HB3	1:C:514:MET:HE3	1.96	0.46
1:D:176:THR:HG21	1:D:333:ILE:HD13	1.97	0.46
1:G:229:ASN:HA	2:G:616:HOH:O	2.15	0.46
1:N:366:GLN:HA	1:N:369:VAL:HG22	1.97	0.46
1:B:149:THR:HG23	1:B:155:ASP:C	2.40	0.46
1:B:178:GLU:HA	1:B:393:LYS:HE3	1.97	0.46
1:B:242:LYS:C	1:B:244:GLY:N	2.73	0.46
1:B:349:ILE:CG2	1:B:369:VAL:HG13	2.45	0.46
1:C:31:LEU:HD13	1:C:90:THR:CG2	2.45	0.46
1:G:16:MET:O	1:G:20:VAL:HG13	2.15	0.46
1:A:301:ILE:HG21	1:A:309:LEU:HD23	1.97	0.46
1:B:203:TYR:C	2:B:661:HOH:O	2.58	0.46
1:D:262:LEU:O	1:D:266:THR:HG23	2.14	0.46
1:E:526:LYS:HE2	2:E:649:HOH:O	2.16	0.46
1:N:463:SER:O	1:N:467:ASN:HB2	2.15	0.46
1:A:479:ASN:HB2	1:A:484:GLU:H	1.80	0.46
1:F:97:GLN:HB3	2:F:645:HOH:O	2.15	0.46
1:F:397:GLU:O	1:F:401:HIS:ND1	2.47	0.46
1:F:479:ASN:C	1:F:481:ALA:H	2.23	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:319:GLN:HA	2:K:636:HOH:O	2.14	0.46
1:K:463:SER:O	1:K:467:ASN:HB2	2.15	0.46
1:F:16:MET:HB3	1:F:514:MET:HE3	1.97	0.46
1:F:359:ASP:O	1:F:363:GLU:HG3	2.16	0.46
1:K:258:ALA:O	1:K:262:LEU:HG	2.16	0.46
1:L:430:ARG:HD2	2:L:633:HOH:O	2.16	0.46
1:D:501:ARG:NH1	1:D:505:GLN:OE1	2.46	0.46
1:F:223:ALA:O	1:F:251:ALA:HA	2.15	0.46
1:G:28:LYS:HD2	1:G:453:GLN:OE1	2.16	0.46
1:H:31:LEU:HD13	1:H:90:THR:CG2	2.45	0.46
1:L:222:LEU:HD23	1:L:250:ILE:HB	1.96	0.46
1:L:400:LEU:O	1:L:404:ARG:HG2	2.16	0.46
1:A:203:TYR:HB2	1:A:263:VAL:HG13	1.97	0.46
1:G:273:VAL:HG12	1:G:274:ALA:N	2.30	0.46
1:H:198:GLY:HA3	1:H:327:LYS:O	2.16	0.46
1:K:222:LEU:HD23	1:K:250:ILE:HB	1.97	0.46
1:L:472:GLY:HA3	1:L:476:TYR:CD2	2.51	0.46
1:L:484:GLU:HA	2:L:646:HOH:O	2.14	0.46
1:M:54:VAL:HG22	1:M:89:THR:CG2	2.44	0.46
1:B:13:ARG:HD2	1:B:104:LEU:HD22	1.97	0.46
1:E:40:LEU:HD13	1:E:59:GLU:HG3	1.98	0.46
1:E:131:LEU:HD13	1:E:422:VAL:HG21	1.97	0.46
1:E:472:GLY:HA3	1:E:476:TYR:CD2	2.51	0.46
1:I:183:LEU:HD23	1:I:383:ALA:HA	1.98	0.46
1:M:27:VAL:CG1	1:M:90:THR:HG23	2.46	0.46
1:C:201:SER:C	1:C:202:PRO:O	2.59	0.46
1:C:289:LEU:HA	1:C:289:LEU:HD23	1.70	0.46
1:C:398:ASP:OD2	1:C:399:ALA:N	2.49	0.46
1:L:193:MET:CE	1:L:292:ILE:HG12	2.45	0.46
1:N:358:SER:O	1:N:362:ARG:HB2	2.16	0.46
1:B:77:VAL:HG12	1:B:506:TYR:HB3	1.97	0.46
1:C:359:ASP:HA	1:C:362:ARG:HH11	1.81	0.46
1:E:372:LEU:HD12	1:E:372:LEU:HA	1.75	0.46
1:F:131:LEU:HD12	1:F:131:LEU:HA	1.77	0.46
1:I:121:ASP:O	1:I:125:THR:HG23	2.16	0.46
1:J:201:SER:HA	1:J:202:PRO:HD3	1.81	0.46
1:K:235:PRO:HG2	1:K:310:GLU:HA	1.98	0.46
1:L:57:ALA:O	1:L:75:LYS:HD2	2.16	0.46
1:A:85:ALA:HB1	1:A:499:VAL:HG12	1.98	0.45
1:C:201:SER:O	1:C:202:PRO:O	2.34	0.45
1:C:220:ILE:HD12	1:C:296:THR:HG21	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:253:ASP:OD1	1:D:254:VAL:N	2.50	0.45
1:E:350:ARG:O	1:E:353:ILE:HB	2.16	0.45
1:F:266:THR:CG2	1:F:273:VAL:H	2.28	0.45
1:H:315:GLU:O	1:H:315:GLU:HG2	2.16	0.45
1:M:479:ASN:O	1:M:481:ALA:N	2.46	0.45
1:N:225:LYS:NZ	1:N:232:GLU:OE2	2.48	0.45
1:C:409:GLU:HB2	2:C:601:HOH:O	2.15	0.45
1:C:494:LEU:HD12	1:C:494:LEU:C	2.41	0.45
1:F:218:PRO:CB	1:F:246:PRO:HG2	2.44	0.45
1:H:16:MET:HB3	1:H:514:MET:HE3	1.98	0.45
1:J:350:ARG:CD	2:J:643:HOH:O	2.61	0.45
1:K:240:VAL:HG13	1:K:271:VAL:HG11	1.97	0.45
1:B:324:VAL:HB	1:B:331:THR:HG23	1.98	0.45
1:E:82:ASN:OD1	1:E:89:THR:OG1	2.31	0.45
1:G:524:LEU:HD12	1:G:524:LEU:HA	1.75	0.45
1:I:319:GLN:HB3	1:I:336:VAL:CG2	2.47	0.45
1:J:432:GLN:NE2	2:J:672:HOH:O	2.49	0.45
1:L:339:GLU:OE2	2:L:659:HOH:O	2.20	0.45
1:M:305:ILE:O	1:M:305:ILE:HG22	2.17	0.45
1:N:144:ILE:HG23	1:N:403:THR:HG21	1.97	0.45
1:E:118:ARG:HD2	1:E:436:GLN:HE22	1.81	0.45
1:F:218:PRO:HD2	1:F:320:ALA:O	2.17	0.45
1:F:266:THR:CG2	1:F:273:VAL:HG22	2.46	0.45
1:G:69:MET:O	1:G:73:MET:HG3	2.16	0.45
1:I:82:ASN:HB2	1:I:89:THR:OG1	2.16	0.45
1:J:421:ARG:NH2	1:J:476:TYR:O	2.49	0.45
1:K:219:PHE:HB3	1:K:317:LEU:HD23	1.97	0.45
1:L:183:LEU:HD13	1:L:184:GLN:N	2.31	0.45
1:N:5:ASP:HB2	1:N:524:LEU:HD12	1.99	0.45
1:N:183:LEU:HD22	1:N:184:GLN:H	1.82	0.45
1:A:372:LEU:HD12	1:A:372:LEU:HA	1.83	0.45
1:B:284:ARG:O	1:B:288:MET:HG3	2.16	0.45
1:D:193:MET:HG3	1:D:371:LYS:HB3	1.98	0.45
1:E:349:ILE:CG2	1:E:369:VAL:HG13	2.47	0.45
1:E:417:VAL:CG1	1:E:488:MET:HE2	2.47	0.45
1:F:182:GLY:O	1:F:183:LEU:C	2.59	0.45
1:F:234:LEU:HB2	1:F:235:PRO:HD3	1.97	0.45
1:H:24:ALA:O	1:H:28:LYS:HG2	2.16	0.45
1:J:455:VAL:HG13	1:J:460:GLU:HB2	1.98	0.45
1:J:463:SER:O	1:J:467:ASN:HB2	2.17	0.45
1:K:124:VAL:HG21	1:K:508:ALA:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:352:GLN:CA	2:L:638:HOH:O	2.65	0.45
1:M:142:LYS:O	1:M:146:GLN:HG3	2.16	0.45
1:B:214:GLU:CD	1:B:322:ARG:HH21	2.25	0.45
1:C:359:ASP:O	1:C:363:GLU:HG3	2.17	0.45
1:E:169:VAL:CG1	1:E:377:ALA:HB2	2.46	0.45
1:G:13:ARG:HD2	1:G:104:LEU:HD22	1.99	0.45
1:G:266:THR:HB	2:G:640:HOH:O	2.16	0.45
1:H:144:ILE:HG23	1:H:403:THR:CG2	2.46	0.45
1:H:519:CYS:HB3	1:N:38:VAL:HB	1.98	0.45
1:K:16:MET:O	1:K:20:VAL:HG13	2.17	0.45
1:L:524:LEU:O	1:L:526:LYS:N	2.46	0.45
1:A:61:GLU:HG2	2:A:638:HOH:O	2.17	0.45
1:B:310:GLU:OE1	1:B:310:GLU:N	2.50	0.45
1:D:16:MET:O	1:D:20:VAL:HG13	2.17	0.45
1:F:463:SER:CB	2:N:650:HOH:O	2.48	0.45
1:G:193:MET:HG3	1:G:371:LYS:HB3	1.98	0.45
1:I:13:ARG:HD2	1:I:104:LEU:HD22	1.98	0.45
1:I:157:THR:HG21	1:I:392:LYS:NZ	2.31	0.45
1:I:314:LEU:O	1:I:317:LEU:HB2	2.16	0.45
1:I:349:ILE:O	1:I:353:ILE:HG13	2.17	0.45
1:I:353:ILE:CB	2:I:637:HOH:O	2.60	0.45
1:J:90:THR:OG1	2:J:640:HOH:O	2.20	0.45
1:K:478:TYR:H	1:K:488:MET:HE2	1.82	0.45
1:N:217:SER:N	1:N:218:PRO:CD	2.80	0.45
1:E:70:GLY:HA2	1:E:73:MET:HE3	1.99	0.45
1:F:247:LEU:HB3	1:F:273:VAL:HG12	1.98	0.45
1:H:270:ILE:O	1:H:271:VAL:HB	2.17	0.45
1:M:54:VAL:CG2	1:M:89:THR:HG21	2.42	0.45
1:M:391:GLU:OE1	1:M:395:ARG:NH1	2.50	0.45
1:B:296:THR:HB	1:B:319:GLN:H	1.82	0.45
1:B:301:ILE:HG21	1:B:309:LEU:HD23	1.97	0.45
1:B:364:LYS:HD3	1:B:364:LYS:HA	1.68	0.45
1:B:473:ASP:OD2	2:B:678:HOH:O	2.21	0.45
1:C:131:LEU:HD21	1:C:500:THR:HG22	1.99	0.45
1:D:271:VAL:O	2:D:651:HOH:O	2.21	0.45
1:F:524:LEU:HD23	1:F:524:LEU:HA	1.83	0.45
1:L:37:ASN:OD1	1:L:51:LYS:HE3	2.16	0.45
1:M:224:ASP:O	1:M:225:LYS:HB3	2.17	0.45
1:N:16:MET:HG3	1:N:520:MET:SD	2.56	0.45
1:F:247:LEU:CD2	1:F:249:ILE:HD11	2.47	0.45
1:G:138:CYS:SG	1:G:147:VAL:HG21	2.57	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:183:LEU:O	1:G:184:GLN:O	2.35	0.45
