



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:14 PM UTC

PDB ID : 1XCK / pdb_00001xck
Title : Crystal structure of apo GroEL
Authors : Bartolucci, C.; Lamba, D.; Grazulis, S.; Manakova, E.; Heumann, H.
Deposited on : 2004-09-02
Resolution : 2.92 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

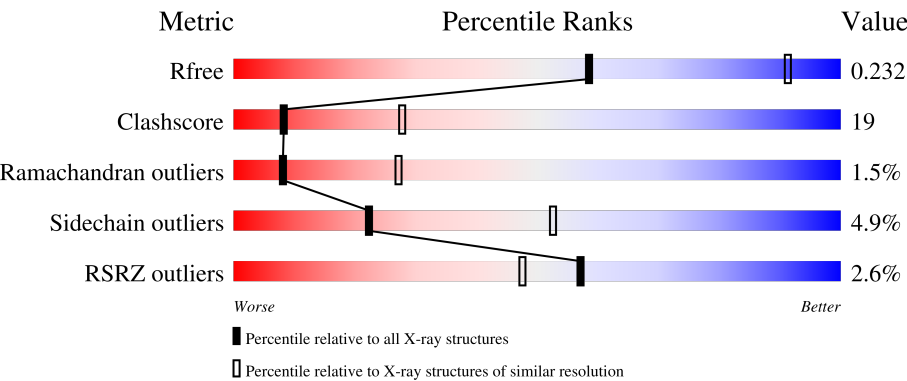
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.92 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	2995 (2.94-2.90)
Clashscore	190562	3213 (2.94-2.90)
Ramachandran outliers	187476	3128 (2.94-2.90)
Sidechain outliers	187428	3130 (2.94-2.90)
RSRZ outliers	180081	2995 (2.94-2.90)

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

Mol	Chain	Length	Quality of chain
1	A	547	% 64%27%5%.
1	B	547	3% 62%29%5%.
1	C	547	2% 61%30%. .
1	D	547	% 63%29%. .
1	E	547	% 63%29%. .

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Mol	Chain	Length	Quality of chain
1	F	547	% 63% 28% . .
1	G	547	% 66% 26% . .
1	H	547	4% 59% 34% . .
1	I	547	3% 59% 33% . .
1	J	547	2% 57% 36% . .
1	K	547	% 58% 35% . .
1	L	547	9% 57% 35% . .
1	M	547	3% 56% 36% . .
1	N	547	2% 58% 35% . .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	B	1136	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 55301 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	524	Total	C	N	O	S	0	0	0
			3855	2397	665	773	20			
1	B	524	Total	C	N	O	S	0	0	0
			3855	2397	665	773	20			
1	C	524	Total	C	N	O	S	0	0	0
			3855	2397	665	773	20			
1	D	524	Total	C	N	O	S	0	0	0
			3855	2397	665	773	20			
1	E	524	Total	C	N	O	S	0	0	0
			3855	2397	665	773	20			
1	F	524	Total	C	N	O	S	0	0	0
			3855	2397	665	773	20			
1	G	524	Total	C	N	O	S	0	0	0
			3855	2397	665	773	20			
1	H	524	Total	C	N	O	S	0	0	0
			3855	2397	665	773	20			
1	I	524	Total	C	N	O	S	0	0	0
			3855	2397	665	773	20			
1	J	524	Total	C	N	O	S	0	0	0
			3855	2397	665	773	20			
1	K	524	Total	C	N	O	S	0	0	0
			3855	2397	665	773	20			
1	L	524	Total	C	N	O	S	0	0	0
			3855	2397	665	773	20			
1	M	524	Total	C	N	O	S	0	0	0
			3855	2397	665	773	20			
1	N	524	Total	C	N	O	S	0	0	0
			3855	2397	665	773	20			

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		
2	I	1	Total	O	S	0	0
			5	4	1		
2	I	1	Total	O	S	0	0
			5	4	1		
2	J	1	Total	O	S	0	0
			5	4	1		
2	J	1	Total	O	S	0	0
			5	4	1		
2	J	1	Total	O	S	0	0
			5	4	1		
2	J	1	Total	O	S	0	0
			5	4	1		
2	K	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	K	1	Total O S 5 4 1	0	0
2	L	1	Total O S 5 4 1	0	0
2	L	1	Total O S 5 4 1	0	0
2	M	1	Total O S 5 4 1	0	0
2	M	1	Total O S 5 4 1	0	0
2	M	1	Total O S 5 4 1	0	0
2	N	1	Total O S 5 4 1	0	0
2	N	1	Total O S 5 4 1	0	0

- Molecule 3 is POTASSIUM ION (CCD ID: K) (formula: K).

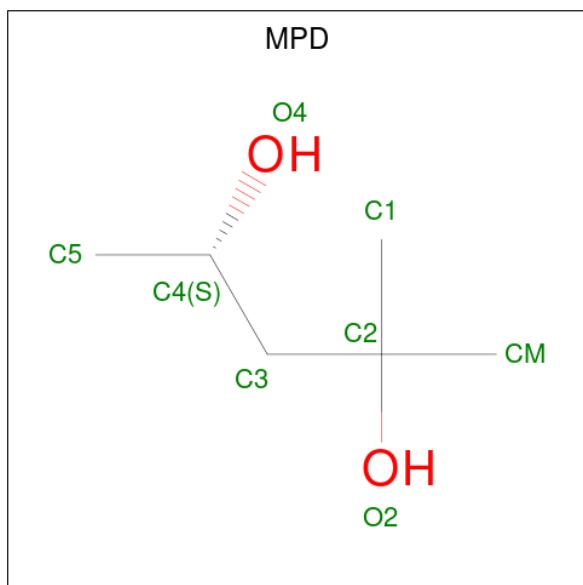
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total K 1 1	0	0
3	B	1	Total K 1 1	0	0
3	C	1	Total K 1 1	0	0
3	D	1	Total K 1 1	0	0
3	E	1	Total K 1 1	0	0
3	F	1	Total K 1 1	0	0
3	G	1	Total K 1 1	0	0
3	H	1	Total K 1 1	0	0
3	I	1	Total K 1 1	0	0
3	J	1	Total K 1 1	0	0
3	K	1	Total K 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	L	1	Total	K	0	0
			1	1		
3	M	1	Total	K	0	0
			1	1		
3	N	1	Total	K	0	0
			1	1		

- Molecule 4 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C₆H₁₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			8	6	2		
4	A	1	Total	C	O	0	0
			8	6	2		
4	B	1	Total	C	O	0	0
			8	6	2		
4	B	1	Total	C	O	0	0
			8	6	2		
4	B	1	Total	C	O	0	0
			8	6	2		
4	C	1	Total	C	O	0	0
			8	6	2		
4	D	1	Total	C	O	0	0
			8	6	2		

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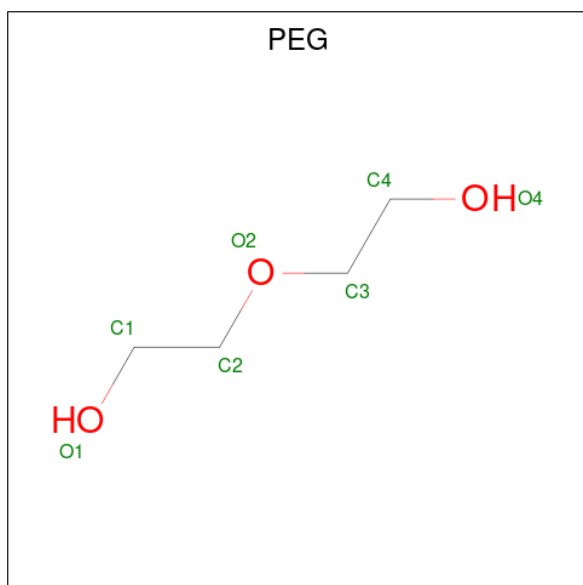
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	E	1	Total	C	O	0	0
			8	6	2		
4	E	1	Total	C	O	0	0
			8	6	2		
4	E	1	Total	C	O	0	0
			8	6	2		
4	E	1	Total	C	O	0	0
			8	6	2		
4	E	1	Total	C	O	0	0
			8	6	2		
4	F	1	Total	C	O	0	0
			8	6	2		
4	F	1	Total	C	O	0	0
			8	6	2		
4	F	1	Total	C	O	0	0
			8	6	2		
4	G	1	Total	C	O	0	0
			8	6	2		
4	G	1	Total	C	O	0	0
			8	6	2		
4	H	1	Total	C	O	0	0
			8	6	2		
4	H	1	Total	C	O	0	0
			8	6	2		
4	I	1	Total	C	O	0	0
			8	6	2		
4	I	1	Total	C	O	0	0
			8	6	2		
4	I	1	Total	C	O	0	0
			8	6	2		
4	J	1	Total	C	O	0	0
			8	6	2		
4	K	1	Total	C	O	0	0
			8	6	2		
4	K	1	Total	C	O	0	0
			8	6	2		
4	L	1	Total	C	O	0	0
			8	6	2		
4	M	1	Total	C	O	0	0
			8	6	2		
4	N	1	Total	C	O	0	0
			8	6	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	N	1	Total	C	O	0	0
			8	6	2		
4	N	1	Total	C	O	0	0
			8	6	2		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	E	1	Total	C	O	0	0
			7	4	3		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	60	Total	O	0	0
			60	60		
6	B	76	Total	O	0	0
			76	76		
6	C	55	Total	O	0	0
			55	55		
6	D	79	Total	O	0	0
			79	79		
6	E	64	Total	O	0	0
			64	64		
6	F	65	Total	O	0	0
			65	65		

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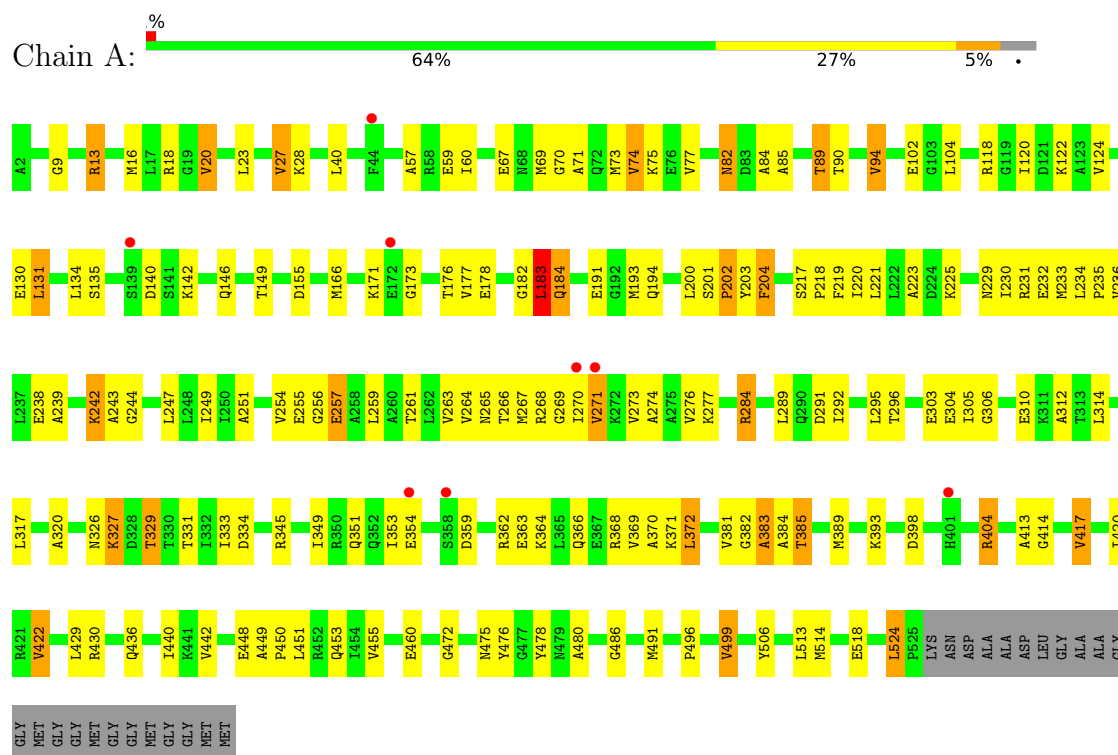
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	G	84	Total O 84 84	0	0
6	H	61	Total O 61 61	0	0
6	I	63	Total O 63 63	0	0
6	J	45	Total O 45 45	0	0
6	K	52	Total O 52 52	0	0
6	L	32	Total O 32 32	0	0
6	M	49	Total O 49 49	0	0
6	N	62	Total O 62 62	0	0

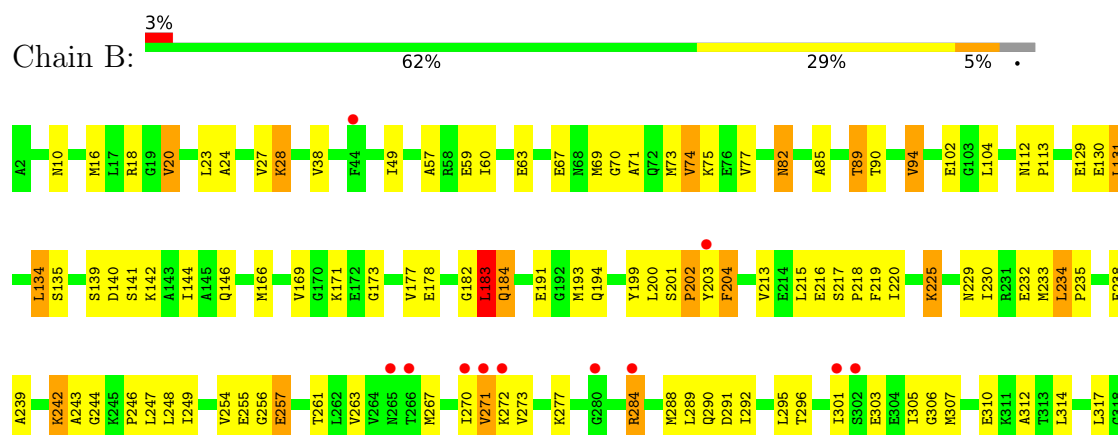
3 Residue-property plots

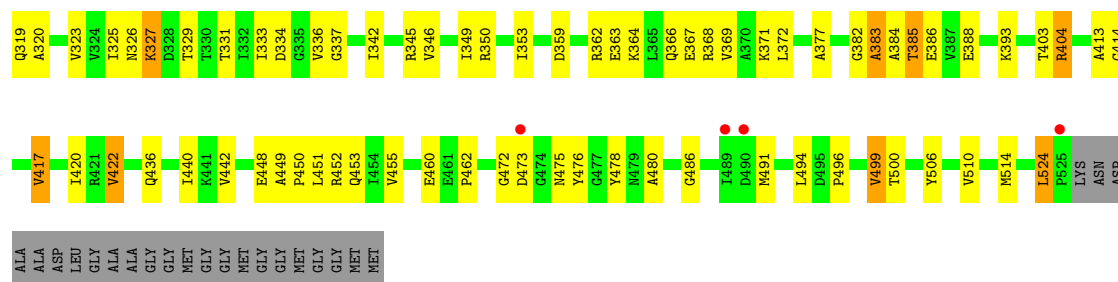
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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