1:H:284:ARG:O	1:H:288:MET:HG3	2.16	0.45
1:J:5:ASP:HB2	1:J:524:LEU:HD12	1.99	0.45
1:K:404:ARG:HH11	1:K:404:ARG:CG	2.30	0.45
1:L:176:THR:HG21	1:L:333:ILE:HD11	1.99	0.45
1:L:455:VAL:HG13	1:L:460:GLU:HB2	2.00	0.45
1:M:220:ILE:O	1:M:221:LEU:C	2.60	0.45
1:A:77:VAL:HG12	1:A:506:TYR:HB3	1.99	0.44
1:A:266:THR:CG2	1:A:273:VAL:H	2.31	0.44
1:A:392:LYS:O	1:A:396:VAL:HG23	2.17	0.44
1:B:486:GLY:C	1:B:491:MET:HE2	2.42	0.44
1:C:219:PHE:CE2	1:C:245:LYS:HD2	2.52	0.44
1:D:479:ASN:OD1	1:D:483:GLU:HA	2.16	0.44
1:E:475:ASN:ND2	2:E:608:HOH:O	2.30	0.44
1:F:26:ALA:HA	1:G:8:PHE:HE1	1.82	0.44
1:F:183:LEU:O	1:F:184:GLN:CB	2.65	0.44
1:F:364:LYS:O	1:F:367:GLU:HG3	2.17	0.44
1:I:336:VAL:HG12	1:I:336:VAL:O	2.16	0.44
1:J:235:PRO:CG	1:J:310:GLU:HA	2.38	0.44
1:L:50:THR:OG1	1:L:51:LYS:N	2.49	0.44
1:N:201:SER:HA	1:N:202:PRO:HD3	1.85	0.44
1:N:420:ILE:HG12	1:N:448:GLU:HG2	2.00	0.44
1:A:130:GLU:HG3	1:A:425:LYS:NZ	2.33	0.44
1:A:214:GLU:OE2	1:A:322:ARG:NH2	2.40	0.44
1:C:391:GLU:OE1	1:C:395:ARG:NH1	2.50	0.44
1:E:487:ASN:O	1:E:491:MET:HG3	2.17	0.44
1:F:239:ALA:HB1	1:F:314:LEU:HG	1.99	0.44
1:K:100:ILE:O	1:K:104:LEU:HG	2.18	0.44
1:B:204:PHE:CD1	1:B:273:VAL:O	2.70	0.44
1:E:169:VAL:HG11	1:E:377:ALA:HB2	1.99	0.44
1:H:165:ALA:O	1:H:169:VAL:HG22	2.18	0.44
1:I:356:ALA:HB3	2:I:653:HOH:O	2.16	0.44
1:J:196:ASP:OD2	2:J:641:HOH:O	2.21	0.44
1:A:158:VAL:HG13	1:A:396:VAL:HG22	2.00	0.44
1:D:219:PHE:O	1:D:247:LEU:HD12	2.16	0.44
1:D:220:ILE:HD12	1:D:296:THR:HG21	1.98	0.44
1:H:42:LYS:C	1:H:44:PHE:N	2.71	0.44
1:I:72:GLN:NE2	1:I:75:LYS:HE3	2.32	0.44
1:K:305:ILE:O	1:K:305:ILE:HG22	2.17	0.44
1:L:142:LYS:O	1:L:146:GLN:HG3	2.17	0.44
1:L:179:ASP:OD1	1:L:389:MET:HE1	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:524:LEU:HD12	1:L:524:LEU:HA	1.82	0.44
1:M:83:ASP:OD2	1:M:327:LYS:HD3	2.17	0.44
1:M:183:LEU:HD22	1:M:184:GLN:H	1.82	0.44
1:N:44:PHE:HD1	1:N:44:PHE:H	1.66	0.44
1:B:158:VAL:HG13	1:B:396:VAL:HG22	1.99	0.44
1:C:223:ALA:O	1:C:251:ALA:HA	2.18	0.44
1:D:463:SER:HB3	1:I:461:GLU:OE2	2.17	0.44
1:F:414:GLY:O	1:F:417:VAL:HG13	2.16	0.44
1:J:291:ASP:OD1	1:J:368:ARG:NH1	2.51	0.44
1:L:223:ALA:O	1:L:251:ALA:HA	2.17	0.44
1:E:29:VAL:HG11	1:F:518:GLU:HB3	1.99	0.44
1:I:57:ALA:O	1:I:75:LYS:HD2	2.18	0.44
1:I:272:LYS:HD2	1:I:272:LYS:N	2.33	0.44
1:J:13:ARG:NH2	1:J:518:GLU:OE2	2.48	0.44
1:N:482:THR:OG1	1:N:484:GLU:HG2	2.18	0.44
1:D:77:VAL:HG12	1:D:506:TYR:HB3	1.99	0.44
1:D:500:THR:O	1:D:501:ARG:C	2.61	0.44
1:E:479:ASN:HB2	1:E:491:MET:HE1	2.00	0.44
1:H:221:LEU:HD23	1:H:249:ILE:HD12	1.99	0.44
1:J:218:PRO:HD2	1:J:320:ALA:O	2.18	0.44
1:J:242:LYS:O	1:J:243:ALA:HB3	2.18	0.44
1:J:291:ASP:OD2	1:J:368:ARG:HD2	2.18	0.44
1:D:383:ALA:O	1:D:384:ALA:CB	2.65	0.44
1:E:131:LEU:HD21	1:E:500:THR:HG22	1.98	0.44
1:F:103:GLY:O	1:F:107:VAL:HG23	2.18	0.44
1:I:183:LEU:HB2	1:I:384:ALA:H	1.82	0.44
1:I:195:PHE:HB2	1:I:279:PRO:HB3	2.00	0.44
1:K:247:LEU:O	1:K:273:VAL:HG13	2.17	0.44
1:L:27:VAL:HG12	1:L:90:THR:HG23	2.00	0.44
1:L:324:VAL:HB	1:L:331:THR:HG23	1.99	0.44
1:A:218:PRO:HD2	1:A:320:ALA:O	2.18	0.44
1:D:77:VAL:HG21	1:D:510:VAL:HG13	1.99	0.44
1:F:197:ARG:HD2	1:F:277:LYS:HB2	2.00	0.44
1:G:165:ALA:O	1:G:169:VAL:HG22	2.18	0.44
1:K:142:LYS:HE3	1:K:146:GLN:HE21	1.82	0.44
1:A:124:VAL:HG21	1:A:508:ALA:CB	2.48	0.43
1:A:230:ILE:HG12	1:A:258:ALA:HA	1.99	0.43
1:B:144:ILE:HG23	1:B:403:THR:HG21	1.99	0.43
1:G:463:SER:HB3	1:M:461:GLU:OE2	2.17	0.43
1:K:227:ILE:CD1	1:K:309:LEU:HD11	2.48	0.43
1:K:488:MET:HA	1:K:491:MET:HE3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:290:GLN:HA	1:L:290:GLN:OE1	2.18	0.43
1:N:233:MET:O	1:N:234:LEU:C	2.61	0.43
1:N:311:LYS:HB3	1:N:311:LYS:HE2	1.82	0.43
1:A:225:LYS:HE3	1:A:225:LYS:HB2	1.89	0.43
1:A:420:ILE:HG12	1:A:448:GLU:HG2	1.99	0.43
1:F:305:ILE:O	1:F:305:ILE:HG22	2.18	0.43
1:G:176:THR:HG21	1:G:333:ILE:HD13	2.00	0.43
1:H:404:ARG:HG2	1:H:404:ARG:HH11	1.83	0.43
1:L:70:GLY:HA2	1:L:73:MET:HE3	2.00	0.43
1:N:191:GLU:O	1:N:334:ASP:HA	2.18	0.43
1:D:74:VAL:HA	1:D:510:VAL:HG11	2.00	0.43
1:D:311:LYS:HB3	1:D:311:LYS:HE2	1.85	0.43
1:E:16:MET:HE1	1:E:517:THR:HB	2.00	0.43
1:E:383:ALA:HB3	1:E:389:MET:HB2	2.00	0.43
1:F:77:VAL:HG11	1:F:510:VAL:HB	2.00	0.43
1:G:215:LEU:HB2	1:G:323:VAL:HG22	2.00	0.43
1:H:100:ILE:O	1:H:104:LEU:HG	2.18	0.43
1:H:158:VAL:HG13	1:H:396:VAL:HG22	2.00	0.43
1:H:202:PRO:O	1:H:203:TYR:CB	2.67	0.43
1:H:204:PHE:O	1:H:213:VAL:HG22	2.18	0.43
1:K:171:LYS:HB2	1:K:171:LYS:HE3	1.84	0.43
1:N:72:GLN:OE1	1:N:75:LYS:HE2	2.19	0.43
1:N:103:GLY:O	1:N:107:VAL:HG23	2.17	0.43
1:A:326:ASN:HD22	1:A:329:THR:HB	1.83	0.43
1:E:219:PHE:HB3	1:E:317:LEU:HD23	2.01	0.43
1:E:314:LEU:HD23	1:E:317:LEU:HD22	2.00	0.43
1:H:304:GLU:C	1:H:306:GLY:H	2.26	0.43
1:H:404:ARG:HG2	1:H:404:ARG:NH1	2.33	0.43
1:I:31:LEU:HD12	1:I:31:LEU:HA	1.85	0.43
1:M:288:MET:CE	2:M:653:HOH:O	2.47	0.43
1:C:350:ARG:CG	1:C:350:ARG:NH1	2.68	0.43
1:D:215:LEU:HB2	1:D:323:VAL:HG22	2.00	0.43
1:D:286:LYS:HB3	1:D:286:LYS:HE2	1.66	0.43
1:E:180:GLY:HA2	1:E:380:LYS:HB3	2.01	0.43
1:I:176:THR:CG2	1:I:177:VAL:N	2.81	0.43
1:I:488:MET:HA	1:I:491:MET:HE2	2.00	0.43
1:K:284:ARG:CZ	1:K:284:ARG:HB2	2.48	0.43
1:L:262:LEU:O	1:L:266:THR:HG23	2.17	0.43
1:M:16:MET:HB3	1:M:514:MET:CE	2.48	0.43
1:M:194:GLN:O	1:M:371:LYS:HE2	2.17	0.43
1:M:200:LEU:HD21	1:M:277:LYS:HG3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:57:ALA:O	1:N:75:LYS:HD2	2.17	0.43
1:D:242:LYS:C	1:D:244:GLY:N	2.76	0.43
1:G:202:PRO:C	1:G:204:PHE:N	2.76	0.43
1:H:66:PHE:CZ	1:H:522:THR:HG22	2.54	0.43
1:J:152:ALA:O	1:J:153:ASN:HB2	2.19	0.43
1:K:150:ILE:HD13	1:K:492:GLY:HA2	2.00	0.43
1:K:230:ILE:HG13	1:K:233:MET:HB3	2.00	0.43
1:M:200:LEU:HG	1:M:276:VAL:HA	2.00	0.43
1:B:202:PRO:C	1:B:204:PHE:H	2.25	0.43
1:E:42:LYS:HB3	1:E:42:LYS:HE2	1.80	0.43
1:F:230:ILE:HD12	1:F:233:MET:HG3	2.00	0.43
1:G:16:MET:HB3	1:G:514:MET:CE	2.49	0.43
1:G:194:GLN:O	1:G:371:LYS:HE3	2.19	0.43
1:G:230:ILE:HD12	1:G:261:THR:HB	1.99	0.43
1:K:383:ALA:HB3	1:K:389:MET:CA	2.49	0.43
1:N:74:VAL:HA	1:N:510:VAL:HG21	1.99	0.43
1:B:205:ILE:CB	2:B:661:HOH:O	2.66	0.43
1:D:224:ASP:O	1:D:225:LYS:HB3	2.19	0.43
1:I:230:ILE:HD13	1:I:261:THR:CG2	2.49	0.43
1:J:49:ILE:HD12	1:K:513:LEU:HD13	1.99	0.43
1:L:301:ILE:HA	1:L:307:MET:SD	2.59	0.43
1:N:494:LEU:C	1:N:494:LEU:HD12	2.44	0.43
1:B:288:MET:HG2	1:B:368:ARG:HD3	2.01	0.43
1:C:286:LYS:HB3	1:C:286:LYS:HE2	1.75	0.43
1:C:413:ALA:HB3	1:C:417:VAL:HG22	2.01	0.43
1:C:455:VAL:HG21	1:C:465:VAL:HG11	2.00	0.43
1:D:7:LYS:NZ	2:D:637:HOH:O	2.19	0.43
1:E:284:ARG:O	1:E:288:MET:HG3	2.18	0.43
1:G:124:VAL:HG21	1:G:508:ALA:HB2	2.01	0.43
1:H:27:VAL:CG1	1:H:90:THR:HG23	2.48	0.43
1:M:42:LYS:C	1:M:44:PHE:H	2.18	0.43
1:M:162:ILE:HD12	1:M:400:LEU:HD13	2.00	0.43
1:D:449:ALA:HB3	1:D:450:PRO:HD3	2.01	0.43
1:E:82:ASN:HB2	1:E:89:THR:CG2	2.49	0.43
1:H:57:ALA:O	1:H:75:LYS:HD2	2.19	0.43
1:I:22:VAL:HG11	1:I:62:LEU:HD21	2.01	0.43
1:I:46:ALA:HA	1:I:47:PRO:HD3	1.90	0.43
1:K:479:ASN:C	1:K:481:ALA:H	2.25	0.43
1:L:66:PHE:CZ	1:L:522:THR:HG22	2.54	0.43
1:L:130:GLU:HB3	1:L:422:VAL:HG22	2.00	0.43
1:M:203:TYR:HB2	1:M:263:VAL:HG13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:VAL:HG12	1:A:274:ALA:N	2.33	0.42
1:B:205:ILE:CG1	2:B:661:HOH:O	2.57	0.42
1:D:524:LEU:O	1:D:526:LYS:N	2.41	0.42
1:F:311:LYS:HA	1:F:311:LYS:HD3	1.82	0.42
1:F:339:GLU:O	1:F:343:GLN:HG2	2.19	0.42
1:J:36:ARG:O	1:J:51:LYS:HG2	2.19	0.42
1:K:39:VAL:CG1	1:L:69:MET:HE2	2.49	0.42
1:L:31:LEU:HD13	1:L:90:THR:CG2	2.49	0.42
1:B:34:LYS:HB2	1:B:458:CYS:SG	2.59	0.42
1:E:359:ASP:N	2:E:659:HOH:O	1.98	0.42
1:F:235:PRO:HG2	1:F:310:GLU:HA	2.01	0.42
1:G:372:LEU:HD12	1:G:372:LEU:HA	1.77	0.42
1:I:247:LEU:HB3	1:I:273:VAL:HG22	2.01	0.42
1:J:215:LEU:O	1:J:322:ARG:HA	2.19	0.42
1:J:338:GLU:O	1:J:340:ALA:N	2.52	0.42
1:J:392:LYS:O	1:J:396:VAL:HG23	2.19	0.42
1:L:420:ILE:HD12	1:L:451:LEU:HD13	2.01	0.42
1:N:140:ASP:OD2	1:N:142:LYS:HB3	2.18	0.42
1:N:166:MET:CE	1:N:171:LYS:HA	2.48	0.42
1:A:291:ASP:OD2	1:A:368:ARG:HD2	2.20	0.42
1:F:463:SER:HA	2:N:650:HOH:O	2.17	0.42
1:J:66:PHE:CZ	1:J:522:THR:HG22	2.54	0.42
1:J:130:GLU:HB3	1:J:422:VAL:HG22	2.01	0.42
1:K:269:GLY:HA3	1:L:257:GLU:HB2	2.02	0.42
1:L:193:MET:HG3	1:L:371:LYS:HB3	2.00	0.42
1:M:242:LYS:C	1:M:244:GLY:H	2.26	0.42
1:A:233:MET:O	1:A:234:LEU:C	2.62	0.42
1:B:429:LEU:HG	1:B:440:ILE:HD13	2.00	0.42
1:D:270:ILE:O	2:D:651:HOH:O	2.21	0.42
1:E:203:TYR:HB2	1:E:263:VAL:HG13	2.01	0.42
1:F:242:LYS:HD3	1:F:242:LYS:N	2.34	0.42
1:G:421:ARG:NH2	1:G:476:TYR:O	2.46	0.42
1:H:235:PRO:HG3	1:H:310:GLU:HA	2.01	0.42
1:J:221:LEU:HD11	1:J:301:ILE:HD12	2.01	0.42
1:J:232:GLU:OE2	1:J:309:LEU:HD12	2.19	0.42
1:J:262:LEU:HD22	1:J:273:VAL:HG11	2.01	0.42
1:J:384:ALA:CA	2:J:644:HOH:O	2.65	0.42
1:J:468:THR:HG1	1:J:485:TYR:HE2	1.64	0.42
1:L:241:ALA:HB2	1:L:271:VAL:HG21	2.00	0.42
1:B:223:ALA:O	1:B:251:ALA:HA	2.19	0.42
1:B:247:LEU:CD2	1:B:249:ILE:HD11	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:46:ALA:HB2	1:D:76:GLU:HG3	2.01	0.42
1:D:13:ARG:HD2	1:D:104:LEU:HD22	2.00	0.42
1:D:202:PRO:C	1:D:204:PHE:H	2.27	0.42
1:G:182:GLY:C	1:G:183:LEU:O	2.63	0.42
1:H:124:VAL:HG21	1:H:508:ALA:CB	2.50	0.42
1:H:136:VAL:HA	1:H:137:PRO:HD3	1.78	0.42
1:H:460:GLU:O	1:H:462:PRO:HD3	2.19	0.42
1:K:420:ILE:CG1	1:K:448:GLU:HG2	2.48	0.42
1:M:404:ARG:O	1:M:407:VAL:HG12	2.20	0.42
1:A:289:LEU:HD23	1:A:289:LEU:HA	1.57	0.42
1:C:24:ALA:O	1:C:28:LYS:HG2	2.19	0.42
1:D:251:ALA:O	1:D:278:ALA:N	2.49	0.42
1:D:484:GLU:HG2	2:D:643:HOH:O	2.19	0.42
1:G:242:LYS:C	1:G:244:GLY:N	2.78	0.42
1:H:28:LYS:HD2	1:H:453:GLN:OE1	2.19	0.42
1:J:286:LYS:HB2	1:J:286:LYS:HE3	1.87	0.42
1:J:462:PRO:HD2	2:J:606:HOH:O	2.20	0.42
1:A:349:ILE:O	1:A:353:ILE:HG13	2.19	0.42
1:C:116:LEU:HD23	1:C:116:LEU:HA	1.84	0.42
1:D:199:TYR:CZ	1:D:327:LYS:HA	2.54	0.42
1:D:296:THR:HB	1:D:319:GLN:H	1.84	0.42
1:G:326:ASN:HD22	1:G:329:THR:HG1	1.68	0.42
1:H:16:MET:O	1:H:20:VAL:HG12	2.19	0.42
1:I:155:ASP:OD1	1:I:157:THR:HB	2.20	0.42
1:N:228:SER:O	1:N:257:GLU:HB3	2.19	0.42
1:A:135:SER:HB2	1:A:497:THR:OG1	2.19	0.42
1:A:176:THR:HG21	1:A:333:ILE:HD13	2.02	0.42
1:A:463:SER:HB3	1:L:461:GLU:OE2	2.20	0.42
1:C:46:ALA:CB	1:D:76:GLU:HG3	2.49	0.42
1:C:193:MET:HE1	1:C:292:ILE:HG12	2.01	0.42
1:D:142:LYS:O	1:D:146:GLN:HG3	2.20	0.42
1:D:372:LEU:HD12	1:D:372:LEU:HA	1.83	0.42
1:E:266:THR:HG22	1:E:273:VAL:H	1.84	0.42
1:E:420:ILE:CD1	1:E:451:LEU:HD13	2.39	0.42
1:F:383:ALA:HB3	1:F:389:MET:HB2	2.01	0.42
1:H:54:VAL:HG21	1:H:82:ASN:HD22	1.83	0.42
1:J:336:VAL:O	1:J:336:VAL:HG12	2.19	0.42
1:L:289:LEU:HD23	1:L:289:LEU:HA	1.86	0.42
1:L:342:ILE:O	1:L:346:VAL:HG23	2.20	0.42
1:M:196:ASP:O	1:M:197:ARG:O	2.38	0.42
1:N:289:LEU:HA	1:N:289:LEU:HD23	1.79	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:ASP:OD2	1:A:142:LYS:HB3	2.20	0.42
1:B:58:ARG:NH1	2:B:660:HOH:O	2.53	0.42
1:B:82:ASN:HD22	1:B:89:THR:HB	1.85	0.42
1:D:286:LYS:NZ	1:D:304:GLU:OE1	2.46	0.42
1:F:182:GLY:HA2	1:G:281:PHE:CE2	2.55	0.42
1:G:7:LYS:HE3	1:G:15:LYS:HE3	2.02	0.42
1:G:205:ILE:HG23	1:G:212:ALA:O	2.20	0.42
1:I:39:VAL:HG12	1:J:69:MET:HE2	2.02	0.42
1:I:248:LEU:HD13	1:I:325:ILE:HD11	2.01	0.42
1:K:25:ASP:OD1	1:K:28:LYS:HE2	2.19	0.42
1:L:164:GLU:OE1	2:L:655:HOH:O	2.21	0.42
1:M:146:GLN:O	1:M:150:ILE:HG13	2.20	0.42
1:M:191:GLU:O	1:M:334:ASP:HA	2.19	0.42
1:N:183:LEU:HA	1:N:383:ALA:N	2.35	0.42
1:A:411:VAL:HG12	1:A:496:PRO:HA	2.02	0.42
1:E:178:GLU:HA	1:E:393:LYS:HE2	2.02	0.42
1:E:242:LYS:O	1:E:243:ALA:HB3	2.19	0.42
1:H:17:LEU:HD22	1:H:104:LEU:HD12	2.02	0.42
1:H:305:ILE:HG22	1:H:305:ILE:O	2.19	0.42
1:H:436:GLN:O	1:H:440:ILE:HG13	2.20	0.42
1:A:180:GLY:HA2	1:A:380:LYS:HB3	2.01	0.41
1:E:46:ALA:HB2	1:F:76:GLU:HG3	2.01	0.41
1:H:23:LEU:HD23	1:H:74:VAL:HG22	2.01	0.41
1:I:183:LEU:HA	1:I:383:ALA:N	2.35	0.41
1:L:441:LYS:HA	1:L:441:LYS:HD3	1.88	0.41
1:M:524:LEU:C	1:M:526:LYS:H	2.28	0.41
1:N:392:LYS:O	1:N:396:VAL:HG23	2.19	0.41
1:C:193:MET:HE2	1:C:193:MET:HB3	1.68	0.41
1:C:198:GLY:HA3	1:C:327:LYS:O	2.19	0.41
1:D:479:ASN:HD22	1:D:491:MET:CE	2.33	0.41
1:F:449:ALA:HB3	1:F:450:PRO:HD3	2.01	0.41
1:G:209:GLU:H	1:G:209:GLU:CD	2.28	0.41
1:I:434:GLU:HG3	2:I:657:HOH:O	2.20	0.41
1:J:345:ARG:NH1	1:J:348:GLN:OE1	2.53	0.41
1:L:287:ALA:HB1	1:L:368:ARG:NH1	2.34	0.41
1:L:405:ALA:O	2:L:601:HOH:O	2.21	0.41
1:L:413:ALA:HB3	1:L:417:VAL:HG22	2.01	0.41
1:M:242:LYS:O	1:M:243:ALA:HB3	2.20	0.41