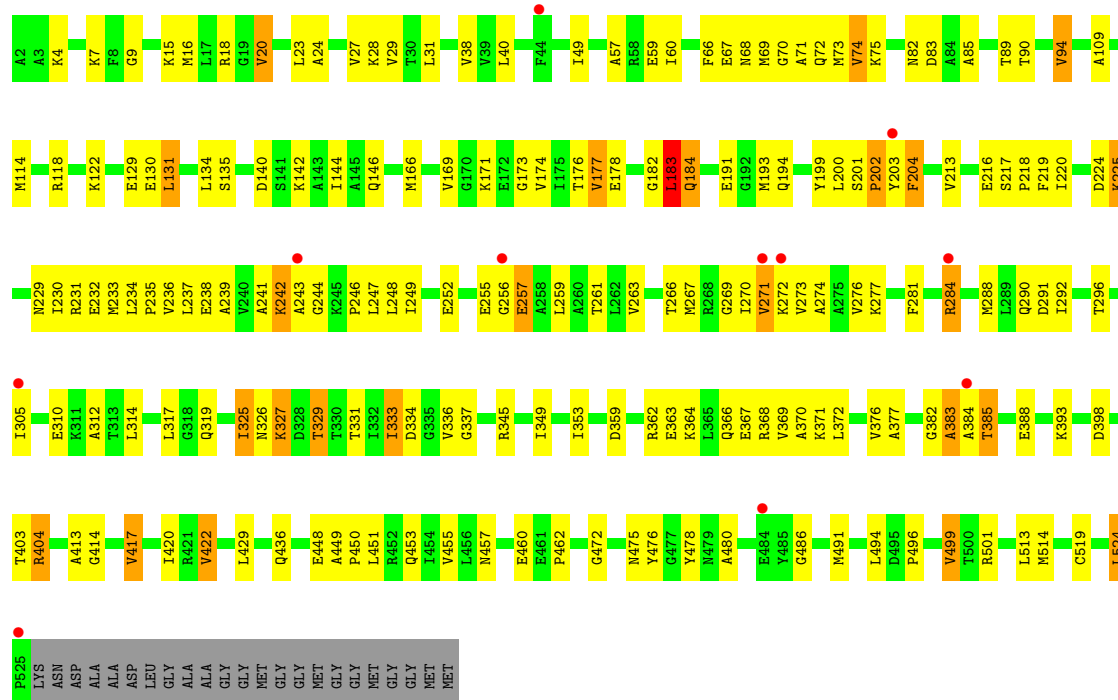


• Molecule 1: 60 kDa chaperonin

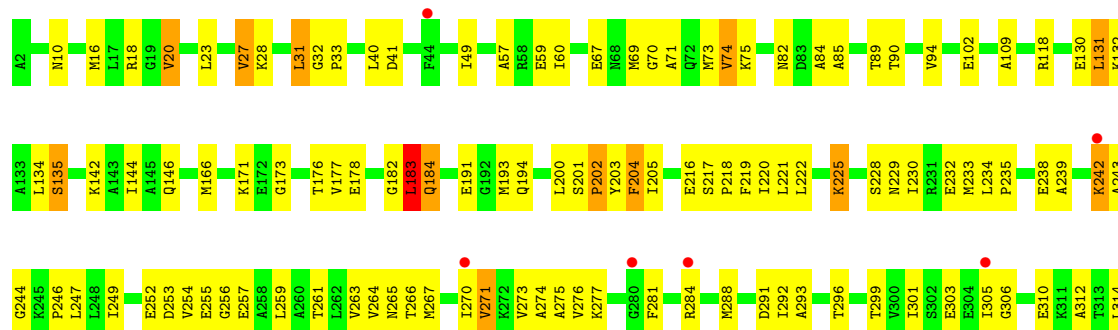


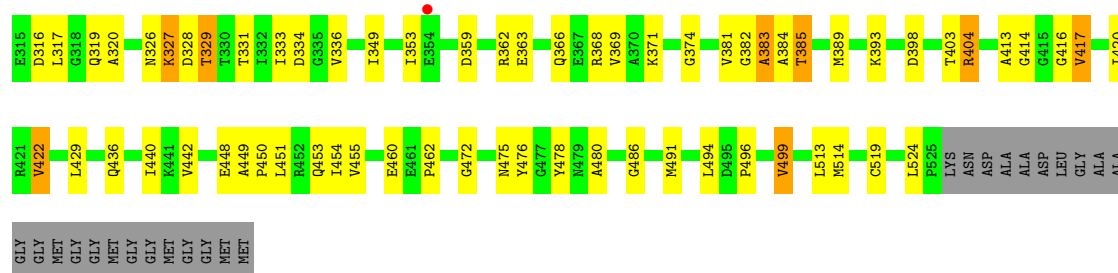


- Molecule 1: 60 kDa chaperonin

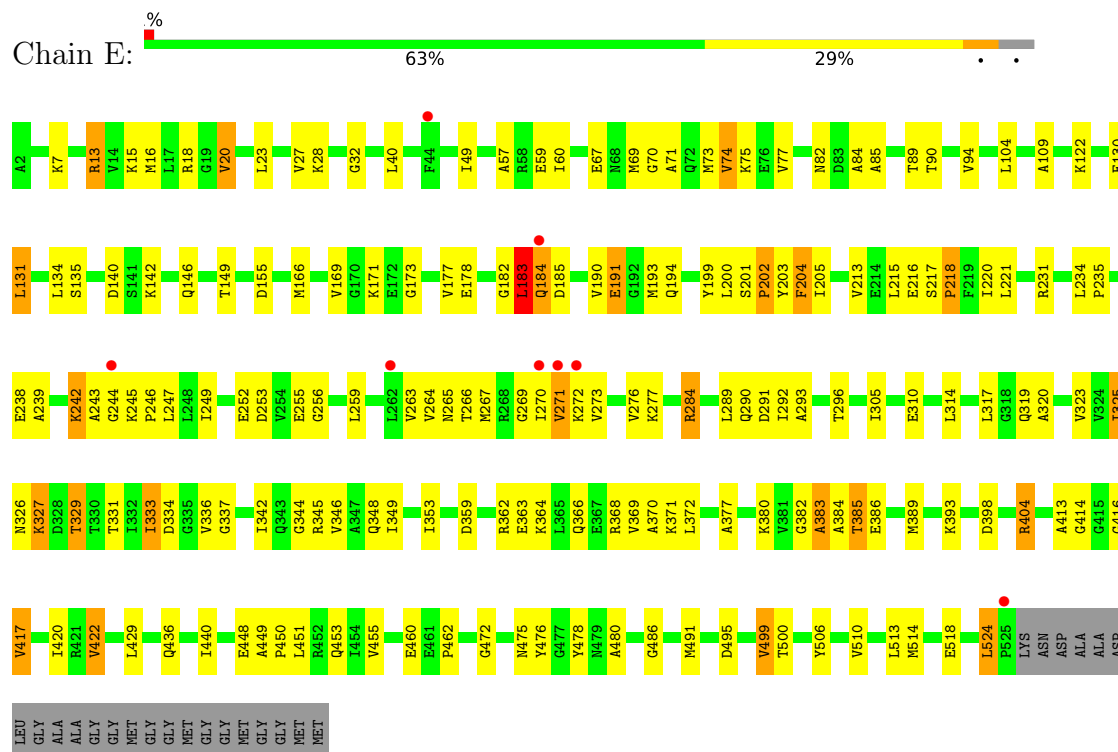


- Molecule 1: 60 kDa chaperonin

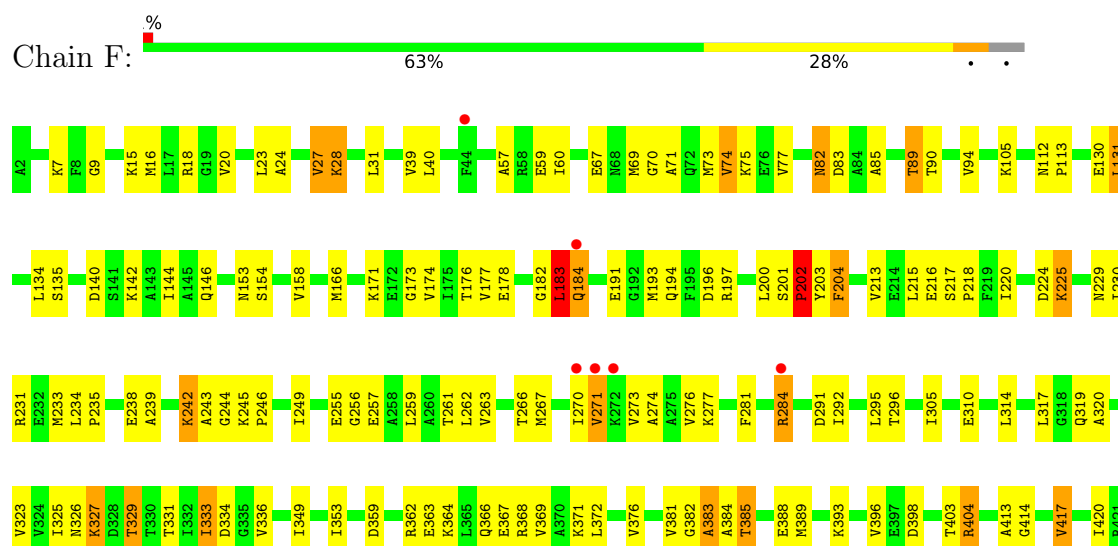


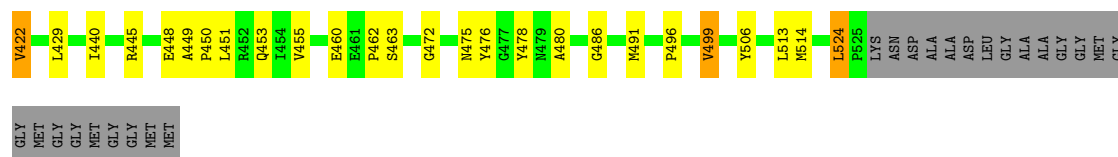


• Molecule 1: 60 kDa chaperonin

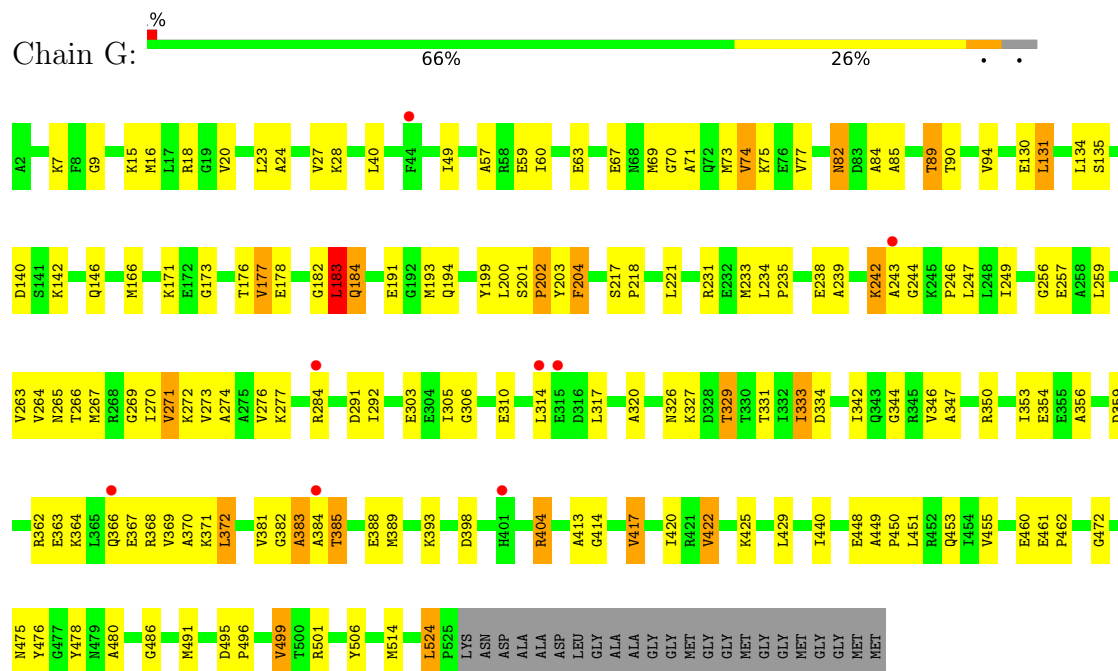


• Molecule 1: 60 kDa chaperonin

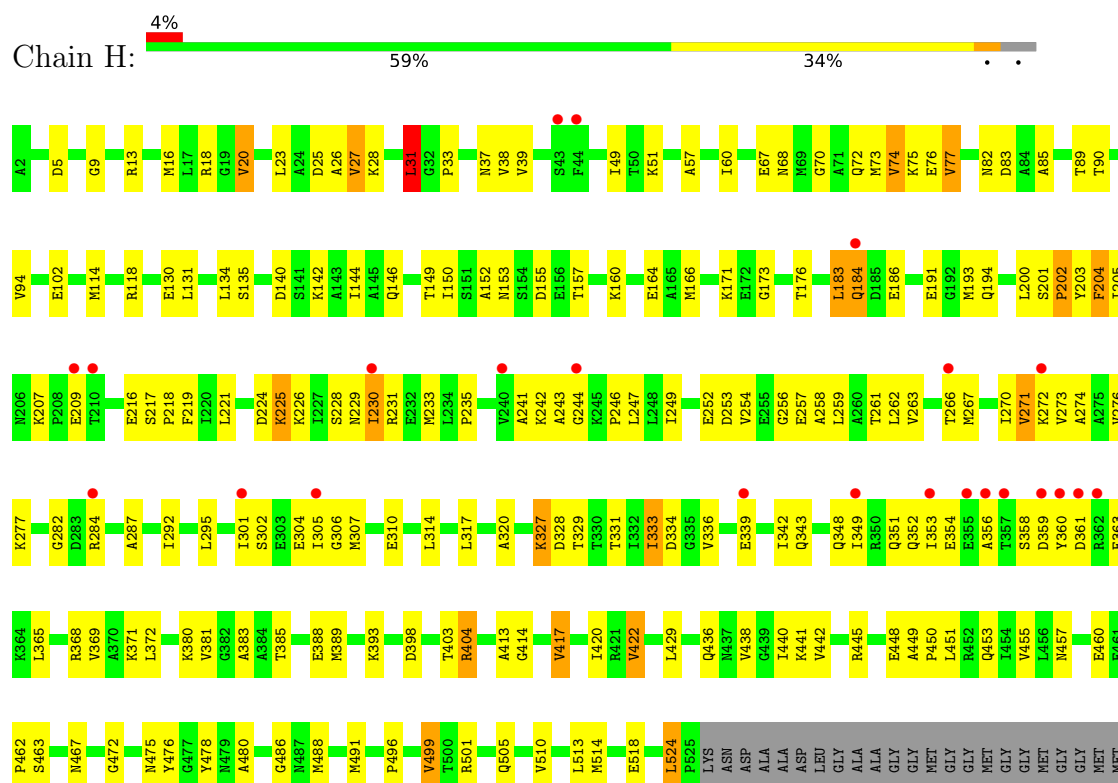




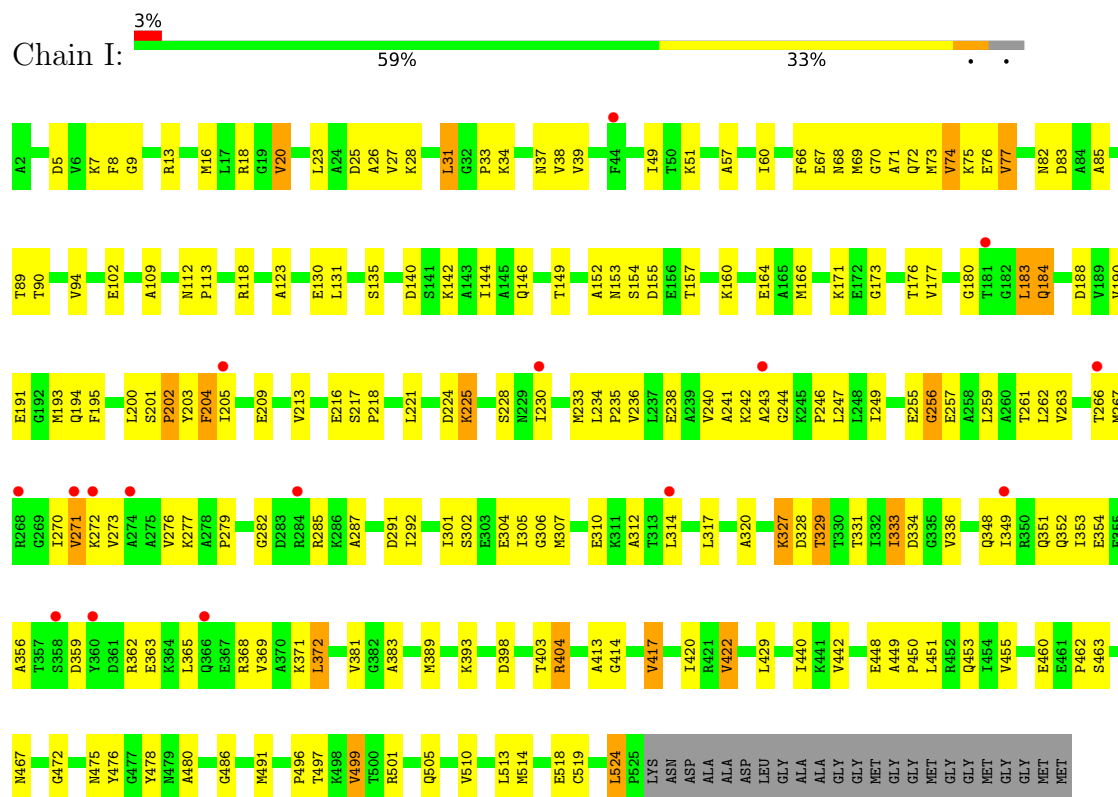
• Molecule 1: 60 kDa chaperonin



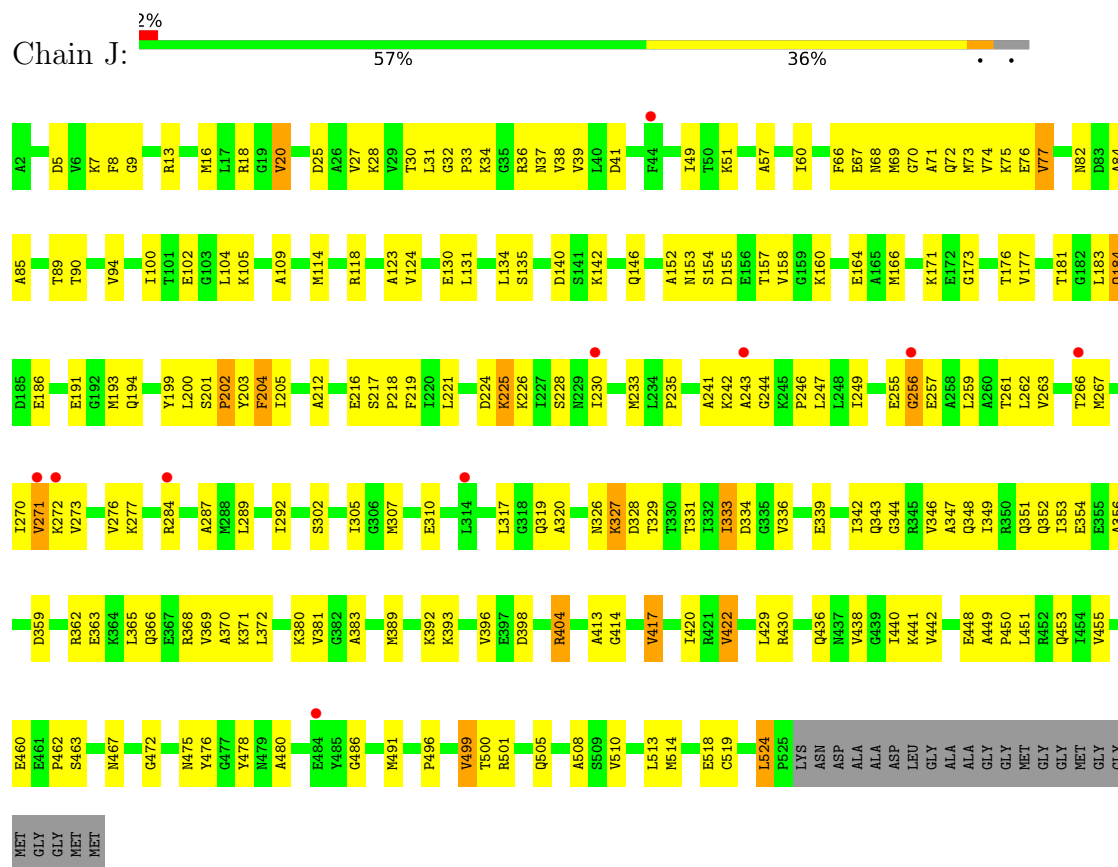
• Molecule 1: 60 kDa chaperonin



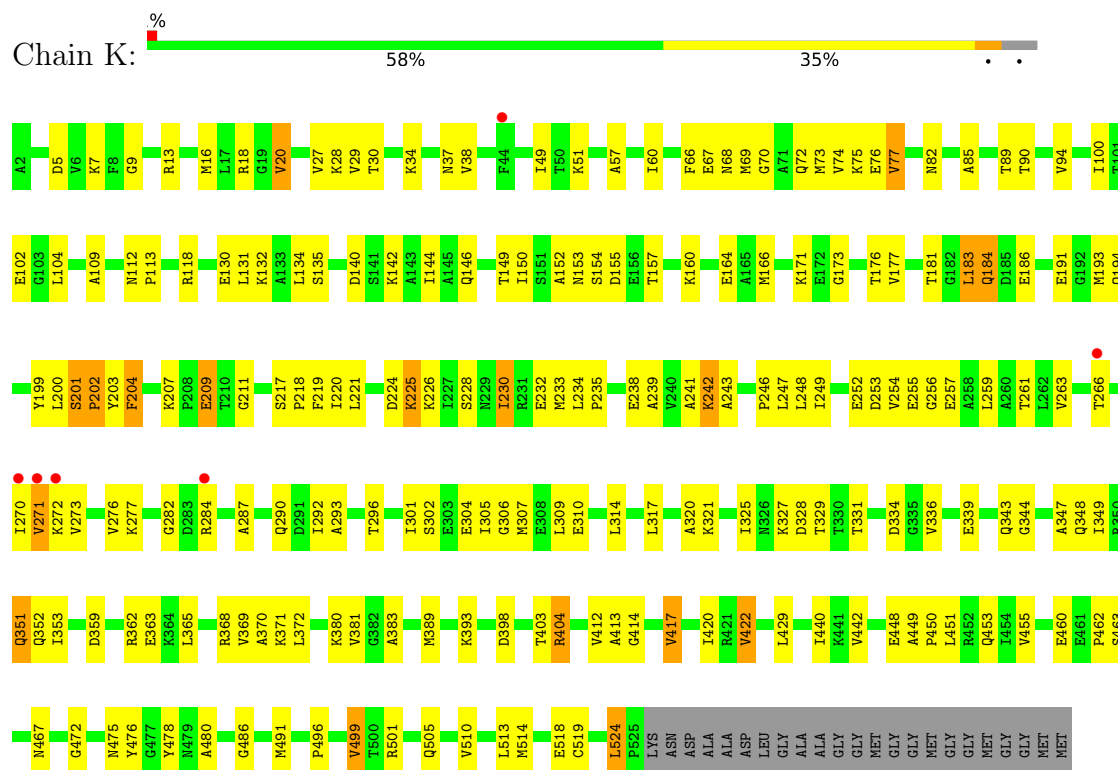
- Molecule 1: 60 kDa chaperonin



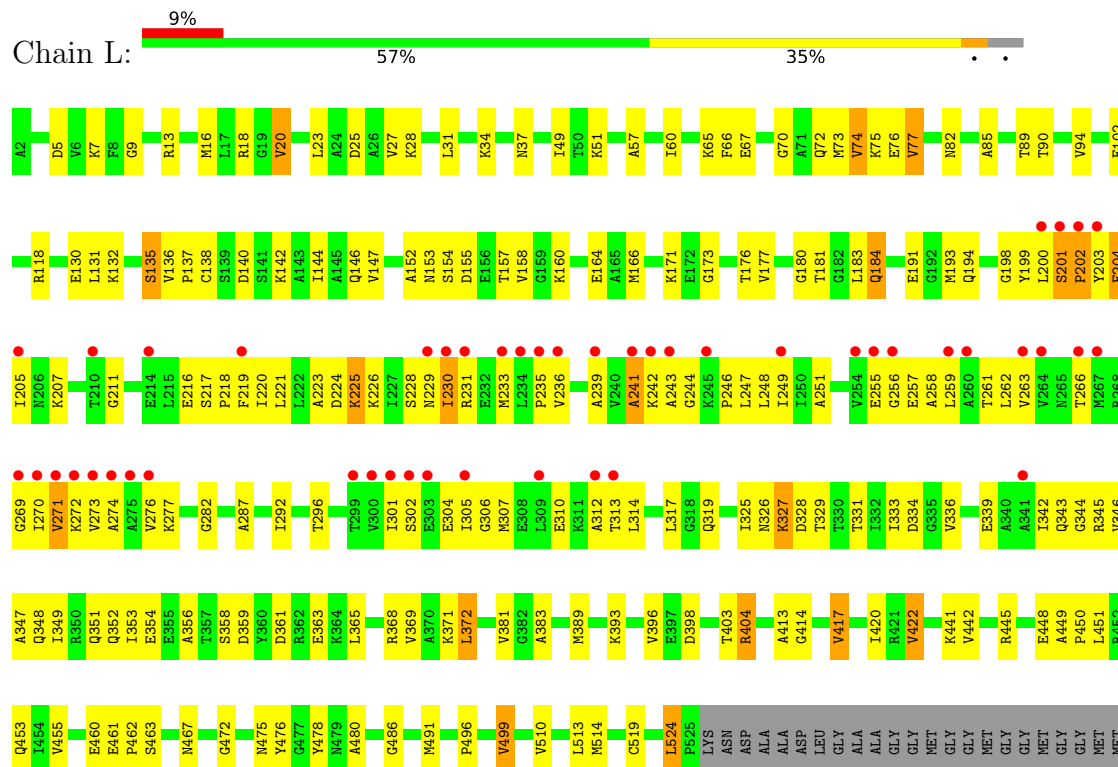
- Molecule 1: 60 kDa chaperonin

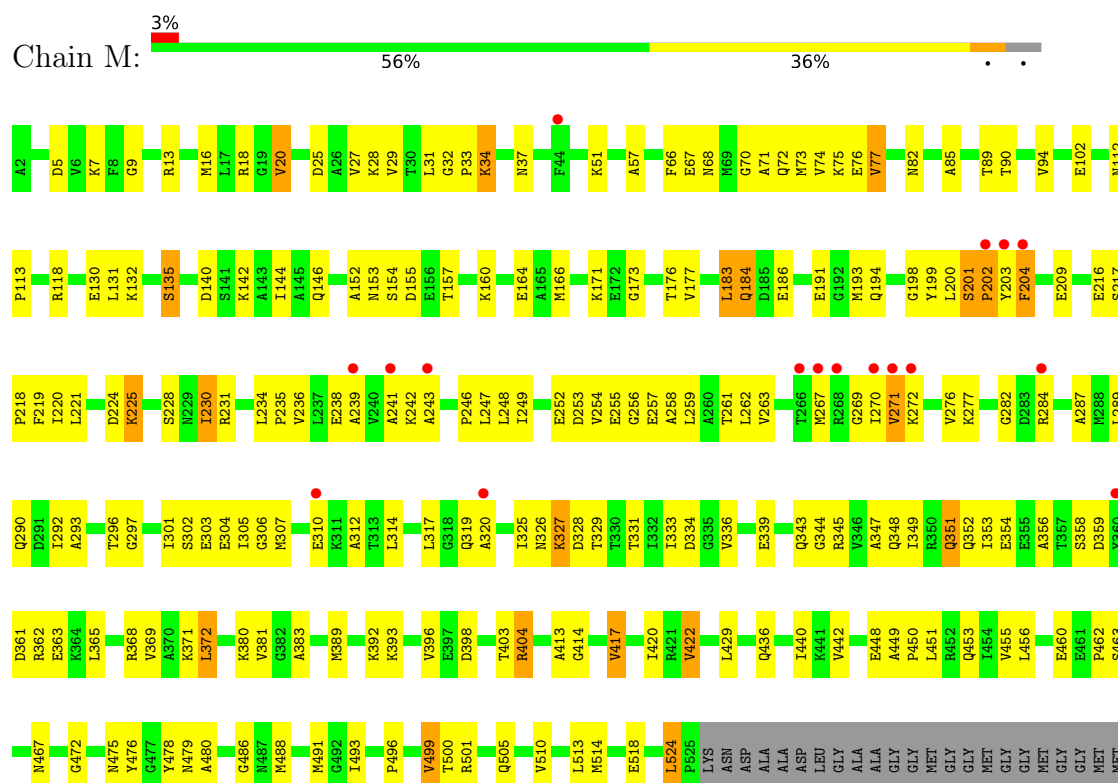


- Molecule 1: 60 kDa chaperonin

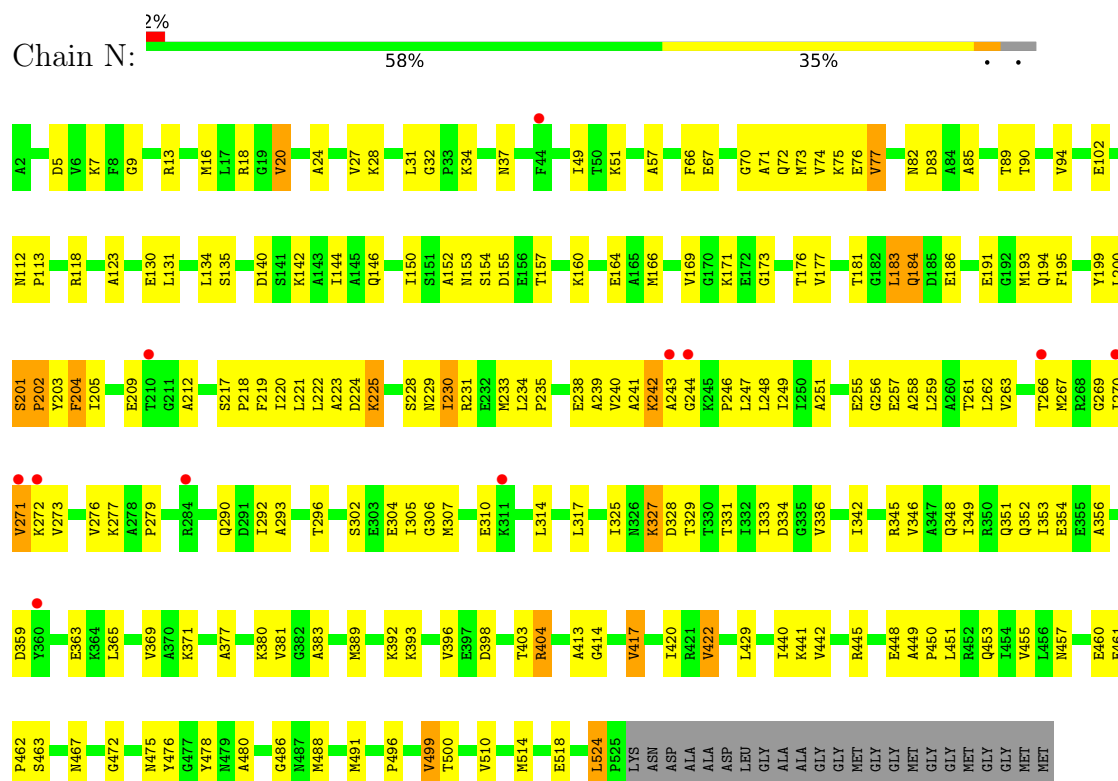


- Molecule 1: 60 kDa chaperonin





• Molecule 1: 60 kDa chaperonin



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	262.80Å 283.60Å 135.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.71 – 2.92 33.71 – 2.92	Depositor EDS
% Data completeness (in resolution range)	83.8 (33.71-2.92) 83.9 (33.71-2.92)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.43 (at 2.90Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.203 , 0.235 0.202 , 0.232	Depositor DCC
R_{free} test set	18290 reflections (9.93%)	wwPDB-VP
Wilson B-factor (Å ²)	53.1	Xtriage
Anisotropy	0.625	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 40.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	55301	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.30% 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

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

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	0.53	0/3883	0.98	14/5243 (0.3%)
1	B	0.52	0/3883	0.94	9/5243 (0.2%)
1	C	0.49	0/3883	0.97	10/5243 (0.2%)
1	D	0.54	0/3883	0.98	11/5243 (0.2%)
1	E	0.50	0/3883	0.98	17/5243 (0.3%)
1	F	0.51	0/3883	0.96	13/5243 (0.2%)
1	G	0.53	0/3883	0.97	9/5243 (0.2%)
1	H	0.49	0/3883	0.95	14/5243 (0.3%)
1	I	0.50	0/3883	0.94	9/5243 (0.2%)
1	J	0.48	0/3883	0.94	12/5243 (0.2%)
1	K	0.47	0/3883	0.94	6/5243 (0.1%)
1	L	0.48	0/3883	0.94	9/5243 (0.2%)
1	M	0.47	0/3883	0.94	9/5243 (0.2%)
1	N	0.47	0/3883	0.94	8/5243 (0.2%)
All	All	0.50	0/54362	0.96	150/73402 (0.2%)

There are no bond length outliers.

All (150) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	31	LEU	N-CA-C	9.65	122.80	111.02
1	H	33	PRO	N-CA-C	-8.98	103.12	114.35
1	F	242	LYS	N-CA-C	-8.33	99.78	110.53
1	G	242	LYS	N-CA-C	-8.15	100.08	110.19
1	C	242	LYS	N-CA-C	-7.95	100.33	110.19
1	D	242	LYS	N-CA-C	-7.94	100.35	110.19
1	A	242	LYS	N-CA-C	-7.44	100.97	110.19
1	E	242	LYS	N-CA-C	-7.30	101.14	110.19
1	D	327	LYS	N-CA-C	-7.15	103.53	111.82
1	B	242	LYS	N-CA-C	-7.04	101.75	110.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	13	ARG	NE-CZ-NH2	-6.93	112.97	119.20
1	G	327	LYS	N-CA-C	-6.90	104.34	112.89
1	M	327	LYS	N-CA-C	-6.87	103.58	112.23
1	H	13	ARG	NE-CZ-NH2	-6.86	113.03	119.20
1	B	204	PHE	N-CA-C	-6.84	104.19	112.54
1	D	31	LEU	N-CA-C	6.83	125.34	110.80
1	L	241	ALA	N-CA-C	-6.82	103.91	111.82
1	N	327	LYS	N-CA-C	-6.82	103.91	111.82
1	C	327	LYS	N-CA-C	-6.75	104.00	111.82
1	A	327	LYS	N-CA-C	-6.64	104.66	112.89
1	F	327	LYS	N-CA-C	-6.63	103.88	112.23
1	K	204	PHE	N-CA-C	-6.60	105.09	113.01
1	I	33	PRO	N-CA-C	-6.59	105.62	113.86
1	B	327	LYS	N-CA-C	-6.59	104.17	111.82
1	I	327	LYS	N-CA-C	-6.59	104.18	111.82
1	A	13	ARG	NE-CZ-NH2	-6.55	113.31	119.20
1	H	327	LYS	N-CA-C	-6.48	104.30	111.82
1	E	204	PHE	N-CA-C	-6.47	104.48	112.38
1	K	255	GLU	N-CA-C	6.47	120.16	110.14
1	N	31	LEU	N-CA-C	6.44	119.32	110.24
1	E	327	LYS	N-CA-C	-6.35	104.45	111.82
1	J	327	LYS	N-CA-C	-6.33	104.25	112.23
1	E	191	GLU	N-CA-C	-6.30	100.84	110.30
1	N	135	SER	N-CA-C	6.29	119.36	110.23
1	I	31	LEU	N-CA-C	6.28	124.17	110.80
1	L	13	ARG	NE-CZ-NH2	-6.25	113.58	119.20
1	M	241	ALA	N-CA-C	-6.19	104.61	111.36
1	K	327	LYS	N-CA-C	-6.18	104.65	111.82
1	J	241	ALA	N-CA-C	-6.16	104.68	111.82
1	M	33	PRO	N-CA-C	-6.13	106.85	114.20
1	I	204	PHE	N-CA-C	-6.12	105.67	113.01
1	A	60	ILE	N-CA-C	6.11	117.58	108.54
1	G	204	PHE	N-CA-C	-6.09	104.95	112.38