1:A:103:GLY:O	1:A:107:VAL:HG23	2.19	0.41
1:B:169:VAL:HG11	1:B:377:ALA:HB2	2.01	0.41
1:B:199:TYR:CZ	1:B:327:LYS:HA	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:102:GLU:HB2	1:D:442:VAL:HG13	2.01	0.41
1:D:326:ASN:HB2	1:D:329:THR:HB	2.02	0.41
1:E:16:MET:HG3	1:E:520:MET:SD	2.60	0.41
1:J:195:PHE:HB2	1:J:279:PRO:HB3	2.02	0.41
1:M:66:PHE:HA	1:M:69:MET:CE	2.47	0.41
1:M:182:GLY:HA2	1:N:281:PHE:CZ	2.55	0.41
1:B:477:GLY:O	1:B:485:TYR:HA	2.20	0.41
1:D:180:GLY:HA2	1:D:380:LYS:HB3	2.01	0.41
1:D:476:TYR:CE1	1:D:485:TYR:HB3	2.55	0.41
1:F:384:ALA:O	1:F:385:THR:HG23	2.20	0.41
1:G:289:LEU:HD23	1:G:289:LEU:HA	1.91	0.41
1:I:281:PHE:HA	1:I:285:ARG:NE	2.35	0.41
1:J:95:LEU:O	1:J:99:ILE:HG13	2.20	0.41
1:L:183:LEU:O	1:L:184:GLN:O	2.38	0.41
1:A:18:ARG:HG2	1:A:67:GLU:CD	2.45	0.41
1:C:455:VAL:HG13	1:C:460:GLU:HB2	2.02	0.41
1:E:100:ILE:O	1:E:104:LEU:HG	2.21	0.41
1:E:487:ASN:ND2	2:E:673:HOH:O	2.28	0.41
1:H:233:MET:HE1	1:H:249:ILE:HD12	2.03	0.41
1:I:16:MET:SD	1:I:73:MET:HE1	2.59	0.41
1:L:259:LEU:O	1:L:263:VAL:HG23	2.21	0.41
1:L:326:ASN:HD22	1:L:326:ASN:HA	1.74	0.41
1:M:223:ALA:O	1:M:251:ALA:HA	2.21	0.41
1:M:270:ILE:HG13	1:N:257:GLU:HG3	2.02	0.41
1:B:223:ALA:C	2:B:658:HOH:O	2.45	0.41
1:D:176:THR:HG22	1:D:177:VAL:N	2.35	0.41
1:D:284:ARG:O	1:D:288:MET:HG3	2.21	0.41
1:E:242:LYS:O	1:E:244:GLY:N	2.46	0.41
1:I:293:ALA:HB2	1:I:300:VAL:HG23	2.03	0.41
1:K:220:ILE:HG23	1:K:248:LEU:HD23	2.03	0.41
1:K:230:ILE:HD13	1:K:261:THR:HG21	2.03	0.41
1:L:124:VAL:HG21	1:L:508:ALA:HB2	2.02	0.41
1:L:222:LEU:CD1	1:L:293:ALA:HA	2.51	0.41
1:L:363:GLU:H	1:L:363:GLU:HG2	1.71	0.41
1:M:383:ALA:O	1:M:384:ALA:HB3	2.21	0.41
1:N:193:MET:CE	1:N:292:ILE:HG12	2.42	0.41
1:N:384:ALA:O	1:N:385:THR:HG23	2.20	0.41
1:A:430:ARG:HH11	1:A:430:ARG:HG2	1.84	0.41
1:C:131:LEU:HD12	1:C:131:LEU:HA	1.76	0.41
1:D:86:GLY:O	1:D:87:ASP:HB2	2.20	0.41
1:E:183:LEU:O	1:E:184:GLN:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:240:VAL:HG11	1:E:247:LEU:HB2	2.03	0.41
1:E:514:MET:HE2	1:E:514:MET:HB3	1.65	0.41
1:G:107:VAL:C	1:G:109:ALA:H	2.28	0.41
1:J:420:ILE:HG12	1:J:448:GLU:HG2	2.02	0.41
1:K:16:MET:HB3	1:K:514:MET:HE3	2.02	0.41
1:L:224:ASP:O	1:L:225:LYS:HB3	2.21	0.41
1:L:447:MET:HE2	1:L:504:LEU:HD21	2.03	0.41
1:N:479:ASN:HB2	1:N:491:MET:SD	2.61	0.41
1:B:319:GLN:O	1:B:336:VAL:HG23	2.21	0.41
1:C:171:LYS:HB3	1:C:407:VAL:HG11	2.03	0.41
1:F:253:ASP:OD1	1:F:254:VAL:N	2.54	0.41
1:H:38:VAL:HG13	1:I:519:CYS:HB3	2.02	0.41
1:I:240:VAL:HG11	1:I:247:LEU:HB2	2.01	0.41
1:I:404:ARG:NE	2:I:608:HOH:O	2.54	0.41
1:K:152:ALA:O	1:K:153:ASN:HB2	2.21	0.41
1:M:82:ASN:HB2	1:M:89:THR:HB	2.01	0.41
1:A:197:ARG:NH1	2:A:607:HOH:O	2.51	0.41
1:C:350:ARG:HG2	1:C:350:ARG:NH1	2.35	0.41
1:D:144:ILE:HG23	1:D:403:THR:HG21	2.03	0.41
1:F:242:LYS:O	1:F:243:ALA:HB3	2.21	0.41
1:H:7:LYS:HG3	1:H:66:PHE:CZ	2.55	0.41
1:H:166:MET:HE2	1:H:404:ARG:NH1	2.35	0.41
1:H:294:THR:HG22	1:H:342:ILE:HD13	2.03	0.41
1:H:349:ILE:O	1:H:353:ILE:HG13	2.21	0.41
1:H:415:GLY:O	1:H:451:LEU:HD12	2.20	0.41
1:I:230:ILE:HG21	1:I:261:THR:HG21	2.03	0.41
1:J:123:ALA:HB2	1:J:440:ILE:HG23	2.02	0.41
1:J:230:ILE:HD12	1:J:233:MET:HG3	2.03	0.41
1:J:236:VAL:HG22	1:J:312:ALA:O	2.21	0.41
1:J:420:ILE:HG13	1:J:448:GLU:HA	2.03	0.41
1:K:229:ASN:HA	1:K:257:GLU:OE1	2.21	0.41
1:K:237:LEU:O	1:K:240:VAL:HG12	2.21	0.41
1:M:190:VAL:HG21	1:M:334:ASP:HB2	2.02	0.41
1:N:242:LYS:O	1:N:243:ALA:HB3	2.20	0.41
1:N:443:ALA:O	1:N:447:MET:HG3	2.21	0.41
1:A:478:TYR:HA	1:A:485:TYR:CE2	2.55	0.41
1:D:524:LEU:HD12	1:D:524:LEU:HA	1.82	0.41
1:G:230:ILE:HB	1:G:257:GLU:OE2	2.21	0.41
1:G:350:ARG:O	1:G:353:ILE:HB	2.20	0.41
1:I:191:GLU:O	1:I:334:ASP:HA	2.20	0.41
1:I:441:LYS:O	1:I:442:VAL:C	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:242:LYS:C	1:J:244:GLY:H	2.29	0.41
1:K:39:VAL:HG12	1:L:69:MET:CE	2.50	0.41
1:A:414:GLY:O	1:A:417:VAL:HG13	2.20	0.40
1:B:381:VAL:CG1	1:B:392:LYS:HD3	2.51	0.40
1:C:514:MET:HE2	1:C:514:MET:HB3	1.88	0.40
1:D:217:SER:N	1:D:218:PRO:HD3	2.35	0.40
1:E:77:VAL:HG12	1:E:506:TYR:HB3	2.03	0.40
1:E:200:LEU:HG	1:E:276:VAL:HA	2.03	0.40
1:F:182:GLY:HA2	1:G:281:PHE:CZ	2.56	0.40
1:F:217:SER:N	1:F:218:PRO:HD3	2.36	0.40
1:M:42:LYS:C	1:M:44:PHE:N	2.79	0.40
1:M:284:ARG:NE	2:M:653:HOH:O	2.53	0.40
1:M:524:LEU:O	1:M:526:LYS:N	2.50	0.40
1:N:216:GLU:C	1:N:218:PRO:HD3	2.46	0.40
1:E:16:MET:HB3	1:E:514:MET:CE	2.51	0.40
1:G:218:PRO:HB3	1:G:246:PRO:HG2	2.02	0.40
1:H:231:ARG:HB2	2:H:608:HOH:O	2.22	0.40
1:I:357:THR:OG1	1:I:358:SER:N	2.54	0.40
1:J:200:LEU:HA	1:J:200:LEU:HD23	1.85	0.40
1:N:199:TYR:CE2	1:N:205:ILE:HD11	2.56	0.40
1:B:514:MET:HE2	1:B:514:MET:HB3	1.90	0.40
1:C:364:LYS:O	1:C:367:GLU:HB3	2.21	0.40
1:D:436:GLN:O	1:D:440:ILE:HG13	2.21	0.40
1:E:269:GLY:O	1:F:229:ASN:ND2	2.55	0.40
1:F:183:LEU:O	1:F:183:LEU:HD13	2.22	0.40
1:I:201:SER:HA	1:I:202:PRO:HD3	1.89	0.40
1:K:5:ASP:HB2	1:K:524:LEU:HD12	2.02	0.40
1:K:17:LEU:HG	1:K:21:ASN:ND2	2.36	0.40
1:A:203:TYR:CB	1:A:263:VAL:HG13	2.52	0.40
1:A:247:LEU:CD2	1:A:249:ILE:HD11	2.51	0.40
1:B:284:ARG:NH1	2:B:612:HOH:O	2.54	0.40
1:C:263:VAL:O	1:C:267:MET:HB2	2.22	0.40
1:D:193:MET:HE1	1:D:292:ILE:CG1	2.51	0.40
1:E:95:LEU:HD13	1:E:504:LEU:HA	2.04	0.40
1:F:296:THR:HB	1:F:319:GLN:H	1.86	0.40
1:F:344:GLY:O	1:F:348:GLN:HG3	2.21	0.40
1:G:183:LEU:O	1:G:184:GLN:C	2.63	0.40
1:G:201:SER:C	1:G:202:PRO:O	2.62	0.40
1:J:217:SER:HA	1:J:320:ALA:O	2.22	0.40
1:J:429:LEU:O	1:J:430:ARG:NH1	2.49	0.40
1:J:455:VAL:HG11	1:J:462:PRO:HA	2.01	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:199:TYR:OH	1:M:205:ILE:HD11	2.22	0.40
1:N:195:PHE:HB2	1:N:279:PRO:HB3	2.02	0.40
1:N:404:ARG:HD2	1:N:404:ARG:HA	1.89	0.40
1:N:524:LEU:O	1:N:526:LYS:N	2.55	0.40
1:A:479:ASN:ND2	1:A:484:GLU:O	2.49	0.40
1:A:487:ASN:O	1:A:490:ASP:HB2	2.22	0.40
1:C:68:ASN:O	1:C:72:GLN:HG2	2.21	0.40
1:D:18:ARG:HG2	1:D:67:GLU:CD	2.46	0.40
1:G:71:ALA:O	1:G:75:LYS:HB2	2.22	0.40
1:I:157:THR:HG21	1:I:392:LYS:HZ1	1.85	0.40
1:I:219:PHE:HB3	1:I:317:LEU:HD23	2.03	0.40
1:K:455:VAL:HG13	1:K:460:GLU:HB2	2.02	0.40
1:M:479:ASN:C	1:M:481:ALA:N	2.80	0.40
1:M:513:LEU:HD23	1:M:513:LEU:HA	1.79	0.40
1:N:200:LEU:HD23	1:N:200:LEU:HA	1.89	0.40

There are no symmetry-related clashes.

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	523/525 (100%)	499 (95%)	15 (3%)	9 (2%)	7	35
1	B	523/525 (100%)	499 (95%)	18 (3%)	6 (1%)	11	43
1	C	523/525 (100%)	496 (95%)	18 (3%)	9 (2%)	7	35
1	D	523/525 (100%)	494 (94%)	21 (4%)	8 (2%)	8	37
1	E	523/525 (100%)	493 (94%)	22 (4%)	8 (2%)	8	37
1	F	523/525 (100%)	496 (95%)	17 (3%)	10 (2%)	6	33
1	G	523/525 (100%)	498 (95%)	17 (3%)	8 (2%)	8	37
1	H	523/525 (100%)	488 (93%)	24 (5%)	11 (2%)	5	31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	523/525 (100%)	492 (94%)	26 (5%)	5 (1%)	12	45
1	J	523/525 (100%)	491 (94%)	24 (5%)	8 (2%)	8	37
1	K	523/525 (100%)	486 (93%)	28 (5%)	9 (2%)	7	35
1	L	523/525 (100%)	486 (93%)	25 (5%)	12 (2%)	5	29
1	M	523/525 (100%)	487 (93%)	18 (3%)	18 (3%)	3	20
1	N	523/525 (100%)	492 (94%)	22 (4%)	9 (2%)	7	35
All	All	7322/7350 (100%)	6897 (94%)	295 (4%)	130 (2%)	6	34