1	E	60	ILE	N-CA-C	6.07	117.53	108.54
1	I	60	ILE	N-CA-C	6.07	116.85	108.84
1	H	13	ARG	CD-NE-CZ	6.07	132.89	124.40
1	F	204	PHE	N-CA-C	-6.06	104.99	112.38
1	J	255	GLU	N-CA-C	6.06	119.53	110.14
1	J	33	PRO	N-CA-C	-6.00	106.36	113.86
1	J	60	ILE	N-CA-C	6.00	116.76	108.84
1	E	135	SER	N-CA-C	6.00	119.06	110.24
1	L	13	ARG	CD-NE-CZ	5.95	132.72	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	60	ILE	N-CA-C	5.89	117.26	108.54
1	D	204	PHE	N-CA-C	-5.89	105.19	112.38
1	H	31	LEU	N-CA-C	5.88	123.33	110.80
1	F	60	ILE	N-CA-C	5.88	117.24	108.54
1	A	204	PHE	N-CA-C	-5.86	105.23	112.38
1	E	32	GLY	CA-C-N	5.84	125.54	119.64
1	E	32	GLY	C-N-CA	5.84	125.54	119.64
1	N	204	PHE	N-CA-C	-5.83	105.87	112.87
1	D	255	GLU	N-CA-C	5.79	118.66	110.14
1	J	32	GLY	N-CA-C	5.79	118.95	112.00
1	C	333	ILE	N-CA-C	5.75	116.38	107.99
1	I	241	ALA	N-CA-C	-5.74	105.10	111.36
1	D	135	SER	N-CA-C	5.74	118.68	110.24
1	M	255	GLU	N-CA-C	5.73	119.06	109.95
1	G	495	ASP	CA-C-N	-5.73	113.64	119.83
1	G	495	ASP	C-N-CA	-5.73	113.64	119.83
1	F	135	SER	N-CA-C	5.72	118.53	110.23
1	C	204	PHE	N-CA-C	-5.72	105.41	112.38
1	D	27	VAL	N-CA-C	5.70	117.22	111.00
1	C	255	GLU	N-CA-C	5.70	118.52	110.14
1	B	255	GLU	N-CA-C	5.67	118.48	110.14
1	D	33	PRO	N-CA-C	-5.66	107.28	114.35
1	L	255	GLU	N-CA-C	5.65	118.90	110.14
1	K	241	ALA	N-CA-C	-5.63	105.23	111.71
1	A	219	PHE	N-CA-C	-5.63	101.69	110.42
1	E	325	ILE	N-CA-C	5.61	115.94	107.75
1	G	135	SER	N-CA-C	5.61	118.36	110.23
1	H	27	VAL	N-CA-C	5.59	116.24	110.82
1	A	135	SER	N-CA-C	5.58	118.42	110.10
1	C	135	SER	N-CA-C	5.58	118.33	110.23
1	F	196	ASP	N-CA-C	5.57	118.25	109.39
1	F	255	GLU	N-CA-C	5.57	118.33	110.14
1	A	255	GLU	N-CA-C	5.57	118.32	110.14
1	A	345	ARG	N-CA-C	-5.55	105.14	111.14
1	M	135	SER	N-CA-C	5.53	118.25	110.23
1	E	13	ARG	NE-CZ-NH1	5.53	127.03	121.50
1	C	252	GLU	N-CA-C	-5.51	105.38	111.71
1	H	241	ALA	N-CA-C	-5.50	105.43	111.82
1	C	241	ALA	N-CA-C	-5.48	105.21	111.07
1	H	60	ILE	N-CA-C	5.47	116.06	108.84
1	E	13	ARG	CD-NE-CZ	5.46	132.05	124.40
1	J	333	ILE	N-CA-C	5.43	115.68	107.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	28	LYS	N-CA-C	5.43	119.01	112.38
1	K	60	ILE	N-CA-C	5.42	116.00	108.84
1	G	60	ILE	N-CA-C	5.42	116.56	108.54
1	H	13	ARG	NE-CZ-NH1	5.41	126.91	121.50
1	E	333	ILE	N-CA-C	5.39	115.62	107.80
1	M	204	PHE	N-CA-C	-5.39	105.81	112.38
1	A	84	ALA	N-CA-C	5.38	116.95	111.14
1	L	327	LYS	N-CA-C	-5.38	105.57	111.82
1	L	13	ARG	NE-CZ-NH1	5.38	126.88	121.50
1	F	325	ILE	N-CA-C	5.38	115.60	107.75
1	N	255	GLU	N-CA-C	5.32	118.39	110.14
1	B	333	ILE	N-CA-C	5.31	115.50	107.80
1	L	135	SER	N-CA-C	5.31	117.93	110.23
1	L	60	ILE	N-CA-C	5.30	116.38	108.54
1	D	60	ILE	N-CA-C	5.30	116.38	108.54
1	H	333	ILE	N-CA-C	5.29	115.39	107.51
1	J	84	ALA	N-CA-C	5.29	117.12	111.36
1	L	204	PHE	N-CA-C	-5.28	105.94	112.38
1	I	255	GLU	N-CA-C	5.27	117.89	110.14
1	M	333	ILE	N-CA-C	5.26	115.43	107.80
1	F	202	PRO	N-CA-C	-5.26	101.64	112.47
1	C	325	ILE	N-CA-C	5.25	115.46	108.11
1	G	84	ALA	N-CA-C	5.24	116.80	111.14
1	K	242	LYS	N-CA-C	-5.23	102.74	110.48
1	I	333	ILE	N-CA-C	5.21	115.35	107.80
1	B	135	SER	N-CA-C	5.20	117.78	110.23
1	M	34	LYS	N-CA-C	-5.20	106.24	112.59
1	E	495	ASP	CA-C-N	-5.19	114.45	119.90
1	E	495	ASP	C-N-CA	-5.19	114.45	119.90
1	E	84	ALA	N-CA-C	5.18	116.74	111.14
1	J	204	PHE	N-CA-C	-5.16	106.68	112.87
1	E	255	GLU	N-CA-C	5.15	117.70	109.81
1	N	242	LYS	N-CA-C	-5.14	102.15	110.32
1	B	139	SER	N-CA-C	5.13	119.29	112.72
1	A	13	ARG	NE-CZ-NH1	5.13	126.63	121.50
1	I	135	SER	N-CA-C	5.13	117.66	110.23
1	D	374	GLY	N-CA-C	5.12	118.44	112.50
1	B	60	ILE	N-CA-C	5.12	116.11	108.54
1	G	333	ILE	N-CA-C	5.11	115.21	107.80
1	H	204	PHE	N-CA-C	-5.09	106.76	112.87
1	N	32	GLY	CA-C-N	5.09	124.58	119.19
1	N	32	GLY	C-N-CA	5.09	124.58	119.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	135	SER	N-CA-C	5.08	117.60	110.23
1	F	27	VAL	N-CA-C	5.08	116.53	111.00
1	F	28	LYS	N-CA-C	5.08	118.57	112.38
1	A	13	ARG	CD-NE-CZ	5.07	131.50	124.40
1	A	27	VAL	N-CA-C	5.07	116.52	111.00
1	H	207	LYS	CA-C-N	5.04	125.32	119.47
1	H	207	LYS	C-N-CA	5.04	125.32	119.47
1	J	105	LYS	N-CA-C	-5.04	105.68	111.07
1	F	31	LEU	N-CA-C	5.04	117.53	110.23
1	J	135	SER	N-CA-C	5.03	117.52	110.23
1	A	13	ARG	N-CA-C	5.02	116.75	111.28
1	F	333	ILE	N-CA-C	5.02	115.32	107.99
1	M	31	LEU	N-CA-C	5.02	121.50	110.80
1	D	84	ALA	N-CA-C	5.01	116.55	111.14