All (130) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	480	ALA
1	B	183	LEU
1	B	184	GLN
1	C	202	PRO
1	E	44	PHE
1	F	184	GLN
1	F	203	TYR
1	G	184	GLN
1	H	43	SER
1	H	184	GLN
1	H	243	ALA
1	I	43	SER
1	K	184	GLN
1	L	184	GLN
1	L	203	TYR
1	L	486	GLY
1	M	43	SER
1	M	199	TYR
1	M	208	PRO
1	M	209	GLU
1	M	221	LEU
1	M	271	VAL
1	A	183	LEU
1	A	244	GLY
1	A	385	THR
1	B	202	PRO
1	B	385	THR
1	C	34	LYS
1	C	385	THR

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Mol	Chain	Res	Type
1	D	385	THR
1	F	183	LEU
1	F	385	THR
1	F	480	ALA
1	G	183	LEU
1	J	183	LEU
1	J	339	GLU
1	K	256	GLY
1	K	480	ALA
1	L	256	GLY
1	M	197	ARG
1	M	256	GLY
1	M	480	ALA
1	A	271	VAL
1	B	271	VAL
1	C	183	LEU
1	C	271	VAL
1	D	183	LEU
1	D	184	GLN
1	D	271	VAL
1	D	482	THR
1	E	183	LEU
1	E	385	THR
1	G	202	PRO
1	G	385	THR
1	H	271	VAL
1	H	481	ALA
1	I	183	LEU
1	I	271	VAL
1	I	383	ALA
1	J	225	LYS
1	J	271	VAL
1	K	271	VAL
1	K	385	THR
1	L	271	VAL
1	L	385	THR
1	L	525	PRO
1	M	196	ASP
1	M	214	GLU
1	M	525	PRO
1	N	43	SER
1	N	182	GLY

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Mol	Chain	Res	Type
1	N	183	LEU
1	N	256	GLY
1	A	203	TYR
1	A	243	ALA
1	B	525	PRO
1	D	225	LYS
1	E	271	VAL
1	E	483	GLU
1	F	271	VAL
1	F	383	ALA
1	F	479	ASN
1	G	108	ALA
1	G	271	VAL
1	G	383	ALA
1	H	202	PRO
1	H	383	ALA
1	I	182	GLY
1	K	225	LYS
1	K	234	LEU
1	K	525	PRO
1	L	225	LYS
1	L	234	LEU
1	M	183	LEU
1	M	225	LYS
1	N	271	VAL
1	N	383	ALA
1	N	525	PRO
1	A	184	GLN
1	A	383	ALA
1	C	184	GLN
1	C	525	PRO
1	D	383	ALA
1	D	483	GLU
1	E	383	ALA
1	E	525	PRO
1	F	525	PRO
1	G	525	PRO
1	H	9	GLY
1	H	480	ALA
1	J	256	GLY
1	J	383	ALA
1	J	525	PRO

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Mol	Chain	Res	Type
1	K	383	ALA
1	L	183	LEU
1	L	358	SER
1	L	383	ALA
1	M	383	ALA
1	N	385	THR
1	C	182	GLY
1	H	183	LEU
1	H	256	GLY
1	J	182	GLY
1	M	182	GLY
1	M	201	SER
1	M	384	ALA
1	N	184	GLN
1	C	33	PRO
1	F	202	PRO
1	E	182	GLY

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	405/405 (100%)	382 (94%)	23 (6%)	18	51
1	B	405/405 (100%)	386 (95%)	19 (5%)	23	57
1	C	405/405 (100%)	380 (94%)	25 (6%)	16	49
1	D	405/405 (100%)	383 (95%)	22 (5%)	20	53
1	E	405/405 (100%)	386 (95%)	19 (5%)	23	57
1	F	405/405 (100%)	377 (93%)	28 (7%)	14	45
1	G	405/405 (100%)	377 (93%)	28 (7%)	14	45
1	H	405/405 (100%)	385 (95%)	20 (5%)	22	55
1	I	405/405 (100%)	376 (93%)	29 (7%)	13	44
1	J	405/405 (100%)	380 (94%)	25 (6%)	16	49
1	K	405/405 (100%)	381 (94%)	24 (6%)	18	50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L	405/405 (100%)	382 (94%)	23 (6%)	18	51
1	M	405/405 (100%)	379 (94%)	26 (6%)	16	48
1	N	405/405 (100%)	379 (94%)	26 (6%)	16	48
All	All	5670/5670 (100%)	5333 (94%)	337 (6%)	18	50

All (337) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	VAL
1	A	82	ASN
1	A	94	VAL
1	A	129	GLU
1	A	134	LEU
1	A	177	VAL
1	A	230	ILE
1	A	232	GLU
1	A	255	GLU
1	A	261	THR
1	A	270	ILE
1	A	295	LEU
1	A	301	ILE
1	A	329	THR
1	A	331	THR
1	A	343	GLN
1	A	351	GLN
1	A	398	ASP
1	A	403	THR
1	A	417	VAL
1	A	420	ILE
1	A	422	VAL
1	A	499	VAL
1	B	82	ASN
1	B	89	THR
1	B	94	VAL
1	B	122	LYS
1	B	131	LEU
1	B	134	LEU
1	B	177	VAL
1	B	183	LEU
1	B	189	VAL
1	B	257	GLU

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Mol	Chain	Res	Type
1	B	261	THR
1	B	284	ARG
1	B	398	ASP
1	B	404	ARG
1	B	417	VAL
1	B	422	VAL
1	B	489	ILE
1	B	499	VAL
1	B	524	LEU
1	C	18	ARG
1	C	20	VAL
1	C	74	VAL
1	C	76	GLU
1	C	82	ASN
1	C	89	THR
1	C	94	VAL
1	C	129	GLU
1	C	131	LEU
1	C	183	LEU
1	C	193	MET
1	C	232	GLU
1	C	255	GLU
1	C	263	VAL
1	C	331	THR
1	C	350	ARG
1	C	372	LEU
1	C	404	ARG
1	C	417	VAL
1	C	420	ILE
1	C	422	VAL
1	C	425	LYS
1	C	489	ILE
1	C	499	VAL
1	C	524	LEU
1	D	20	VAL
1	D	74	VAL
1	D	76	GLU
1	D	82	ASN
1	D	94	VAL
1	D	129	GLU
1	D	131	LEU
1	D	134	LEU

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Mol	Chain	Res	Type
1	D	177	VAL
1	D	183	LEU
1	D	257	GLU
1	D	317	LEU
1	D	328	ASP
1	D	329	THR
1	D	331	THR
1	D	398	ASP
1	D	404	ARG
1	D	417	VAL
1	D	422	VAL
1	D	499	VAL
1	D	510	VAL
1	D	524	LEU
1	E	42	LYS
1	E	82	ASN
1	E	89	THR
1	E	94	VAL
1	E	131	LEU
1	E	134	LEU
1	E	177	VAL
1	E	183	LEU
1	E	232	GLU
1	E	284	ARG
1	E	319	GLN
1	E	329	THR
1	E	331	THR
1	E	372	LEU
1	E	404	ARG
1	E	417	VAL
1	E	422	VAL
1	E	483	GLU
1	E	499	VAL
1	F	20	VAL
1	F	74	VAL
1	F	76	GLU
1	F	77	VAL
1	F	82	ASN
1	F	94	VAL
1	F	129	GLU
1	F	131	LEU
1	F	183	LEU

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Mol	Chain	Res	Type
1	F	228	SER
1	F	232	GLU
1	F	267	MET
1	F	270	ILE
1	F	284	ARG
1	F	295	LEU
1	F	328	ASP
1	F	329	THR
1	F	331	THR
1	F	367	GLU
1	F	387	VAL
1	F	398	ASP
1	F	417	VAL
1	F	420	ILE
1	F	422	VAL
1	F	489	ILE
1	F	499	VAL
1	F	524	LEU
1	F	526	LYS
1	G	20	VAL
1	G	42	LYS
1	G	74	VAL
1	G	82	ASN
1	G	89	THR
1	G	94	VAL
1	G	129	GLU
1	G	131	LEU
1	G	134	LEU
1	G	139	SER
1	G	141	SER
1	G	142	LYS
1	G	183	LEU
1	G	240	VAL
1	G	255	GLU
1	G	257	GLU
1	G	270	ILE
1	G	314	LEU
1	G	328	ASP
1	G	329	THR
1	G	331	THR
1	G	358	SER
1	G	372	LEU

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Mol	Chain	Res	Type
1	G	417	VAL
1	G	422	VAL
1	G	467	ASN
1	G	499	VAL
1	G	524	LEU
1	H	20	VAL
1	H	74	VAL
1	H	94	VAL
1	H	183	LEU
1	H	209	GLU
1	H	210	THR
1	H	228	SER
1	H	232	GLU
1	H	255	GLU
1	H	257	GLU
1	H	327	LYS
1	H	328	ASP
1	H	329	THR
1	H	331	THR
1	H	398	ASP
1	H	404	ARG
1	H	417	VAL
1	H	422	VAL
1	H	482	THR
1	H	499	VAL
1	I	20	VAL
1	I	76	GLU
1	I	82	ASN
1	I	89	THR
1	I	94	VAL
1	I	131	LEU
1	I	134	LEU
1	I	138	CYS
1	I	172	GLU
1	I	183	LEU
1	I	209	GLU
1	I	210	THR
1	I	232	GLU
1	I	257	GLU
1	I	286	LYS
1	I	305	ILE
1	I	328	ASP

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Mol	Chain	Res	Type
1	I	329	THR
1	I	331	THR
1	I	372	LEU
1	I	385	THR
1	I	398	ASP
1	I	417	VAL
1	I	420	ILE
1	I	422	VAL
1	I	467	ASN
1	I	489	ILE
1	I	499	VAL
1	I	524	LEU
1	J	20	VAL
1	J	74	VAL
1	J	76	GLU
1	J	77	VAL
1	J	79	SER
1	J	89	THR
1	J	94	VAL
1	J	134	LEU
1	J	183	LEU
1	J	225	LYS
1	J	231	ARG
1	J	232	GLU
1	J	259	LEU
1	J	328	ASP
1	J	329	THR
1	J	331	THR
1	J	343	GLN
1	J	398	ASP
1	J	404	ARG
1	J	412	VAL
1	J	417	VAL
1	J	420	ILE
1	J	422	VAL
1	J	499	VAL
1	J	524	LEU
1	K	20	VAL
1	K	58	ARG
1	K	74	VAL
1	K	76	GLU
1	K	82	ASN