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3855	0	3976	133	0
1	B	3855	0	3976	155	0
1	C	3855	0	3976	165	0
1	D	3855	0	3976	139	0
1	E	3855	0	3976	151	0
1	F	3855	0	3976	141	0
1	G	3855	0	3976	126	0
1	H	3855	0	3976	170	0
1	I	3855	0	3976	172	0
1	J	3855	0	3976	166	0
1	K	3855	0	3976	166	0
1	L	3855	0	3976	178	0
1	M	3855	0	3976	189	0
1	N	3855	0	3976	188	0
2	A	20	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	25	0	0	2	0
2	C	20	0	0	0	0
2	D	25	0	0	0	0
2	E	10	0	0	0	0
2	F	10	0	0	1	0
2	G	15	0	0	0	0
2	H	15	0	0	0	0
2	I	10	0	0	0	0
2	J	20	0	0	0	0
2	K	10	0	0	0	0
2	L	10	0	0	0	0
2	M	15	0	0	0	0
2	N	10	0	0	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
3	K	1	0	0	0	0
3	L	1	0	0	0	0
3	M	1	0	0	0	0
3	N	1	0	0	0	0
4	A	16	0	28	0	0
4	B	32	0	56	2	0
4	C	8	0	14	2	0
4	D	8	0	14	0	0
4	E	40	0	70	1	0
4	F	24	0	42	1	0
4	G	16	0	28	1	0
4	H	16	0	28	2	0
4	I	24	0	42	0	0
4	J	8	0	14	0	0
4	K	16	0	28	2	0
4	L	8	0	14	0	0
4	M	8	0	14	3	0
4	N	24	0	42	9	0
5	E	7	0	10	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	60	0	0	1	0
6	B	76	0	0	4	0
6	C	55	0	0	2	0
6	D	79	0	0	5	0
6	E	64	0	0	1	0
6	F	65	0	0	1	0
6	G	84	0	0	2	0
6	H	61	0	0	3	0
6	I	63	0	0	2	0
6	J	45	0	0	6	0
6	K	52	0	0	3	0
6	L	32	0	0	1	0
6	M	49	0	0	3	0
6	N	62	0	0	1	0
All	All	55301	0	56108	2133	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 19.