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Mol	Chain	Res	Type
1	K	94	VAL
1	K	134	LEU
1	K	141	SER
1	K	183	LEU
1	K	188	ASP
1	K	225	LYS
1	K	255	GLU
1	K	328	ASP
1	K	329	THR
1	K	331	THR
1	K	363	GLU
1	K	385	THR
1	K	398	ASP
1	K	404	ARG
1	K	417	VAL
1	K	420	ILE
1	K	422	VAL
1	K	499	VAL
1	K	524	LEU
1	L	20	VAL
1	L	74	VAL
1	L	76	GLU
1	L	82	ASN
1	L	94	VAL
1	L	138	CYS
1	L	156	GLU
1	L	183	LEU
1	L	242	LYS
1	L	326	ASN
1	L	328	ASP
1	L	329	THR
1	L	331	THR
1	L	339	GLU
1	L	363	GLU
1	L	385	THR
1	L	398	ASP
1	L	417	VAL
1	L	420	ILE
1	L	422	VAL
1	L	440	ILE
1	L	499	VAL
1	L	524	LEU

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Mol	Chain	Res	Type
1	M	20	VAL
1	M	74	VAL
1	M	82	ASN
1	M	94	VAL
1	M	134	LEU
1	M	183	LEU
1	M	193	MET
1	M	210	THR
1	M	232	GLU
1	M	234	LEU
1	M	257	GLU
1	M	267	MET
1	M	284	ARG
1	M	304	GLU
1	M	313	THR
1	M	328	ASP
1	M	329	THR
1	M	331	THR
1	M	339	GLU
1	M	404	ARG
1	M	417	VAL
1	M	422	VAL
1	M	424	SER
1	M	451	LEU
1	M	499	VAL
1	M	524	LEU
1	N	20	VAL
1	N	38	VAL
1	N	44	PHE
1	N	54	VAL
1	N	74	VAL
1	N	82	ASN
1	N	94	VAL
1	N	183	LEU
1	N	209	GLU
1	N	210	THR
1	N	295	LEU
1	N	313	THR
1	N	328	ASP
1	N	329	THR
1	N	331	THR
1	N	339	GLU

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Mol	Chain	Res	Type
1	N	351	GLN
1	N	372	LEU
1	N	393	LYS
1	N	398	ASP
1	N	417	VAL
1	N	420	ILE
1	N	422	VAL
1	N	451	LEU
1	N	499	VAL
1	N	524	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	146	GLN
1	A	194	GLN
1	A	229	ASN
1	A	290	GLN
1	A	326	ASN
1	A	401	HIS
1	B	37	ASN
1	B	82	ASN
1	C	37	ASN
1	C	319	GLN
1	C	343	GLN
1	C	401	HIS
1	D	229	ASN
1	D	326	ASN
1	D	366	GLN
1	E	37	ASN
1	E	97	GLN
1	E	184	GLN
1	E	229	ASN
1	E	290	GLN
1	E	352	GLN
1	E	366	GLN
1	E	401	HIS
1	E	433	ASN
1	F	82	ASN
1	F	194	GLN
1	F	265	ASN
1	F	319	GLN

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Mol	Chain	Res	Type
1	F	467	ASN
1	G	326	ASN
1	H	194	GLN
1	H	229	ASN
1	I	72	GLN
1	I	352	GLN
1	J	37	ASN
1	J	265	ASN
1	K	146	GLN
1	K	265	ASN
1	L	326	ASN
1	L	351	GLN
1	M	97	GLN
1	M	352	GLN
1	N	146	GLN
1	N	326	ASN
1	N	351	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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 ⓘ

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	525/525 (100%)	-0.43	6 (1%) 78 61	10, 32, 68, 153	0
1	B	525/525 (100%)	-0.47	2 (0%) 88 79	11, 35, 69, 95	0
1	C	525/525 (100%)	-0.36	3 (0%) 85 73	13, 40, 77, 102	0
1	D	525/525 (100%)	-0.28	8 (1%) 72 52	13, 39, 88, 153	0
1	E	525/525 (100%)	-0.48	9 (1%) 69 49	11, 30, 63, 180	0
1	F	525/525 (100%)	-0.40	6 (1%) 78 61	9, 38, 73, 163	0
1	G	525/525 (100%)	-0.43	7 (1%) 75 55	10, 34, 74, 122	0
1	H	525/525 (100%)	-0.37	6 (1%) 78 61	11, 38, 74, 140	0
1	I	525/525 (100%)	-0.38	4 (0%) 82 67	12, 41, 79, 170	0
1	J	525/525 (100%)	-0.36	2 (0%) 88 79	13, 40, 82, 122	0
1	K	525/525 (100%)	-0.02	22 (4%) 40 25	10, 48, 121, 151	0
1	L	525/525 (100%)	-0.26	6 (1%) 78 61	12, 46, 94, 126	0
1	M	525/525 (100%)	-0.35	5 (0%) 79 63	11, 37, 80, 160	0
1	N	525/525 (100%)	-0.37	8 (1%) 72 52	9, 37, 72, 140	0
All	All	7350/7350 (100%)	-0.35	94 (1%) 75 55	9, 38, 85, 180	0

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	478	TYR	6.3
1	H	478	TYR	5.3
1	F	478	TYR	5.3
1	A	480	ALA	4.9
1	H	480	ALA	4.7
1	N	480	ALA	4.3
1	N	478	TYR	4.0
1	M	478	TYR	4.0

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Mol	Chain	Res	Type	RSRZ
1	K	270	ILE	3.9
1	A	478	TYR	3.8
1	E	44	PHE	3.8
1	F	480	ALA	3.7
1	K	314	LEU	3.6
1	A	271	VAL	3.6
1	D	480	ALA	3.6
1	D	478	TYR	3.6
1	I	480	ALA	3.5
1	K	480	ALA	3.5
1	G	480	ALA	3.4
1	H	43	SER	3.4
1	E	480	ALA	3.3
1	K	210	THR	3.3
1	I	478	TYR	3.3
1	M	270	ILE	3.3
1	G	478	TYR	3.2
1	J	487	ASN	3.1
1	A	481	ALA	3.1
1	K	266	THR	3.1
1	A	485	TYR	3.0
1	D	479	ASN	3.0
1	L	266	THR	3.0
1	E	481	ALA	2.9
1	G	481	ALA	2.9
1	N	485	TYR	2.9
1	M	480	ALA	2.9
1	D	483	GLU	2.9
1	K	256	GLY	2.8
1	E	482	THR	2.8
1	E	479	ASN	2.8
1	N	44	PHE	2.8
1	L	486	GLY	2.7
1	C	271	VAL	2.7
1	K	264	VAL	2.7
1	G	485	TYR	2.7
1	M	485	TYR	2.7
1	E	477	GLY	2.6
1	K	259	LEU	2.6
1	K	271	VAL	2.5
1	L	480	ALA	2.5
1	K	485	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
1	L	481	ALA	2.4
1	C	485	TYR	2.4
1	F	476	TYR	2.4
1	K	476	TYR	2.4
1	F	184	GLN	2.4
1	A	483	GLU	2.4
1	H	44	PHE	2.4
1	E	478	TYR	2.3
1	G	272	LYS	2.3
1	D	270	ILE	2.3
1	D	477	GLY	2.3
1	K	255	GLU	2.3
1	D	481	ALA	2.3
1	K	243	ALA	2.3
1	K	477	GLY	2.2
1	G	44	PHE	2.2
1	B	477	GLY	2.2
1	N	43	SER	2.2
1	K	209	GLU	2.2
1	K	211	GLY	2.2
1	F	482	THR	2.2
1	E	476	TYR	2.2
1	H	82	ASN	2.2
1	I	483	GLU	2.2
1	N	481	ALA	2.2
1	N	366	GLN	2.1
1	K	263	VAL	2.1
1	J	479	ASN	2.1
1	I	485	TYR	2.1
1	K	269	GLY	2.1
1	D	485	TYR	2.1
1	L	203	TYR	2.1
1	B	271	VAL	2.1
1	N	271	VAL	2.1
1	H	485	TYR	2.1
1	C	481	ALA	2.1
1	K	272	LYS	2.0
1	K	203	TYR	2.0
1	K	317	LEU	2.0
1	M	481	ALA	2.0
1	E	484	GLU	2.0
1	F	271	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	G	284	ARG	2.0
1	L	271	VAL	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.