All (2133) 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:B:270:ILE:HG23	1:C:231:ARG:HH12	1.20	1.03
1:B:329:THR:HG22	6:B:3165:HOH:O	1.60	1.01
1:I:193:MET:HE1	1:I:292:ILE:HG12	1.45	0.99
1:K:193:MET:HE1	1:K:292:ILE:HG12	1.45	0.99
1:D:242:LYS:HG2	1:E:231:ARG:NH2	1.78	0.97
1:B:326:ASN:HD22	1:B:329:THR:HB	1.31	0.94
1:K:272:LYS:NZ	1:L:229:ASN:HD21	1.65	0.94
1:E:270:ILE:HG23	1:F:231:ARG:HH12	1.33	0.93
1:M:235:PRO:HG3	1:M:310:GLU:HA	1.51	0.92
1:C:176:THR:HG21	1:C:333:ILE:HD13	1.49	0.92
1:C:193:MET:HE1	1:C:292:ILE:HG12	1.52	0.90
1:D:193:MET:HE1	1:D:292:ILE:HG12	1.53	0.90
1:H:235:PRO:HG3	1:H:310:GLU:HA	1.53	0.89
1:M:193:MET:HE1	1:M:292:ILE:HG12	1.55	0.88
1:K:272:LYS:HZ3	1:L:229:ASN:HD21	1.21	0.88
1:L:193:MET:HE1	1:L:292:ILE:HG12	1.57	0.87
1:E:270:ILE:HG23	1:F:231:ARG:NH1	1.88	0.87
1:K:235:PRO:HG3	1:K:310:GLU:HA	1.56	0.87
1:J:235:PRO:HG3	1:J:310:GLU:HA	1.57	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:235:PRO:HG3	1:L:310:GLU:HA	1.56	0.86
1:B:331:THR:HG22	6:B:3165:HOH:O	1.77	0.84
1:I:183:LEU:O	1:I:184:GLN:HB2	1.77	0.83
1:M:290:GLN:HG3	6:M:3113:HOH:O	1.77	0.83
1:N:235:PRO:HG3	1:N:310:GLU:HA	1.60	0.82
1:M:85:ALA:HB1	1:M:499:VAL:HG12	1.61	0.82
1:J:183:LEU:O	1:J:184:GLN:HB2	1.80	0.82
1:G:176:THR:HG21	1:G:333:ILE:HD13	1.60	0.81
1:K:183:LEU:O	1:K:184:GLN:HB2	1.77	0.81
1:M:34:LYS:HE2	1:N:118:ARG:HH22	1.45	0.81
1:H:176:THR:HG21	1:H:333:ILE:HD13	1.61	0.81
1:J:193:MET:HE1	1:J:292:ILE:HG12	1.61	0.81
1:B:239:ALA:HB1	1:B:314:LEU:HG	1.63	0.81
1:J:85:ALA:HB1	1:J:499:VAL:HG12	1.62	0.80
1:B:270:ILE:HG23	1:C:231:ARG:NH1	1.97	0.80
1:H:183:LEU:O	1:H:184:GLN:HB2	1.82	0.80
1:C:239:ALA:HB1	1:C:314:LEU:HG	1.63	0.79
1:F:235:PRO:HG3	1:F:310:GLU:HA	1.64	0.79
1:G:235:PRO:HG3	1:G:310:GLU:HA	1.62	0.78
1:M:183:LEU:O	1:M:184:GLN:HB2	1.81	0.78
1:M:272:LYS:NZ	1:N:229:ASN:ND2	2.30	0.78
1:N:183:LEU:O	1:N:184:GLN:HB2	1.82	0.78
1:G:27:VAL:HG12	1:G:90:THR:HG23	1.66	0.78
1:L:85:ALA:HB1	1:L:499:VAL:HG12	1.63	0.78
1:H:85:ALA:HB1	1:H:499:VAL:HG12	1.64	0.78
1:L:183:LEU:O	1:L:184:GLN:HB2	1.82	0.78
1:I:235:PRO:HG3	1:I:310:GLU:HA	1.64	0.78
1:A:184:GLN:H	1:A:382:GLY:HA3	1.49	0.78
1:I:85:ALA:HB1	1:I:499:VAL:HG12	1.63	0.78
1:N:85:ALA:HB1	1:N:499:VAL:HG12	1.66	0.77
1:N:193:MET:HE1	1:N:292:ILE:HG12	1.66	0.77
1:C:235:PRO:HG3	1:C:310:GLU:HA	1.65	0.77
1:L:272:LYS:NZ	1:M:228:SER:HB3	2.00	0.77
1:K:200:LEU:HD21	1:K:277:LYS:HG3	1.65	0.77
1:J:218:PRO:HB3	1:J:246:PRO:HG2	1.67	0.77
1:E:200:LEU:HD21	1:E:277:LYS:HG3	1.67	0.76
1:L:228:SER:O	1:L:257:GLU:HB3	1.84	0.76
1:E:27:VAL:HG12	1:E:90:THR:HG23	1.66	0.76
1:K:85:ALA:HB1	1:K:499:VAL:HG12	1.66	0.76
1:J:413:ALA:HB2	1:J:475:ASN:HD22	1.51	0.76
1:D:184:GLN:H	1:D:382:GLY:HA3	1.51	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:184:GLN:H	1:E:382:GLY:HA3	1.50	0.75
1:J:200:LEU:HD21	1:J:277:LYS:HG3	1.68	0.75
1:E:16:MET:SD	1:E:73:MET:HE1	2.26	0.75
1:F:404:ARG:HG2	1:F:404:ARG:HH11	1.50	0.75
1:F:16:MET:SD	1:F:73:MET:HE1	2.26	0.75
1:N:445:ARG:HH22	4:N:1515:MPD:H12	1.51	0.75
1:M:218:PRO:HB3	1:M:246:PRO:HG2	1.68	0.74
1:N:200:LEU:HD21	1:N:277:LYS:HG3	1.67	0.74
1:B:184:GLN:H	1:B:382:GLY:HA3	1.52	0.74
1:A:193:MET:HE1	1:A:292:ILE:HG12	1.70	0.74
1:C:404:ARG:HG2	1:C:404:ARG:HH11	1.52	0.74
1:J:183:LEU:HD13	1:J:184:GLN:HG3	1.69	0.74
1:H:183:LEU:HD13	1:H:184:GLN:HG3	1.68	0.74
1:L:176:THR:HG21	1:L:333:ILE:HD13	1.69	0.74
1:F:176:THR:HG21	1:F:333:ILE:HD13	1.70	0.74
1:G:200:LEU:HD21	1:G:277:LYS:HG3	1.70	0.74
1:G:234:LEU:O	1:G:238:GLU:HG3	1.88	0.74
1:I:183:LEU:HD13	1:I:184:GLN:HG3	1.70	0.74
1:G:359:ASP:O	1:G:363:GLU:HG3	1.88	0.74
1:M:413:ALA:H	1:M:475:ASN:ND2	1.86	0.74
1:H:404:ARG:HG2	1:H:404:ARG:HH11	1.51	0.73
1:C:326:ASN:HD22	1:C:329:THR:HB	1.53	0.73
1:E:314:LEU:HD23	1:E:317:LEU:HD22	1.70	0.73
1:F:57:ALA:O	1:F:75:LYS:HE3	1.87	0.73
1:D:359:ASP:O	1:D:363:GLU:HG3	1.89	0.73
1:F:184:GLN:H	1:F:382:GLY:HA3	1.53	0.73
1:A:230:ILE:HD13	1:A:261:THR:HG21	1.69	0.73
1:B:16:MET:SD	1:B:73:MET:HE1	2.29	0.73
1:F:27:VAL:HG12	1:F:90:THR:HG23	1.69	0.73
1:G:183:LEU:O	1:G:183:LEU:HD13	1.88	0.73
1:C:118:ARG:NH2	6:C:3133:HOH:O	2.21	0.73
1:C:242:LYS:C	1:C:244:GLY:H	1.97	0.73
1:L:413:ALA:HB2	1:L:475:ASN:HD22	1.54	0.73
1:F:326:ASN:HD22	1:F:329:THR:HB	1.54	0.73
1:H:193:MET:HE1	1:H:292:ILE:HG12	1.70	0.73
1:L:218:PRO:HB3	1:L:246:PRO:HG2	1.71	0.73
1:K:413:ALA:HB2	1:K:475:ASN:HD22	1.54	0.72
1:E:131:LEU:HD13	1:E:422:VAL:HG21	1.70	0.72
1:J:404:ARG:HG2	1:J:404:ARG:HH11	1.54	0.72
1:N:445:ARG:HH22	4:N:1515:MPD:C1	2.02	0.72
1:B:218:PRO:HB3	1:B:246:PRO:HG2	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:183:LEU:HD13	1:N:184:GLN:HG3	1.70	0.72
1:K:272:LYS:NZ	1:L:229:ASN:ND2	2.37	0.72
1:K:302:SER:H	1:K:307:MET:HE3	1.54	0.72
1:C:27:VAL:HG12	1:C:90:THR:HG23	1.71	0.72
1:J:284:ARG:NH2	6:J:3072:HOH:O	2.23	0.72
1:B:272:LYS:NZ	1:C:229:ASN:HD22	1.88	0.71
1:L:219:PHE:HB3	1:L:317:LEU:HD23	1.71	0.71
1:N:176:THR:HG21	1:N:333:ILE:HD13	1.72	0.71
1:E:235:PRO:HG3	1:E:310:GLU:HA	1.72	0.71
1:H:413:ALA:HB2	1:H:475:ASN:HD22	1.55	0.71
1:A:449:ALA:HB3	1:A:450:PRO:HD3	1.71	0.71
1:C:16:MET:SD	1:C:73:MET:HE1	2.31	0.71
1:L:404:ARG:HG2	1:L:404:ARG:HH11	1.54	0.71
1:A:183:LEU:O	1:A:183:LEU:HD13	1.89	0.71
1:H:247:LEU:HD21	1:H:249:ILE:HD11	1.71	0.71
1:J:224:ASP:O	1:J:225:LYS:HB3	1.90	0.71
1:C:184:GLN:H	1:C:382:GLY:HA3	1.56	0.71
1:E:239:ALA:HB1	1:E:314:LEU:HG	1.72	0.71
1:F:105:LYS:HA	4:F:1522:MPD:HM2	1.73	0.71
1:A:200:LEU:HD21	1:A:277:LYS:HG3	1.71	0.71
1:I:359:ASP:O	1:I:363:GLU:HG2	1.89	0.71
1:I:131:LEU:HD13	1:I:422:VAL:HG21	1.72	0.71
1:M:228:SER:O	1:M:257:GLU:HB3	1.91	0.71
1:G:57:ALA:O	1:G:75:LYS:HE3	1.91	0.71
1:G:184:GLN:H	1:G:382:GLY:HA3	1.56	0.71
1:J:160:LYS:O	1:J:164:GLU:HG3	1.91	0.71
1:K:228:SER:O	1:K:257:GLU:HB3	1.91	0.71
1:N:359:ASP:O	1:N:363:GLU:HG2	1.91	0.70
1:A:235:PRO:HG3	1:A:310:GLU:HA	1.71	0.70
1:G:16:MET:SD	1:G:73:MET:HE1	2.31	0.70
1:H:200:LEU:HD21	1:H:277:LYS:HG3	1.71	0.70
1:B:27:VAL:HG12	1:B:90:THR:HG23	1.72	0.70
1:J:348:GLN:O	1:J:352:GLN:HG2	1.92	0.70
1:K:420:ILE:HG13	1:K:448:GLU:HG2	1.72	0.70
1:G:420:ILE:HG13	1:G:448:GLU:HG2	1.74	0.70
1:H:449:ALA:HB3	1:H:450:PRO:HD3	1.74	0.70
1:G:291:ASP:OD2	1:G:368:ARG:HD2	1.91	0.70
1:F:242:LYS:HG2	1:G:231:ARG:NH2	2.07	0.70
1:G:239:ALA:HB1	1:G:314:LEU:HG	1.73	0.70
1:I:404:ARG:HG2	1:I:404:ARG:HH11	1.55	0.70
1:D:27:VAL:HG12	1:D:90:THR:HG23	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:420:ILE:HG13	1:N:448:GLU:HG2	1.74	0.70
1:D:176:THR:HG21	1:D:333:ILE:HD13	1.73	0.69
1:B:291:ASP:OD2	1:B:368:ARG:HD2	1.92	0.69
1:B:362:ARG:HG2	1:B:366:GLN:NE2	2.07	0.69
1:K:219:PHE:HB3	1:K:317:LEU:HD23	1.72	0.69
1:M:131:LEU:HD13	1:M:422:VAL:HG21	1.74	0.69
1:A:27:VAL:HG12	1:A:90:THR:HG23	1.74	0.69
1:K:348:GLN:O	1:K:352:GLN:HG2	1.92	0.69
1:A:420:ILE:HG13	1:A:448:GLU:HG2	1.72	0.69
1:N:131:LEU:HD13	1:N:422:VAL:HG21	1.75	0.69
1:N:193:MET:HG3	1:N:371:LYS:HB3	1.73	0.69
1:N:413:ALA:HB2	1:N:475:ASN:HD22	1.56	0.69
1:D:200:LEU:HD21	1:D:277:LYS:HG3	1.74	0.69
1:E:404:ARG:HG2	1:E:404:ARG:HH11	1.58	0.69
1:K:183:LEU:HD13	1:K:184:GLN:HG3	1.75	0.69
1:M:183:LEU:HD13	1:M:184:GLN:HG3	1.73	0.69
1:M:413:ALA:HB2	1:M:475:ASN:HD22	1.56	0.69
1:B:385:THR:H	1:C:281:PHE:HE1	1.38	0.69
1:I:413:ALA:H	1:I:475:ASN:ND2	1.89	0.69
1:C:183:LEU:HD13	1:C:183:LEU:O	1.93	0.69
1:F:404:ARG:HG2	1:F:404:ARG:NH1	2.07	0.69
1:F:420:ILE:HG13	1:F:448:GLU:HG2	1.74	0.69
1:G:242:LYS:C	1:G:244:GLY:H	2.01	0.69
1:D:183:LEU:O	1:D:183:LEU:HD13	1.92	0.69
1:L:27:VAL:HG12	1:L:90:THR:HG23	1.74	0.69
1:L:302:SER:H	1:L:307:MET:HE3	1.58	0.69
1:I:193:MET:HE1	1:I:292:ILE:CG1	2.22	0.69
1:M:29:VAL:HG12	4:M:1518:MPD:H12	1.75	0.69
1:D:242:LYS:C	1:D:244:GLY:H	2.00	0.68
1:K:404:ARG:HG2	1:K:404:ARG:HH11	1.59	0.68
1:M:270:ILE:HG23	1:N:231:ARG:NH1	2.07	0.68
1:M:272:LYS:NZ	1:N:229:ASN:HD22	1.89	0.68
1:C:383:ALA:O	1:C:384:ALA:HB3	1.93	0.68
1:F:384:ALA:O	1:F:385:THR:HG23	1.93	0.68
1:I:176:THR:HG21	1:I:333:ILE:HD13	1.74	0.68
1:H:420:ILE:HG13	1:H:448:GLU:HG2	1.76	0.68
1:L:287:ALA:HB1	1:L:368:ARG:NH1	2.08	0.68
1:A:242:LYS:C	1:A:244:GLY:H	2.01	0.68
1:E:57:ALA:O	1:E:75:LYS:HE3	1.93	0.68
1:I:218:PRO:HB3	1:I:246:PRO:HG2	1.75	0.68
1:B:272:LYS:NZ	1:C:229:ASN:ND2	2.41	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:404:ARG:HG2	1:N:404:ARG:HH11	1.59	0.68
1:H:404:ARG:HG2	1:H:404:ARG:NH1	2.08	0.68
1:H:413:ALA:H	1:H:475:ASN:ND2	1.91	0.68
1:I:413:ALA:HB2	1:I:475:ASN:HD22	1.59	0.68
1:J:176:THR:HG21	1:J:333:ILE:HD13	1.74	0.68
1:L:413:ALA:H	1:L:475:ASN:ND2	1.92	0.68
1:E:269:GLY:HA2	1:E:272:LYS:HZ2	1.57	0.68
1:I:420:ILE:HG13	1:I:448:GLU:HG2	1.76	0.68
1:J:202:PRO:O	1:J:203:TYR:HB2	1.93	0.68
1:J:359:ASP:O	1:J:363:GLU:HG2	1.94	0.68
1:K:413:ALA:H	1:K:475:ASN:ND2	1.91	0.68
1:N:83:ASP:OD2	1:N:327:LYS:HD2	1.93	0.68
1:B:420:ILE:HG13	1:B:448:GLU:HG2	1.75	0.68
1:M:200:LEU:HD21	1:M:277:LYS:HG3	1.76	0.68
1:B:359:ASP:HA	1:B:362:ARG:NH1	2.09	0.68
1:K:455:VAL:HG13	1:K:460:GLU:HB2	1.76	0.68
1:B:193:MET:HE1	1:B:292:ILE:HG12	1.74	0.67
1:D:57:ALA:O	1:D:75:LYS:HE3	1.94	0.67
1:E:291:ASP:OD2	1:E:368:ARG:HD2	1.93	0.67
1:N:413:ALA:H	1:N:475:ASN:ND2	1.92	0.67
1:D:326:ASN:HD22	1:D:329:THR:HB	1.59	0.67
1:J:455:VAL:HG13	1:J:460:GLU:HB2	1.76	0.67
1:M:420:ILE:HG13	1:M:448:GLU:HG2	1.76	0.67
1:E:420:ILE:HG13	1:E:448:GLU:HG2	1.76	0.67
1:L:200:LEU:HD21	1:L:277:LYS:HG3	1.74	0.67
1:N:218:PRO:HB3	1:N:246:PRO:HG2	1.77	0.67
1:D:239:ALA:HB1	1:D:314:LEU:HG	1.76	0.67
1:E:242:LYS:C	1:E:244:GLY:H	2.03	0.67
1:F:202:PRO:O	1:F:203:TYR:HB2	1.93	0.67
1:J:352:GLN:HB2	1:J:365:LEU:HD13	1.77	0.67
1:M:70:GLY:HA2	1:M:73:MET:HE3	1.77	0.67
1:M:142:LYS:O	1:M:146:GLN:HG3	1.94	0.67
1:M:269:GLY:HA3	1:N:229:ASN:CG	2.20	0.67
1:D:235:PRO:HG3	1:D:310:GLU:HA	1.76	0.67
1:I:70:GLY:HA2	1:I:73:MET:HE3	1.76	0.67
1:B:183:LEU:O	1:B:183:LEU:HD13	1.94	0.67
1:F:193:MET:HE1	1:F:292:ILE:HG12	1.77	0.67
1:I:202:PRO:O	1:I:203:TYR:HB2	1.95	0.67
1:L:221:LEU:HD23	1:L:249:ILE:HD12	1.77	0.67
1:E:69:MET:O	1:E:73:MET:HG3	1.95	0.67
1:J:420:ILE:HG13	1:J:448:GLU:HG2	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:224:ASP:O	1:N:225:LYS:HB3	1.94	0.67
1:B:404:ARG:HG2	1:B:404:ARG:HH11	1.58	0.67
1:C:219:PHE:O	1:C:247:LEU:HD12	1.95	0.67
1:M:272:LYS:HZ2	1:N:229:ASN:ND2	1.92	0.66
1:N:455:VAL:HG13	1:N:460:GLU:HB2	1.76	0.66
1:A:326:ASN:HD22	1:A:329:THR:HB	1.59	0.66
1:C:69:MET:O	1:C:73:MET:HG3	1.94	0.66
1:C:404:ARG:HG2	1:C:404:ARG:NH1	2.09	0.66
1:J:131:LEU:HD13	1:J:422:VAL:HG21	1.77	0.66
1:H:131:LEU:HD13	1:H:422:VAL:HG21	1.77	0.66
1:K:218:PRO:HB3	1:K:246:PRO:HG2	1.77	0.66
1:D:132:LYS:HE2	6:D:3055:HOH:O	1.95	0.66
1:E:193:MET:HE1	1:E:292:ILE:HG12	1.77	0.66
1:G:69:MET:O	1:G:73:MET:HG3	1.96	0.66
1:A:16:MET:SD	1:A:73:MET:HE1	2.35	0.66
1:D:234:LEU:O	1:D:238:GLU:HG3	1.96	0.66
1:H:202:PRO:O	1:H:203:TYR:HB2	1.94	0.66
1:A:247:LEU:HD21	1:A:249:ILE:HD11	1.77	0.66
1:B:202:PRO:O	1:B:204:PHE:N	2.28	0.66
1:E:142:LYS:O	1:E:146:GLN:HG3	1.95	0.66
1:F:291:ASP:OD2	1:F:368:ARG:HD2	1.96	0.66
1:H:194:GLN:O	1:H:371:LYS:HE3	1.95	0.66
1:H:348:GLN:O	1:H:352:GLN:HG2	1.95	0.66
1:I:5:ASP:HB2	1:I:524:LEU:HD12	1.77	0.66
1:K:359:ASP:O	1:K:363:GLU:HG2	1.96	0.66
1:L:224:ASP:O	1:L:225:LYS:HB3	1.95	0.66
1:M:348:GLN:O	1:M:352:GLN:HG2	1.96	0.66
1:D:420:ILE:HG13	1:D:448:GLU:HG2	1.77	0.66
1:G:404:ARG:HG2	1:G:404:ARG:HH11	1.60	0.66
1:K:284:ARG:NH2	6:K:3052:HOH:O	2.27	0.66
1:D:414:GLY:O	1:D:417:VAL:HG13	1.94	0.66
1:I:270:ILE:O	1:I:271:VAL:HB	1.95	0.66
1:L:230:ILE:HD13	1:L:261:THR:CG2	2.25	0.66
1:N:27:VAL:HG12	1:N:90:THR:HG23	1.78	0.66
1:D:16:MET:SD	1:D:73:MET:HE1	2.36	0.66
1:D:247:LEU:HD21	1:D:249:ILE:HD11	1.77	0.66
1:E:183:LEU:O	1:E:183:LEU:HD13	1.95	0.66
1:A:404:ARG:HG2	1:A:404:ARG:HH11	1.61	0.65
1:C:31:LEU:HD13	1:C:90:THR:HG21	1.78	0.65
1:F:130:GLU:HB3	1:F:422:VAL:HG22	1.78	0.65
1:B:314:LEU:HD23	1:B:317:LEU:HD22	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:291:ASP:OD2	1:D:368:ARG:HD2	1.96	0.65
1:F:183:LEU:HD13	1:F:183:LEU:O	1.95	0.65
1:N:194:GLN:O	1:N:371:LYS:HE3	1.96	0.65
1:B:272:LYS:HZ2	1:C:229:ASN:ND2	1.93	0.65
1:C:27:VAL:CG1	1:C:90:THR:HG23	2.26	0.65
1:C:420:ILE:HG13	1:C:448:GLU:HG2	1.79	0.65
1:E:218:PRO:HB3	1:E:246:PRO:HG2	1.77	0.65
1:H:455:VAL:HG13	1:H:460:GLU:HB2	1.78	0.65
1:I:200:LEU:HD21	1:I:277:LYS:HG3	1.77	0.65
1:L:455:VAL:HG13	1:L:460:GLU:HB2	1.78	0.65
1:A:142:LYS:O	1:A:146:GLN:HG3	1.97	0.65
1:N:142:LYS:O	1:N:146:GLN:HG3	1.97	0.65
1:N:414:GLY:O	1:N:417:VAL:HG13	1.96	0.65
1:F:234:LEU:O	1:F:238:GLU:HG3	1.96	0.65
1:J:27:VAL:HG12	1:J:90:THR:HG23	1.78	0.65
1:L:131:LEU:HD13	1:L:422:VAL:HG21	1.78	0.65
1:I:455:VAL:HG13	1:I:460:GLU:HB2	1.78	0.65
1:A:131:LEU:HD13	1:A:422:VAL:HG21	1.78	0.65
1:E:183:LEU:HB2	1:E:384:ALA:HB2	1.78	0.65
1:E:247:LEU:HD21	1:E:249:ILE:HD11	1.77	0.65
1:E:326:ASN:HD22	1:E:329:THR:HB	1.61	0.65
1:K:224:ASP:O	1:K:225:LYS:HB3	1.95	0.65
1:L:449:ALA:HB3	1:L:450:PRO:HD3	1.79	0.65
1:M:27:VAL:HG12	1:M:90:THR:HG23	1.79	0.65
1:D:142:LYS:O	1:D:146:GLN:HG3	1.97	0.64
1:I:449:ALA:HB3	1:I:450:PRO:HD3	1.79	0.64
1:M:193:MET:HG2	1:M:194:GLN:N	2.12	0.64
1:M:455:VAL:HG13	1:M:460:GLU:HB2	1.79	0.64
1:D:384:ALA:O	1:D:385:THR:HG23	1.98	0.64
1:G:131:LEU:HD13	1:G:422:VAL:HG21	1.80	0.64
1:I:142:LYS:O	1:I:146:GLN:HG3	1.97	0.64
1:K:70:GLY:HA2	1:K:73:MET:HE3	1.79	0.64
1:K:414:GLY:O	1:K:417:VAL:HG13	1.97	0.64
1:J:413:ALA:H	1:J:475:ASN:ND2	1.94	0.64
1:L:404:ARG:HG2	1:L:404:ARG:NH1	2.11	0.64
1:L:420:ILE:HG13	1:L:448:GLU:HG2	1.78	0.64
1:C:193:MET:HE1	1:C:292:ILE:CG1	2.25	0.64
1:K:272:LYS:HZ3	1:L:229:ASN:ND2	1.93	0.64
1:B:384:ALA:O	1:B:385:THR:HG23	1.98	0.64
1:C:384:ALA:O	1:C:385:THR:HG23	1.97	0.64
1:I:414:GLY:O	1:I:417:VAL:HG13	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:29:VAL:HG12	4:K:1506:MPD:H12	1.79	0.64
1:L:5:ASP:HB2	1:L:524:LEU:HD12	1.80	0.64
1:E:359:ASP:HA	1:E:362:ARG:NH1	2.13	0.64
1:J:5:ASP:HB2	1:J:524:LEU:HD12	1.78	0.64
1:N:5:ASP:HB2	1:N:524:LEU:HD12	1.79	0.64
1:B:69:MET:O	1:B:73:MET:HG3	1.98	0.64
1:H:218:PRO:HB3	1:H:246:PRO:HG2	1.80	0.64
1:H:284:ARG:NH2	6:H:3055:HOH:O	2.30	0.64
1:B:449:ALA:HB3	1:B:450:PRO:HD3	1.79	0.64
1:C:57:ALA:O	1:C:75:LYS:HE3	1.98	0.64
1:H:160:LYS:O	1:H:164:GLU:HG3	1.98	0.64
1:H:414:GLY:O	1:H:417:VAL:HG13	1.97	0.64
1:C:131:LEU:HD13	1:C:422:VAL:HG21	1.78	0.64
1:E:234:LEU:O	1:E:238:GLU:HG3	1.97	0.64
1:G:449:ALA:HB3	1:G:450:PRO:HD3	1.80	0.64
1:I:233:MET:HE1	1:I:249:ILE:HD12	1.78	0.64
1:J:414:GLY:O	1:J:417:VAL:HG13	1.97	0.64
1:D:233:MET:HE1	1:D:249:ILE:HD12	1.79	0.64
1:M:5:ASP:HB2	1:M:524:LEU:HD12	1.79	0.64
1:A:359:ASP:O	1:A:363:GLU:HG3	1.98	0.63
1:E:193:MET:HG3	1:E:371:LYS:HB3	1.81	0.63
1:K:34:LYS:HE2	1:L:118:ARG:HH22	1.63	0.63
1:L:348:GLN:O	1:L:352:GLN:HG2	1.98	0.63
1:H:5:ASP:HB2	1:H:524:LEU:HD12	1.80	0.63
1:A:13:ARG:NH2	1:A:518:GLU:OE2	2.30	0.63
1:A:239:ALA:HB1	1:A:314:LEU:HG	1.81	0.63
1:B:142:LYS:O	1:B:146:GLN:HG3	1.99	0.63
1:B:414:GLY:O	1:B:417:VAL:HG13	1.97	0.63
1:D:173:GLY:O	1:D:404:ARG:NH2	2.31	0.63
1:K:5:ASP:HB2	1:K:524:LEU:HD12	1.78	0.63
1:N:445:ARG:HH12	4:N:1515:MPD:H31	1.62	0.63
1:B:234:LEU:O	1:B:238:GLU:HG3	1.99	0.63
1:J:449:ALA:HB3	1:J:450:PRO:HD3	1.81	0.63
1:L:142:LYS:O	1:L:146:GLN:HG3	1.99	0.63
1:A:57:ALA:O	1:A:75:LYS:HE3	1.99	0.63
1:A:451:LEU:C	1:A:451:LEU:HD23	2.24	0.63
1:A:513:LEU:HD13	1:G:49:ILE:HD12	1.80	0.63
1:D:28:LYS:HD2	1:D:453:GLN:OE1	1.99	0.63
1:L:181:THR:O	1:M:282:GLY:HA3	1.98	0.63
1:M:414:GLY:O	1:M:417:VAL:HG13	1.99	0.63
1:B:57:ALA:O	1:B:75:LYS:HE3	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:326:ASN:ND2	1:B:329:THR:HB	2.11	0.63
1:B:404:ARG:HG2	1:B:404:ARG:NH1	2.13	0.63
1:M:224:ASP:O	1:M:225:LYS:HB3	1.99	0.63
1:M:270:ILE:HA	1:N:231:ARG:NH1	2.14	0.63
1:N:228:SER:O	1:N:257:GLU:HB3	1.99	0.63
1:F:239:ALA:HB1	1:F:314:LEU:HG	1.79	0.63
1:F:383:ALA:O	1:F:384:ALA:HB3	1.99	0.63
1:H:287:ALA:HB1	1:H:368:ARG:NH1	2.14	0.63
1:J:142:LYS:O	1:J:146:GLN:HG3	1.98	0.62
1:B:295:LEU:HA	1:B:342:ILE:HD11	1.81	0.62
1:H:242:LYS:O	1:H:243:ALA:HB3	2.00	0.62
1:M:230:ILE:HD13	1:M:261:THR:CG2	2.29	0.62
1:D:131:LEU:HD13	1:D:422:VAL:HG21	1.81	0.62
1:D:404:ARG:HH11	1:D:404:ARG:HG2	1.63	0.62
1:N:449:ALA:HB3	1:N:450:PRO:HD3	1.81	0.62
1:H:359:ASP:O	1:H:363:GLU:HG2	2.00	0.62
1:K:449:ALA:HB3	1:K:450:PRO:HD3	1.80	0.62
1:C:174:VAL:HG12	1:C:376:VAL:HG13	1.81	0.62
1:E:269:GLY:HA3	1:F:229:ASN:CG	2.23	0.62
1:H:70:GLY:HA2	1:H:73:MET:HE3	1.79	0.62
1:K:142:LYS:O	1:K:146:GLN:HG3	1.99	0.62
1:M:16:MET:SD	1:M:73:MET:HE1	2.40	0.62
1:N:70:GLY:HA2	1:N:73:MET:HE3	1.80	0.62
1:F:200:LEU:HD21	1:F:277:LYS:HG3	1.82	0.62
1:H:27:VAL:HG12	1:H:90:THR:HG23	1.82	0.62
1:I:27:VAL:HG12	1:I:90:THR:HG23	1.81	0.62
1:J:194:GLN:O	1:J:371:LYS:HE3	1.99	0.62
1:K:131:LEU:HD13	1:K:422:VAL:HG21	1.82	0.62
1:F:142:LYS:O	1:F:146:GLN:HG3	1.98	0.62
1:J:242:LYS:O	1:J:243:ALA:HB3	2.00	0.62
1:E:384:ALA:O	1:E:385:THR:HG23	2.00	0.62
1:L:183:LEU:HD13	1:L:184:GLN:HG3	1.81	0.62
1:N:404:ARG:HG2	1:N:404:ARG:NH1	2.14	0.62
1:H:230:ILE:HD13	1:H:261:THR:CG2	2.30	0.62
1:I:404:ARG:HG2	1:I:404:ARG:NH1	2.13	0.62
1:N:27:VAL:CG1	1:N:90:THR:HG23	2.30	0.62
1:K:404:ARG:HG2	1:K:404:ARG:NH1	2.15	0.61
1:L:230:ILE:HG21	1:L:261:THR:HG21	1.81	0.61
1:A:69:MET:O	1:A:73:MET:HG3	2.01	0.61
1:A:404:ARG:HG2	1:A:404:ARG:NH1	2.15	0.61
1:D:383:ALA:O	1:D:384:ALA:HB3	1.98	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:27:VAL:CG1	1:F:90:THR:HG23	2.30	0.61
1:G:414:GLY:O	1:G:417:VAL:HG13	1.99	0.61
1:F:183:LEU:HB2	1:F:384:ALA:HB2	1.82	0.61
1:A:314:LEU:HD23	1:A:317:LEU:HD22	1.83	0.61
1:B:183:LEU:HB2	1:B:384:ALA:HB2	1.82	0.61
1:C:142:LYS:O	1:C:146:GLN:HG3	2.00	0.61
1:E:359:ASP:O	1:E:363:GLU:HG3	2.00	0.61
1:J:27:VAL:CG1	1:J:90:THR:HG23	2.30	0.61
1:L:70:GLY:HA2	1:L:73:MET:HE3	1.82	0.61
1:M:352:GLN:HB2	1:M:365:LEU:HD13	1.82	0.61
1:M:359:ASP:O	1:M:363:GLU:HG2	2.00	0.61
1:G:221:LEU:HD23	1:G:249:ILE:HD12	1.82	0.61
1:M:160:LYS:O	1:M:164:GLU:HG3	2.00	0.61
1:M:404:ARG:HG2	1:M:404:ARG:HH11	1.64	0.61
1:C:234:LEU:O	1:C:238:GLU:HG3	1.99	0.61
1:E:13:ARG:NH2	1:E:518:GLU:OE2	2.34	0.61
1:G:359:ASP:HA	1:G:362:ARG:NH1	2.16	0.61
1:A:27:VAL:CG1	1:A:90:THR:HG23	2.30	0.61
1:A:130:GLU:HB3	1:A:422:VAL:HG22	1.83	0.61
1:C:233:MET:HE1	1:C:249:ILE:HD12	1.82	0.61
1:L:16:MET:HB3	1:L:514:MET:HE3	1.82	0.61
1:J:404:ARG:HG2	1:J:404:ARG:NH1	2.11	0.61
1:L:359:ASP:O	1:L:363:GLU:HG2	2.01	0.61
1:C:414:GLY:O	1:C:417:VAL:HG13	2.01	0.60
1:E:130:GLU:HB3	1:E:422:VAL:HG22	1.83	0.60
1:I:28:LYS:HD2	1:I:453:GLN:OE1	2.00	0.60
1:A:414:GLY:O	1:A:417:VAL:HG13	2.02	0.60
1:F:359:ASP:O	1:F:363:GLU:HG3	2.01	0.60
1:G:404:ARG:HG2	1:G:404:ARG:NH1	2.15	0.60
1:I:224:ASP:O	1:I:225:LYS:HB3	2.01	0.60
1:B:235:PRO:HG3	1:B:310:GLU:HA	1.84	0.60
1:C:359:ASP:O	1:C:363:GLU:HG3	2.01	0.60
1:H:263:VAL:O	1:H:267:MET:HB2	2.01	0.60
1:H:496:PRO:HB2	1:H:499:VAL:HG13	1.83	0.60
1:L:269:GLY:HA3	1:M:257:GLU:HB2	1.81	0.60
1:E:70:GLY:HA2	1:E:73:MET:HE3	1.82	0.60
1:F:242:LYS:O	1:F:243:ALA:HB3	2.00	0.60
1:D:449:ALA:HB3	1:D:450:PRO:HD3	1.83	0.60
1:F:242:LYS:C	1:F:244:GLY:H	2.10	0.60
1:C:291:ASP:OD2	1:C:368:ARG:HD2	2.01	0.60
1:E:27:VAL:CG1	1:E:90:THR:HG23	2.29	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:449:ALA:HB3	1:E:450:PRO:HD3	1.83	0.60
1:N:348:GLN:O	1:N:352:GLN:HG2	2.01	0.60
1:F:414:GLY:O	1:F:417:VAL:HG13	2.01	0.60
1:H:27:VAL:CG1	1:H:90:THR:HG23	2.31	0.60
1:J:70:GLY:HA2	1:J:73:MET:HE3	1.82	0.60
1:D:404:ARG:HG2	1:D:404:ARG:NH1	2.16	0.60
1:G:384:ALA:O	1:G:385:THR:HG23	2.01	0.60
1:L:225:LYS:HD2	1:L:226:LYS:O	2.01	0.60
1:M:272:LYS:HZ2	1:N:229:ASN:HD22	1.49	0.60
1:D:193:MET:HE1	1:D:292:ILE:CG1	2.29	0.60
1:C:413:ALA:HB2	1:C:475:ASN:HD22	1.67	0.60
1:C:449:ALA:HB3	1:C:450:PRO:HD3	1.84	0.60
1:E:220:ILE:HD12	1:E:296:THR:HG21	1.84	0.60
1:M:242:LYS:O	1:M:243:ALA:HB3	2.02	0.60
1:A:173:GLY:O	1:A:404:ARG:NH2	2.34	0.59
1:B:451:LEU:HD23	1:B:451:LEU:C	2.27	0.59
1:E:191:GLU:O	1:E:334:ASP:HA	2.02	0.59
1:B:16:MET:HB3	1:B:514:MET:HE3	1.84	0.59
1:B:242:LYS:C	1:B:244:GLY:H	2.08	0.59
1:E:202:PRO:O	1:E:204:PHE:N	2.30	0.59
1:G:70:GLY:HA2	1:G:73:MET:HE3	1.83	0.59
1:F:131:LEU:HD13	1:F:422:VAL:HG21	1.84	0.59
1:F:359:ASP:HA	1:F:362:ARG:NH1	2.17	0.59
1:F:362:ARG:HG2	1:F:366:GLN:NE2	2.17	0.59
1:G:314:LEU:HD23	1:G:317:LEU:HD22	1.84	0.59
1:C:173:GLY:O	1:C:404:ARG:NH2	2.35	0.59
1:G:27:VAL:CG1	1:G:90:THR:HG23	2.32	0.59
1:G:451:LEU:HD23	1:G:451:LEU:C	2.27	0.59
1:J:181:THR:O	1:K:282:GLY:HA3	2.03	0.59
1:B:166:MET:HE2	1:B:171:LYS:HA	1.84	0.59
1:B:359:ASP:O	1:B:363:GLU:HG3	2.02	0.59
1:H:224:ASP:O	1:H:225:LYS:HB3	2.02	0.59
1:L:414:GLY:O	1:L:417:VAL:HG13	2.01	0.59
1:C:200:LEU:HD21	1:C:277:LYS:HG3	1.84	0.59
1:F:233:MET:HE1	1:F:249:ILE:HD12	1.84	0.59
1:I:352:GLN:HB2	1:I:365:LEU:HD13	1.84	0.59
1:L:272:LYS:HZ3	1:M:228:SER:HB3	1.67	0.59
1:C:202:PRO:O	1:C:203:TYR:HB2	2.02	0.59
1:E:218:PRO:HD2	1:E:320:ALA:O	2.03	0.59
1:F:455:VAL:HG13	1:F:460:GLU:HB2	1.84	0.59
1:G:455:VAL:HG13	1:G:460:GLU:HB2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:235:PRO:CG	1:L:310:GLU:HA	2.31	0.59
1:L:272:LYS:HZ1	1:M:228:SER:HB3	1.64	0.59
1:M:28:LYS:HD2	1:M:453:GLN:OE1	2.03	0.59
1:M:193:MET:HE1	1:M:292:ILE:CG1	2.30	0.59
1:B:319:GLN:O	1:B:336:VAL:HG23	2.02	0.59
1:E:221:LEU:HD23	1:E:249:ILE:HD12	1.84	0.59
1:J:228:SER:O	1:J:257:GLU:HB3	2.02	0.59
1:D:130:GLU:HB3	1:D:422:VAL:HG22	1.84	0.59
1:J:191:GLU:O	1:J:334:ASP:HA	2.03	0.59
1:H:142:LYS:O	1:H:146:GLN:HG3	2.03	0.58
1:J:472:GLY:HA3	1:J:476:TYR:CD2	2.38	0.58
1:K:242:LYS:O	1:K:243:ALA:HB3	2.02	0.58
1:M:272:LYS:HZ1	1:N:229:ASN:ND2	1.99	0.58
1:H:228:SER:O	1:H:257:GLU:HB3	2.02	0.58
1:I:193:MET:HG3	1:I:371:LYS:HB3	1.84	0.58
1:K:27:VAL:HG12	1:K:90:THR:HG23	1.84	0.58
1:L:27:VAL:CG1	1:L:90:THR:HG23	2.32	0.58
1:N:302:SER:H	1:N:307:MET:HE3	1.69	0.58
1:E:451:LEU:HD23	1:E:451:LEU:C	2.28	0.58
1:H:183:LEU:HD22	1:H:184:GLN:H	1.68	0.58
1:J:413:ALA:CB	1:J:475:ASN:HD22	2.16	0.58
1:M:270:ILE:HA	1:N:231:ARG:HH11	1.67	0.58
1:C:70:GLY:HA2	1:C:73:MET:HE3	1.86	0.58
1:C:455:VAL:HG13	1:C:460:GLU:HB2	1.84	0.58
1:E:319:GLN:O	1:E:336:VAL:HG23	2.03	0.58
1:E:404:ARG:HG2	1:E:404:ARG:NH1	2.15	0.58
1:G:183:LEU:HB2	1:G:384:ALA:HB2	1.85	0.58
1:H:270:ILE:O	1:H:271:VAL:HB	2.04	0.58
1:K:254:VAL:HG12	1:K:259:LEU:HB2	1.85	0.58
1:M:413:ALA:N	1:M:475:ASN:ND2	2.51	0.58
1:A:218:PRO:HD2	1:A:320:ALA:O	2.04	0.58
1:A:455:VAL:HG13	1:A:460:GLU:HB2	1.85	0.58
1:I:38:VAL:HG13	1:J:519:CYS:HB3	1.86	0.58
1:I:336:VAL:O	1:I:336:VAL:HG12	2.02	0.58
1:J:34:LYS:HE2	1:K:118:ARG:HH22	1.68	0.58
1:L:305:ILE:HB	1:L:307:MET:HE2	1.85	0.58
1:A:291:ASP:OD2	1:A:368:ARG:HD2	2.04	0.58
1:B:233:MET:HE1	1:B:249:ILE:HD12	1.86	0.58
1:D:230:ILE:HD13	1:D:261:THR:HG21	1.86	0.58
1:E:16:MET:HB3	1:E:514:MET:HE3	1.86	0.58
1:G:142:LYS:O	1:G:146:GLN:HG3	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:200:LEU:HG	1:L:276:VAL:HA	1.86	0.58
1:M:221:LEU:HD23	1:M:249:ILE:HD12	1.86	0.58
1:D:69:MET:O	1:D:73:MET:HG3	2.04	0.58
1:F:270:ILE:O	1:F:271:VAL:HB	2.04	0.58
1:I:242:LYS:O	1:I:243:ALA:HB3	2.01	0.58
1:J:221:LEU:HD23	1:J:249:ILE:HD12	1.85	0.58
1:K:140:ASP:OD2	1:K:142:LYS:HB3	2.03	0.58
1:M:449:ALA:HB3	1:M:450:PRO:HD3	1.86	0.58
1:A:230:ILE:HD13	1:A:261:THR:CG2	2.34	0.58
1:E:166:MET:HE2	1:E:171:LYS:HA	1.85	0.58
1:C:18:ARG:HG2	1:C:67:GLU:CD	2.29	0.58
1:C:290:GLN:HB3	1:C:345:ARG:NH2	2.19	0.58
1:M:383:ALA:HB3	1:M:389:MET:HB2	1.84	0.58
1:N:352:GLN:HB2	1:N:365:LEU:HD13	1.86	0.58
1:C:202:PRO:O	1:C:204:PHE:N	2.33	0.57
1:E:455:VAL:HG13	1:E:460:GLU:HB2	1.84	0.57
1:I:16:MET:HB3	1:I:514:MET:HE3	1.86	0.57
1:K:218:PRO:HD2	1:K:320:ALA:O	2.04	0.57
1:M:472:GLY:HA3	1:M:476:TYR:CD2	2.39	0.57
1:C:451:LEU:HD23	1:C:451:LEU:C	2.28	0.57
1:G:273:VAL:HG12	1:G:274:ALA:N	2.19	0.57
1:J:140:ASP:OD2	1:J:142:LYS:HB3	2.03	0.57
1:K:221:LEU:HD23	1:K:249:ILE:HD12	1.87	0.57
1:M:259:LEU:O	1:M:263:VAL:HG23	2.04	0.57
1:M:404:ARG:HG2	1:M:404:ARG:NH1	2.19	0.57
1:N:445:ARG:NH1	4:N:1515:MPD:H31	2.19	0.57
1:A:349:ILE:CG2	1:A:369:VAL:HG13	2.35	0.57
1:K:413:ALA:CB	1:K:475:ASN:HD22	2.18	0.57
1:C:413:ALA:H	1:C:475:ASN:ND2	2.02	0.57
1:F:69:MET:O	1:F:73:MET:HG3	2.05	0.57
1:G:201:SER:C	1:G:202:PRO:O	2.46	0.57
1:I:160:LYS:O	1:I:164:GLU:HG3	2.04	0.57
1:L:242:LYS:O	1:L:243:ALA:HB3	2.03	0.57
1:L:496:PRO:HB2	1:L:499:VAL:HG13	1.86	0.57
1:H:28:LYS:HD2	1:H:453:GLN:OE1	2.04	0.57
1:B:173:GLY:O	1:B:404:ARG:NH2	2.37	0.57
1:D:202:PRO:O	1:D:203:TYR:HB2	2.04	0.57
1:D:242:LYS:HG2	1:E:231:ARG:CZ	2.33	0.57
1:H:193:MET:HG3	1:H:371:LYS:HB3	1.87	0.57
1:I:348:GLN:O	1:I:352:GLN:HG2	2.05	0.57
1:K:202:PRO:O	1:K:204:PHE:N	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:130:GLU:HB3	1:C:422:VAL:HG22	1.85	0.57
1:H:310:GLU:N	1:H:310:GLU:OE1	2.38	0.57
1:J:270:ILE:O	1:J:271:VAL:HB	2.04	0.57
1:K:166:MET:HE2	1:K:171:LYS:HA	1.87	0.57
1:L:233:MET:HE1	1:L:249:ILE:CD1	2.35	0.57
1:M:16:MET:HB3	1:M:514:MET:HE3	1.85	0.57
1:N:413:ALA:N	1:N:475:ASN:ND2	2.53	0.57
1:A:384:ALA:O	1:A:385:THR:HG23	2.05	0.57
1:A:486:GLY:C	1:A:491:MET:HE2	2.30	0.57
1:B:455:VAL:HG13	1:B:460:GLU:HB2	1.87	0.57
1:G:173:GLY:O	1:G:404:ARG:NH2	2.38	0.57
1:G:359:ASP:HA	1:G:362:ARG:HH12	1.70	0.57
1:G:383:ALA:O	1:G:384:ALA:HB3	2.04	0.57
1:D:455:VAL:HG13	1:D:460:GLU:HB2	1.86	0.57
1:G:326:ASN:HD22	1:G:329:THR:HB	1.70	0.57
1:H:305:ILE:HG22	1:H:305:ILE:O	2.04	0.57
1:J:287:ALA:HB1	1:J:368:ARG:NH1	2.20	0.57
1:N:383:ALA:HB3	1:N:389:MET:HB2	1.87	0.57
1:A:234:LEU:O	1:A:238:GLU:HG3	2.04	0.56
1:A:383:ALA:O	1:A:384:ALA:HB3	2.05	0.56
1:B:413:ALA:HB2	1:B:475:ASN:HD22	1.69	0.56
1:C:270:ILE:O	1:C:271:VAL:HB	2.04	0.56
1:C:359:ASP:HA	1:C:362:ARG:NH1	2.20	0.56
1:G:425:LYS:NZ	6:G:3204:HOH:O	2.38	0.56
1:H:140:ASP:OD2	1:H:142:LYS:HB3	2.05	0.56
1:A:413:ALA:HB2	1:A:475:ASN:HD22	1.70	0.56
1:C:183:LEU:HB2	1:C:384:ALA:HB2	1.86	0.56
1:H:266:THR:HG21	1:H:273:VAL:HB	1.87	0.56
1:J:173:GLY:O	1:J:404:ARG:NH2	2.38	0.56
1:K:28:LYS:HD2	1:K:453:GLN:OE1	2.05	0.56
1:M:305:ILE:HB	1:M:307:MET:HE2	1.86	0.56
1:N:140:ASP:OD2	1:N:142:LYS:HB3	2.05	0.56
1:B:220:ILE:HD12	1:B:296:THR:HG21	1.87	0.56
1:B:359:ASP:HA	1:B:362:ARG:HH12	1.70	0.56
1:F:449:ALA:HB3	1:F:450:PRO:HD3	1.86	0.56
1:G:202:PRO:O	1:G:203:TYR:HB2	2.05	0.56
1:H:413:ALA:N	1:H:475:ASN:ND2	2.53	0.56
1:J:218:PRO:CB	1:J:246:PRO:HG2	2.35	0.56
1:J:225:LYS:HD2	1:J:226:LYS:O	2.06	0.56
1:L:72:GLN:OE1	1:L:75:LYS:HE3	2.05	0.56
1:L:155:ASP:OD1	1:L:157:THR:HB	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:202:PRO:O	1:M:203:TYR:HB2	2.04	0.56
1:N:230:ILE:HD13	1:N:261:THR:CG2	2.35	0.56
1:N:472:GLY:HA3	1:N:476:TYR:CD2	2.40	0.56
1:C:194:GLN:O	1:C:371:LYS:HE3	2.05	0.56
1:H:231:ARG:NH1	1:N:241:ALA:CB	2.69	0.56
1:I:27:VAL:CG1	1:I:90:THR:HG23	2.34	0.56
1:I:171:LYS:HG2	6:I:3095:HOH:O	2.04	0.56
1:B:200:LEU:HD21	1:B:277:LYS:HG3	1.86	0.56
1:I:173:GLY:O	1:I:404:ARG:NH2	2.39	0.56
1:I:193:MET:CE	1:I:292:ILE:HG12	2.29	0.56
1:M:413:ALA:CB	1:M:475:ASN:HD22	2.19	0.56
1:H:191:GLU:O	1:H:334:ASP:HA	2.05	0.56
1:B:140:ASP:OD2	1:B:142:LYS:HB3	2.05	0.56
1:G:270:ILE:O	1:G:271:VAL:HB	2.05	0.56
1:J:233:MET:HE1	1:J:249:ILE:HD12	1.88	0.56
1:A:359:ASP:HA	1:A:362:ARG:NH1	2.20	0.56
1:B:70:GLY:HA2	1:B:73:MET:HE3	1.86	0.56
1:D:27:VAL:CG1	1:D:90:THR:HG23	2.34	0.56
1:E:23:LEU:HD23	1:E:74:VAL:HG22	1.87	0.56
1:K:413:ALA:N	1:K:475:ASN:ND2	2.53	0.56
1:L:28:LYS:HD2	1:L:453:GLN:OE1	2.06	0.56
1:A:194:GLN:O	1:A:371:LYS:HE3	2.06	0.56
1:B:130:GLU:HB3	1:B:422:VAL:HG22	1.88	0.56
1:D:118:ARG:NH2	6:D:3039:HOH:O	2.38	0.56
1:M:230:ILE:HD13	1:M:261:THR:HG21	1.86	0.56
1:A:140:ASP:OD2	1:A:142:LYS:HB3	2.06	0.56
1:B:27:VAL:CG1	1:B:90:THR:HG23	2.36	0.56
1:H:225:LYS:HD2	1:H:226:LYS:O	2.06	0.56
1:I:383:ALA:HB3	1:I:389:MET:HB2	1.86	0.56
1:K:160:LYS:O	1:K:164:GLU:HG3	2.06	0.56
1:B:218:PRO:HD2	1:B:320:ALA:O	2.05	0.55
1:G:202:PRO:O	1:G:204:PHE:N	2.35	0.55
1:I:305:ILE:O	1:I:305:ILE:HG22	2.05	0.55
1:J:319:GLN:HB3	1:J:336:VAL:HG21	1.88	0.55
1:K:16:MET:HB3	1:K:514:MET:HE3	1.87	0.55
1:L:413:ALA:CB	1:L:475:ASN:HD22	2.19	0.55
1:C:140:ASP:OD2	1:C:142:LYS:HB3	2.06	0.55
1:E:109:ALA:HB2	1:I:109:ALA:HB2	1.89	0.55
1:G:23:LEU:HD23	1:G:74:VAL:HG22	1.87	0.55
1:A:259:LEU:O	1:A:263:VAL:HG23	2.05	0.55
1:D:416:GLY:HA2	6:D:3097:HOH:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:28:LYS:HD2	1:J:453:GLN:OE1	2.06	0.55
1:M:183:LEU:HD22	1:M:184:GLN:H	1.71	0.55
1:A:183:LEU:HB2	1:A:384:ALA:HB2	1.87	0.55
1:B:131:LEU:HD13	1:B:422:VAL:HG21	1.87	0.55
1:I:140:ASP:OD2	1:I:142:LYS:HB3	2.06	0.55
1:J:383:ALA:HB3	1:J:389:MET:HB2	1.88	0.55
1:B:201:SER:O	1:B:202:PRO:O	2.24	0.55
1:G:200:LEU:HG	1:G:276:VAL:HA	1.89	0.55
1:K:193:MET:HG3	1:K:371:LYS:HB3	1.89	0.55
1:K:220:ILE:HD12	1:K:296:THR:HG21	1.89	0.55
1:K:472:GLY:HA3	1:K:476:TYR:CD2	2.41	0.55
1:M:270:ILE:HG23	1:N:231:ARG:CZ	2.36	0.55
1:D:451:LEU:C	1:D:451:LEU:HD23	2.32	0.55
1:J:155:ASP:OD1	1:J:157:THR:HB	2.07	0.55
1:K:234:LEU:O	1:K:238:GLU:HG3	2.06	0.55
1:A:220:ILE:HD12	1:A:296:THR:HG21	1.88	0.55
1:D:183:LEU:HB2	1:D:384:ALA:HB2	1.89	0.55
1:D:242:LYS:O	1:D:244:GLY:N	2.35	0.55
1:H:83:ASP:OD2	1:H:327:LYS:HD3	2.06	0.55
1:J:230:ILE:HD13	1:J:261:THR:CG2	2.37	0.55
1:J:263:VAL:O	1:J:267:MET:HB2	2.07	0.55
1:N:242:LYS:O	1:N:243:ALA:HB3	2.07	0.55
1:C:16:MET:HB3	1:C:514:MET:HE3	1.88	0.55
1:D:23:LEU:HD23	1:D:74:VAL:HG22	1.89	0.55
1:E:385:THR:H	1:F:281:PHE:HE1	1.54	0.55
1:E:414:GLY:O	1:E:417:VAL:HG13	2.06	0.55
1:F:18:ARG:HG2	1:F:67:GLU:CD	2.32	0.55
1:H:228:SER:HB3	1:N:272:LYS:NZ	2.22	0.55
1:H:259:LEU:O	1:H:263:VAL:HG23	2.07	0.55
1:I:413:ALA:N	1:I:475:ASN:ND2	2.54	0.55
1:L:345:ARG:HA	1:L:348:GLN:HE21	1.72	0.55
1:L:352:GLN:HB2	1:L:365:LEU:HD13	1.89	0.55
1:M:27:VAL:CG1	1:M:90:THR:HG23	2.36	0.55
1:N:160:LYS:O	1:N:164:GLU:HG3	2.07	0.55
1:A:200:LEU:HG	1:A:276:VAL:HA	1.89	0.55
1:H:16:MET:HB3	1:H:514:MET:HE3	1.89	0.55
1:M:269:GLY:CA	1:N:229:ASN:CG	2.79	0.55
1:A:178:GLU:HA	1:A:393:LYS:HE2	1.89	0.55
1:A:413:ALA:H	1:A:475:ASN:ND2	2.05	0.55
1:B:193:MET:HG3	1:B:371:LYS:HB3	1.89	0.55
1:I:472:GLY:HA3	1:I:476:TYR:CD2	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:194:GLN:O	1:L:371:LYS:HE3	2.07	0.55
1:L:472:GLY:HA3	1:L:476:TYR:CD2	2.41	0.55
1:M:193:MET:CE	1:M:292:ILE:HG12	2.34	0.55
1:C:193:MET:CE	1:C:292:ILE:HG12	2.31	0.54
1:C:230:ILE:HD13	1:C:261:THR:HG21	1.89	0.54
1:E:18:ARG:HG2	1:E:67:GLU:CD	2.32	0.54
1:K:27:VAL:CG1	1:K:90:THR:HG23	2.37	0.54
1:K:349:ILE:HA	1:K:352:GLN:HG3	1.88	0.54
1:L:16:MET:SD	1:L:73:MET:HE1	2.47	0.54
1:C:362:ARG:HG2	1:C:366:GLN:NE2	2.23	0.54
1:G:263:VAL:O	1:G:267:MET:HB2	2.08	0.54
1:L:413:ALA:N	1:L:475:ASN:ND2	2.54	0.54
1:A:23:LEU:HD23	1:A:74:VAL:HG22	1.88	0.54
1:C:242:LYS:O	1:C:244:GLY:N	2.38	0.54
1:D:259:LEU:O	1:D:263:VAL:HG23	2.06	0.54
1:H:39:VAL:HG12	1:I:69:MET:HE2	1.89	0.54
1:H:302:SER:H	1:H:307:MET:HE3	1.73	0.54
1:M:235:PRO:CG	1:M:310:GLU:HA	2.32	0.54
1:M:239:ALA:HB1	1:M:314:LEU:HG	1.89	0.54
1:A:16:MET:HB3	1:A:514:MET:HE3	1.90	0.54
1:B:242:LYS:O	1:B:243:ALA:HB3	2.08	0.54
1:D:359:ASP:HA	1:D:362:ARG:NH1	2.23	0.54
1:E:194:GLN:O	1:E:371:LYS:HE3	2.07	0.54
1:I:72:GLN:OE1	1:I:75:LYS:HE3	2.07	0.54
1:K:16:MET:SD	1:K:73:MET:HE1	2.46	0.54
1:L:191:GLU:O	1:L:334:ASP:HA	2.08	0.54
1:D:70:GLY:HA2	1:D:73:MET:HE3	1.88	0.54
1:G:140:ASP:OD2	1:G:142:LYS:HB3	2.07	0.54
1:J:305:ILE:O	1:J:305:ILE:HG22	2.08	0.54
1:K:221:LEU:HD11	1:K:301:ILE:HD12	1.90	0.54
1:L:77:VAL:HG21	1:L:510:VAL:HB	1.89	0.54
1:A:166:MET:HE2	1:A:171:LYS:HA	1.90	0.54
1:D:362:ARG:HG2	1:D:366:GLN:NE2	2.22	0.54
1:E:140:ASP:OD2	1:E:142:LYS:HB3	2.06	0.54
1:F:28:LYS:HD2	1:F:453:GLN:OE1	2.07	0.54
1:H:413:ALA:CB	1:H:475:ASN:HD22	2.19	0.54
1:H:472:GLY:HA3	1:H:476:TYR:CD2	2.42	0.54
1:J:262:LEU:O	1:J:266:THR:HG23	2.07	0.54
1:L:216:GLU:C	1:L:218:PRO:HD3	2.31	0.54
1:L:236:VAL:HG22	1:L:312:ALA:O	2.07	0.54
1:N:413:ALA:CB	1:N:475:ASN:HD22	2.20	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:LYS:O	1:A:243:ALA:HB3	2.07	0.54
1:D:314:LEU:HD23	1:D:317:LEU:HD22	1.89	0.54
1:G:18:ARG:HG2	1:G:67:GLU:CD	2.33	0.54
1:J:413:ALA:N	1:J:475:ASN:ND2	2.56	0.54
1:M:219:PHE:HB3	1:M:317:LEU:HD23	1.90	0.54
1:D:18:ARG:HG2	1:D:67:GLU:CD	2.33	0.54
1:E:201:SER:C	1:E:202:PRO:O	2.49	0.54
1:F:16:MET:HB3	1:F:514:MET:HE3	1.90	0.54
1:H:230:ILE:HD13	1:H:261:THR:HG21	1.89	0.54
1:H:252:GLU:O	1:H:253:ASP:HB2	2.08	0.54
1:J:193:MET:HG3	1:J:371:LYS:HB3	1.90	0.54
1:B:383:ALA:O	1:B:384:ALA:HB3	2.08	0.54
1:D:193:MET:CE	1:D:292:ILE:HG12	2.34	0.54
1:G:130:GLU:HB3	1:G:422:VAL:HG22	1.89	0.54
1:H:16:MET:SD	1:H:73:MET:HE1	2.47	0.54
1:I:31:LEU:HD13	1:I:90:THR:CG2	2.38	0.54
1:J:305:ILE:HB	1:J:307:MET:HE2	1.90	0.54
1:N:349:ILE:HA	1:N:352:GLN:HG3	1.90	0.54
1:B:202:PRO:C	1:B:204:PHE:H	2.15	0.54
1:E:247:LEU:CD2	1:E:249:ILE:HD11	2.38	0.54
1:H:383:ALA:HB3	1:H:389:MET:HB2	1.88	0.54
1:F:218:PRO:HB3	1:F:246:PRO:HG2	1.90	0.53
1:F:314:LEU:HD23	1:F:317:LEU:HD22	1.90	0.53
1:H:57:ALA:O	1:H:75:LYS:HD2	2.08	0.53
1:L:342:ILE:O	1:L:346:VAL:HG23	2.08	0.53
1:L:349:ILE:O	1:L:353:ILE:HG13	2.08	0.53
1:D:32:GLY:HA3	1:D:454:ILE:HG23	1.89	0.53
1:G:233:MET:HE1	1:G:249:ILE:HD12	1.90	0.53
1:H:72:GLN:OE1	1:H:75:LYS:HE3	2.08	0.53
1:J:217:SER:N	1:J:218:PRO:CD	2.72	0.53
1:K:130:GLU:HB3	1:K:422:VAL:HG22	1.90	0.53
1:L:266:THR:HG21	1:L:273:VAL:HB	1.89	0.53
1:M:57:ALA:O	1:M:75:LYS:HD2	2.08	0.53
1:N:202:PRO:O	1:N:203:TYR:HB2	2.09	0.53
1:K:72:GLN:OE1	1:K:75:LYS:HE3	2.08	0.53
1:K:230:ILE:HD13	1:K:261:THR:CG2	2.38	0.53
1:N:202:PRO:C	1:N:204:PHE:H	2.16	0.53
1:N:349:ILE:O	1:N:353:ILE:HG13	2.09	0.53
1:A:70:GLY:HA2	1:A:73:MET:HE3	1.90	0.53
1:D:270:ILE:O	1:D:271:VAL:HB	2.08	0.53
1:F:140:ASP:OD2	1:F:142:LYS:HB3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:349:ILE:HA	1:H:352:GLN:HG3	1.90	0.53
1:K:201:SER:O	1:K:202:PRO:O	2.27	0.53
1:M:194:GLN:O	1:M:371:LYS:HE3	2.08	0.53
1:M:287:ALA:HB1	1:M:368:ARG:NH1	2.23	0.53
1:M:349:ILE:HA	1:M:352:GLN:HG3	1.91	0.53
1:D:349:ILE:CG2	1:D:369:VAL:HG13	2.38	0.53
1:E:173:GLY:O	1:E:404:ARG:NH2	2.41	0.53
1:E:182:GLY:O	1:E:183:LEU:C	2.52	0.53
1:H:339:GLU:O	1:H:343:GLN:HB2	2.08	0.53
1:I:218:PRO:HD2	1:I:320:ALA:O	2.09	0.53
1:B:178:GLU:HA	1:B:393:LYS:HE2	1.91	0.53
1:C:284:ARG:NH1	1:C:364:LYS:HD2	2.24	0.53
1:E:199:TYR:CZ	1:E:327:LYS:HA	2.44	0.53
1:L:217:SER:N	1:L:218:PRO:CD	2.72	0.53
1:N:270:ILE:O	1:N:271:VAL:HB	2.09	0.53
1:A:202:PRO:O	1:A:203:TYR:HB2	2.08	0.53
1:C:31:LEU:HD13	1:C:90:THR:CG2	2.38	0.53
1:D:202:PRO:O	1:D:204:PHE:N	2.37	0.53
1:E:383:ALA:O	1:E:384:ALA:HB3	2.08	0.53
1:I:302:SER:H	1:I:307:MET:HE3	1.74	0.53
1:J:218:PRO:HD2	1:J:320:ALA:O	2.09	0.53
1:G:201:SER:O	1:G:202:PRO:O	2.26	0.53
1:H:183:LEU:HD22	1:H:184:GLN:N	2.24	0.53
1:H:235:PRO:CG	1:H:310:GLU:HA	2.33	0.53
1:K:200:LEU:HG	1:K:276:VAL:HA	1.91	0.53
1:E:413:ALA:H	1:E:475:ASN:ND2	2.07	0.53
1:N:305:ILE:HB	1:N:307:MET:HE2	1.90	0.53
1:C:200:LEU:HG	1:C:276:VAL:HA	1.90	0.53
1:I:233:MET:HE1	1:I:249:ILE:CD1	2.39	0.53
1:L:319:GLN:HB3	1:L:336:VAL:HG21	1.91	0.53
1:L:349:ILE:HA	1:L:352:GLN:HG3	1.90	0.53
1:N:496:PRO:HB2	1:N:499:VAL:HG13	1.91	0.53
1:B:10:ASN:ND2	4:B:1510:MPD:H51	2.24	0.52
1:D:183:LEU:O	1:D:184:GLN:HG3	2.10	0.52
1:D:201:SER:C	1:D:202:PRO:O	2.50	0.52
1:F:23:LEU:HD23	1:F:74:VAL:HG22	1.91	0.52
1:G:71:ALA:O	1:G:75:LYS:HB2	2.10	0.52
1:L:258:ALA:O	1:L:262:LEU:HG	2.09	0.52
1:M:37:ASN:ND2	1:M:51:LYS:HG3	2.23	0.52
1:M:496:PRO:HB2	1:M:499:VAL:HG13	1.91	0.52
1:C:166:MET:HE2	1:C:171:LYS:HA	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:155:ASP:OD1	1:M:157:THR:HB	2.09	0.52
1:M:173:GLY:O	1:M:404:ARG:NH2	2.42	0.52
1:E:359:ASP:HA	1:E:362:ARG:HH12	1.73	0.52
1:G:191:GLU:O	1:G:334:ASP:HA	2.10	0.52
1:H:155:ASP:OD1	1:H:157:THR:HB	2.09	0.52
1:H:173:GLY:O	1:H:404:ARG:NH2	2.42	0.52
4:H:1516:MPD:HM1	1:I:518:GLU:HG3	1.90	0.52
1:I:349:ILE:HA	1:I:352:GLN:HG3	1.90	0.52
1:J:114:MET:HB3	6:J:3085:HOH:O	2.09	0.52
1:K:352:GLN:HB2	1:K:365:LEU:HD13	1.91	0.52
1:A:18:ARG:HG2	1:A:67:GLU:CD	2.35	0.52
1:A:242:LYS:O	1:A:244:GLY:N	2.41	0.52
1:F:182:GLY:O	1:F:183:LEU:C	2.52	0.52
1:G:28:LYS:HD2	1:G:453:GLN:OE1	2.10	0.52
1:L:49:ILE:HD12	1:M:513:LEU:HD13	1.90	0.52
1:B:71:ALA:O	1:B:75:LYS:HB2	2.10	0.52
1:C:71:ALA:O	1:C:75:LYS:HB2	2.09	0.52
1:C:109:ALA:HB2	1:K:109:ALA:HB2	1.92	0.52
1:D:242:LYS:O	1:D:243:ALA:HB3	2.09	0.52
1:F:70:GLY:HA2	1:F:73:MET:HE3	1.90	0.52
1:J:72:GLN:OE1	1:J:75:LYS:HE3	2.10	0.52
1:B:18:ARG:HG2	1:B:67:GLU:CD	2.34	0.52
1:B:182:GLY:O	1:B:183:LEU:C	2.53	0.52
1:C:23:LEU:HD23	1:C:74:VAL:HG22	1.92	0.52
1:K:77:VAL:HG21	1:K:510:VAL:HB	1.92	0.52
1:K:239:ALA:HB1	1:K:314:LEU:HG	1.90	0.52
1:C:273:VAL:HG12	1:C:274:ALA:N	2.25	0.52
1:E:201:SER:O	1:E:202:PRO:O	2.28	0.52
1:G:242:LYS:O	1:G:243:ALA:HB3	2.09	0.52
1:J:230:ILE:HD13	1:J:261:THR:HG21	1.92	0.52
1:K:202:PRO:C	1:K:204:PHE:H	2.17	0.52
1:N:16:MET:HB3	1:N:514:MET:HE3	1.91	0.52
1:A:71:ALA:O	1:A:75:LYS:HB2	2.10	0.52
1:J:49:ILE:HD12	1:K:513:LEU:HD13	1.91	0.52
1:K:305:ILE:HG22	1:K:305:ILE:O	2.10	0.52
1:L:230:ILE:HD13	1:L:261:THR:HG21	1.91	0.52
1:M:199:TYR:C	1:M:201:SER:H	2.18	0.52
1:N:130:GLU:HB3	1:N:422:VAL:HG22	1.92	0.52
1:A:230:ILE:HG22	1:A:257:GLU:OE2	2.10	0.52
1:D:486:GLY:C	1:D:491:MET:HE2	2.35	0.52
1:G:460:GLU:O	1:G:462:PRO:HD3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:7:LYS:HG3	1:M:66:PHE:CZ	2.43	0.52
1:B:85:ALA:HB1	1:B:499:VAL:HG12	1.92	0.51
1:D:193:MET:HG3	1:D:371:LYS:HB3	1.92	0.51
1:D:194:GLN:O	1:D:371:LYS:HE3	2.10	0.51
1:F:174:VAL:HG12	1:F:376:VAL:HG13	1.91	0.51
1:H:38:VAL:HG13	1:I:519:CYS:HB3	1.91	0.51
1:H:513:LEU:HD13	1:N:49:ILE:HD12	1.92	0.51
1:I:230:ILE:HD13	1:I:261:THR:CG2	2.40	0.51
1:I:305:ILE:HB	1:I:307:MET:HE2	1.90	0.51
1:L:140:ASP:OD2	1:L:142:LYS:HB3	2.10	0.51
1:D:218:PRO:HD2	1:D:320:ALA:O	2.10	0.51
1:F:413:ALA:H	1:F:475:ASN:ND2	2.08	0.51
1:F:486:GLY:C	1:F:491:MET:HE2	2.36	0.51
1:I:354:GLU:C	1:I:356:ALA:H	2.17	0.51
1:J:496:PRO:HB2	1:J:499:VAL:HG13	1.92	0.51
1:C:319:GLN:O	1:C:336:VAL:HG23	2.11	0.51
1:E:486:GLY:C	1:E:491:MET:HE2	2.35	0.51
1:G:202:PRO:C	1:G:204:PHE:H	2.16	0.51
1:L:7:LYS:HG3	1:L:66:PHE:CZ	2.45	0.51
1:L:102:GLU:HB2	1:L:442:VAL:HG13	1.92	0.51
1:L:233:MET:HE1	1:L:249:ILE:HD12	1.92	0.51
1:L:310:GLU:OE1	1:L:310:GLU:N	2.43	0.51
1:N:155:ASP:OD1	1:N:157:THR:HB	2.10	0.51
1:N:191:GLU:O	1:N:334:ASP:HA	2.10	0.51
1:F:183:LEU:HA	1:F:383:ALA:N	2.26	0.51
1:G:16:MET:HB3	1:G:514:MET:HE3	1.92	0.51
1:H:191:GLU:OE1	1:H:342:ILE:HD13	2.11	0.51
1:K:194:GLN:O	1:K:371:LYS:HE3	2.10	0.51
1:L:130:GLU:HB3	1:L:422:VAL:HG22	1.92	0.51
1:M:413:ALA:H	1:M:475:ASN:HD22	1.58	0.51
1:A:176:THR:HG21	1:A:333:ILE:HD13	1.93	0.51
1:B:199:TYR:CZ	1:B:327:LYS:HA	2.46	0.51
1:B:219:PHE:HB3	1:B:317:LEU:HD23	1.91	0.51
1:E:362:ARG:HG2	1:E:366:GLN:NE2	2.26	0.51
1:F:202:PRO:C	1:F:204:PHE:H	2.18	0.51
1:I:102:GLU:HB2	1:I:442:VAL:HG13	1.92	0.51
1:A:201:SER:C	1:A:202:PRO:O	2.50	0.51
1:B:201:SER:C	1:B:202:PRO:O	2.51	0.51
1:C:220:ILE:HD12	1:C:296:THR:HG21	1.92	0.51
1:D:201:SER:O	1:D:202:PRO:O	2.28	0.51
1:D:242:LYS:C	1:D:244:GLY:N	2.64	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:263:VAL:O	1:F:267:MET:HB2	2.11	0.51
1:H:193:MET:HG2	1:H:194:GLN:N	2.25	0.51
1:J:16:MET:HB3	1:J:514:MET:HE3	1.92	0.51
1:L:219:PHE:O	1:L:247:LEU:HD12	2.10	0.51
1:N:193:MET:HE1	1:N:292:ILE:CG1	2.39	0.51
1:A:193:MET:HE1	1:A:292:ILE:CG1	2.41	0.51
1:B:486:GLY:C	1:B:491:MET:HE2	2.36	0.51
1:C:85:ALA:HB1	1:C:499:VAL:HG12	1.92	0.51
1:F:193:MET:HG3	1:F:371:LYS:HB3	1.93	0.51
1:G:146:GLN:NE2	4:G:1509:MPD:H4	2.26	0.51
1:K:102:GLU:HB2	1:K:442:VAL:HG13	1.91	0.51
1:B:191:GLU:O	1:B:334:ASP:HA	2.11	0.51
1:C:201:SER:C	1:C:202:PRO:O	2.52	0.51
1:I:155:ASP:OD1	1:I:157:THR:HB	2.11	0.51
1:I:413:ALA:CB	1:I:475:ASN:HD22	2.23	0.51
1:J:336:VAL:O	1:J:336:VAL:HG12	2.09	0.51
1:N:16:MET:SD	1:N:73:MET:HE1	2.51	0.51
1:G:193:MET:HE1	1:G:292:ILE:HG12	1.92	0.51
1:J:349:ILE:HA	1:J:352:GLN:HG3	1.93	0.51
1:K:336:VAL:HG12	1:K:336:VAL:O	2.10	0.51
1:M:230:ILE:HG21	1:M:261:THR:HG21	1.93	0.51
1:M:270:ILE:O	1:M:271:VAL:HB	2.09	0.51
1:A:201:SER:O	1:A:202:PRO:O	2.29	0.51
1:H:221:LEU:HD23	1:H:249:ILE:HD12	1.92	0.51
1:H:233:MET:HE1	1:H:249:ILE:HD12	1.91	0.51
1:I:201:SER:C	1:I:202:PRO:O	2.51	0.51
1:J:102:GLU:HB2	1:J:442:VAL:HG13	1.93	0.51
1:E:247:LEU:HB3	1:E:273:VAL:HG22	1.92	0.50
1:G:193:MET:HE1	1:G:292:ILE:CG1	2.41	0.50
1:J:118:ARG:NH2	6:J:3085:HOH:O	2.41	0.50
1:C:202:PRO:C	1:C:204:PHE:H	2.18	0.50
1:F:305:ILE:O	1:F:305:ILE:HG22	2.11	0.50
1:K:230:ILE:HD13	1:K:261:THR:HG21	1.92	0.50
1:K:463:SER:O	1:K:467:ASN:HB2	2.11	0.50
1:L:31:LEU:HD13	1:L:90:THR:CG2	2.41	0.50
1:B:166:MET:CE	1:B:171:LYS:HA	2.41	0.50
1:C:314:LEU:HD23	1:C:317:LEU:HD22	1.92	0.50
1:I:191:GLU:O	1:I:334:ASP:HA	2.11	0.50
1:I:460:GLU:O	1:I:462:PRO:HD3	2.11	0.50
1:N:223:ALA:O	1:N:251:ALA:HA	2.12	0.50
1:N:336:VAL:HG12	1:N:336:VAL:O	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:230:ILE:HD13	1:B:261:THR:HG21	1.94	0.50
1:B:270:ILE:HA	1:C:231:ARG:NH1	2.26	0.50
1:D:16:MET:HB3	1:D:514:MET:HE3	1.92	0.50
1:H:247:LEU:CD2	1:H:249:ILE:HD11	2.41	0.50
1:I:18:ARG:HG3	1:I:67:GLU:CD	2.36	0.50
1:J:259:LEU:O	1:J:263:VAL:HG23	2.12	0.50
1:N:248:LEU:HD13	1:N:325:ILE:HD11	1.94	0.50
1:D:263:VAL:O	1:D:267:MET:HB2	2.12	0.50
1:E:264:VAL:HG12	1:E:265:ASN:N	2.27	0.50
1:F:259:LEU:O	1:F:263:VAL:HG23	2.11	0.50
1:J:7:LYS:HG3	1:J:66:PHE:CZ	2.47	0.50
1:K:155:ASP:OD1	1:K:157:THR:HB	2.11	0.50
1:L:193:MET:HG3	1:L:371:LYS:HB3	1.94	0.50
1:M:193:MET:HG3	1:M:371:LYS:HB3	1.92	0.50
1:N:230:ILE:HG21	1:N:261:THR:HG21	1.94	0.50
1:C:230:ILE:HG22	1:C:257:GLU:OE2	2.11	0.50
1:I:218:PRO:CB	1:I:246:PRO:HG2	2.41	0.50
1:M:37:ASN:HD21	1:M:51:LYS:HE3	1.75	0.50
1:M:191:GLU:O	1:M:334:ASP:HA	2.12	0.50
1:E:270:ILE:O	1:E:271:VAL:HB	2.12	0.50
1:G:183:LEU:O	1:G:184:GLN:HG3	2.12	0.50
1:G:242:LYS:O	1:G:244:GLY:N	2.44	0.50
1:G:461:GLU:HB3	6:G:3186:HOH:O	2.10	0.50
1:H:83:ASP:OD2	1:H:327:LYS:CD	2.60	0.50
1:I:228:SER:O	1:I:257:GLU:HB3	2.11	0.50
1:K:173:GLY:O	1:K:404:ARG:NH2	2.44	0.50
1:N:72:GLN:OE1	1:N:75:LYS:HE3	2.10	0.50
1:N:173:GLY:O	1:N:404:ARG:NH2	2.45	0.50
1:N:201:SER:O	1:N:202:PRO:O	2.30	0.50
1:A:183:LEU:O	1:A:184:GLN:HG3	2.12	0.50
1:J:77:VAL:HG21	1:J:510:VAL:HB	1.93	0.50
1:K:193:MET:HE1	1:K:292:ILE:CG1	2.30	0.50
1:A:202:PRO:O	1:A:204:PHE:N	2.38	0.50
1:B:104:LEU:HB3	4:B:1510:MPD:H31	1.94	0.50
1:C:486:GLY:C	1:C:491:MET:HE2	2.36	0.50
1:D:413:ALA:H	1:D:475:ASN:ND2	2.10	0.50
1:G:23:LEU:CD2	1:G:74:VAL:HG22	2.41	0.50
1:G:413:ALA:CB	1:G:417:VAL:HG22	2.42	0.50
1:I:130:GLU:HB3	1:I:422:VAL:HG22	1.94	0.50
1:L:229:ASN:HA	1:L:257:GLU:OE1	2.12	0.50
1:M:153:ASN:O	1:M:154:SER:HB2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:381:VAL:HG21	1:M:393:LYS:HA	1.93	0.50
1:M:413:ALA:N	1:M:475:ASN:HD22	2.10	0.50
1:B:183:LEU:HA	1:B:383:ALA:N	2.27	0.49
1:G:346:VAL:O	1:G:350:ARG:HB2	2.12	0.49
1:H:349:ILE:O	1:H:353:ILE:HG13	2.11	0.49
1:I:77:VAL:HG21	1:I:510:VAL:HB	1.94	0.49
1:K:287:ALA:HB1	1:K:368:ARG:NH1	2.27	0.49
1:K:310:GLU:OE1	1:K:310:GLU:N	2.44	0.49
1:L:239:ALA:HB1	1:L:314:LEU:HG	1.93	0.49
1:M:140:ASP:OD2	1:M:142:LYS:HB3	2.12	0.49
1:N:263:VAL:O	1:N:267:MET:HB2	2.12	0.49
1:B:193:MET:HE1	1:B:292:ILE:CG1	2.40	0.49
1:C:225:LYS:NZ	1:C:232:GLU:OE2	2.46	0.49
1:D:166:MET:HE2	1:D:171:LYS:HA	1.93	0.49
1:F:193:MET:HE1	1:F:292:ILE:CG1	2.41	0.49
1:F:201:SER:C	1:F:202:PRO:O	2.52	0.49
1:G:413:ALA:H	1:G:475:ASN:ND2	2.08	0.49
1:K:201:SER:C	1:K:202:PRO:O	2.55	0.49
1:L:202:PRO:O	1:L:204:PHE:N	2.43	0.49
1:L:202:PRO:O	1:L:203:TYR:HB2	2.12	0.49
1:L:230:ILE:HB	1:L:258:ALA:HA	1.94	0.49
1:N:28:LYS:HD2	1:N:453:GLN:OE1	2.13	0.49
1:D:178:GLU:HA	1:D:393:LYS:HE2	1.94	0.49
1:E:49:ILE:HD12	1:F:513:LEU:HD13	1.94	0.49
1:F:178:GLU:HA	1:F:393:LYS:HE2	1.93	0.49
1:I:26:ALA:HA	1:J:8:PHE:HE1	1.77	0.49
1:J:37:ASN:ND2	1:J:51:LYS:HG3	2.27	0.49
1:K:209:GLU:H	1:K:209:GLU:CD	2.19	0.49
1:K:247:LEU:HD21	1:K:249:ILE:HD11	1.95	0.49
1:M:72:GLN:OE1	1:M:75:LYS:HE3	2.12	0.49
1:M:336:VAL:O	1:M:336:VAL:HG12	2.11	0.49
1:D:40:LEU:HD13	1:D:59:GLU:HG3	1.93	0.49
1:D:202:PRO:C	1:D:204:PHE:H	2.19	0.49
1:F:451:LEU:HD23	1:F:451:LEU:C	2.37	0.49
1:H:37:ASN:ND2	1:H:51:LYS:HG3	2.27	0.49
1:H:231:ARG:NH1	1:N:241:ALA:C	2.70	0.49
1:H:352:GLN:HB2	1:H:365:LEU:HD13	1.94	0.49
1:J:18:ARG:HG3	1:J:67:GLU:CD	2.37	0.49
1:K:383:ALA:HB3	1:K:389:MET:HB2	1.94	0.49
1:M:102:GLU:HB2	1:M:442:VAL:HG13	1.94	0.49
1:N:218:PRO:CB	1:N:246:PRO:HG2	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:LYS:C	1:A:244:GLY:N	2.66	0.49
1:B:413:ALA:H	1:B:475:ASN:ND2	2.11	0.49
1:C:413:ALA:CB	1:C:475:ASN:HD22	2.25	0.49
1:D:200:LEU:HG	1:D:276:VAL:HA	1.95	0.49
1:E:284:ARG:NH1	1:E:364:LYS:HD2	2.27	0.49
1:G:178:GLU:HA	1:G:393:LYS:HE2	1.94	0.49
1:K:270:ILE:O	1:K:271:VAL:HB	2.12	0.49
1:K:496:PRO:HB2	1:K:499:VAL:HG13	1.94	0.49
1:L:202:PRO:C	1:L:204:PHE:H	2.19	0.49
1:L:218:PRO:CB	1:L:246:PRO:HG2	2.43	0.49
1:L:313:THR:O	1:L:317:LEU:HD13	2.13	0.49
1:N:200:LEU:HG	1:N:276:VAL:HA	1.94	0.49
1:D:183:LEU:HA	1:D:383:ALA:N	2.28	0.49
1:E:178:GLU:HA	1:E:393:LYS:HE2	1.95	0.49
1:I:217:SER:N	1:I:218:PRO:CD	2.75	0.49
1:L:16:MET:O	1:L:20:VAL:HG13	2.12	0.49
1:L:486:GLY:C	1:L:491:MET:HE2	2.37	0.49
1:M:77:VAL:HG21	1:M:510:VAL:HB	1.95	0.49
1:M:166:MET:HE2	1:M:171:LYS:HA	1.95	0.49
1:M:221:LEU:HD11	1:M:301:ILE:HD12	1.94	0.49
1:C:166:MET:CE	1:C:171:LYS:HA	2.42	0.49
1:E:183:LEU:HA	1:E:383:ALA:N	2.27	0.49
1:F:183:LEU:O	1:F:184:GLN:HG3	2.12	0.49
1:G:247:LEU:HD21	1:G:249:ILE:HD11	1.93	0.49
1:H:231:ARG:HH11	1:N:241:ALA:C	2.21	0.49
1:I:263:VAL:O	1:I:267:MET:HB2	2.13	0.49
1:K:248:LEU:HD13	1:K:325:ILE:HD11	1.95	0.49
1:M:248:LEU:HD13	1:M:325:ILE:HD11	1.94	0.49
1:M:263:VAL:O	1:M:267:MET:HB2	2.12	0.49
1:N:219:PHE:HB3	1:N:317:LEU:HD23	1.95	0.49
1:F:284:ARG:NH1	1:F:364:LYS:HD2	2.28	0.49
1:H:314:LEU:HA	1:H:317:LEU:HD22	1.95	0.49
1:L:34:LYS:HE2	1:M:118:ARG:HH22	1.77	0.49
1:L:160:LYS:O	1:L:164:GLU:HG3	2.12	0.49
1:N:259:LEU:O	1:N:263:VAL:HG23	2.12	0.49
1:N:460:GLU:O	1:N:462:PRO:HD3	2.13	0.49
1:A:430:ARG:NH2	6:A:3018:HOH:O	2.45	0.49
1:B:23:LEU:HD23	1:B:74:VAL:HG22	1.94	0.49
1:C:183:LEU:O	1:C:184:GLN:HG3	2.13	0.49
1:F:233:MET:HE1	1:F:249:ILE:CD1	2.43	0.49
1:H:77:VAL:HG21	1:H:510:VAL:HB	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:305:ILE:HB	1:H:307:MET:HE2	1.93	0.49
1:K:68:ASN:O	1:K:72:GLN:HG2	2.13	0.49
1:L:221:LEU:HB3	1:L:249:ILE:HD13	1.94	0.49
1:L:383:ALA:HB3	1:L:389:MET:HB2	1.93	0.49
1:D:496:PRO:HB2	1:D:499:VAL:HG13	1.95	0.49
1:E:413:ALA:HB2	1:E:475:ASN:HD22	1.78	0.49
1:H:68:ASN:O	1:H:72:GLN:HG2	2.13	0.49
1:H:102:GLU:HB2	1:H:442:VAL:HG13	1.94	0.49
1:K:259:LEU:O	1:K:263:VAL:HG23	2.13	0.49
1:M:216:GLU:C	1:M:218:PRO:HD3	2.38	0.49
1:N:102:GLU:HB2	1:N:442:VAL:HG13	1.95	0.49
1:N:201:SER:C	1:N:202:PRO:O	2.55	0.49
1:C:49:ILE:HD12	1:D:513:LEU:HD13	1.95	0.48
1:D:413:ALA:CB	1:D:417:VAL:HG22	2.43	0.48
1:E:242:LYS:O	1:E:243:ALA:HB3	2.12	0.48
1:F:83:ASP:OD2	1:F:327:LYS:HD3	2.12	0.48
1:F:273:VAL:HG12	1:F:274:ALA:N	2.28	0.48
1:F:413:ALA:HB2	1:F:475:ASN:HD22	1.78	0.48
1:G:413:ALA:HB2	1:G:475:ASN:HD22	1.77	0.48
1:H:463:SER:O	1:H:467:ASN:HB2	2.12	0.48
1:I:230:ILE:HD13	1:I:261:THR:HG21	1.93	0.48
1:J:310:GLU:OE1	1:J:310:GLU:N	2.43	0.48
1:L:132:LYS:O	1:L:135:SER:HB3	2.13	0.48
1:M:305:ILE:O	1:M:305:ILE:HG22	2.12	0.48
1:A:40:LEU:HD13	1:A:59:GLU:HG3	1.95	0.48
1:A:383:ALA:HB3	1:A:389:MET:HB2	1.95	0.48
1:B:183:LEU:O	1:B:184:GLN:HG3	2.13	0.48
1:C:266:THR:CG2	1:C:273:VAL:H	2.26	0.48
1:D:273:VAL:HG12	1:D:274:ALA:N	2.27	0.48
1:F:266:THR:CG2	1:F:273:VAL:HB	2.43	0.48
1:H:457:ASN:OD1	4:H:1516:MPD:H13	2.13	0.48
1:J:319:GLN:HB3	1:J:336:VAL:CG2	2.43	0.48
1:L:463:SER:O	1:L:467:ASN:HB2	2.13	0.48
1:F:85:ALA:HB1	1:F:499:VAL:HG12	1.95	0.48
1:J:57:ALA:O	1:J:75:LYS:HD2	2.13	0.48
1:L:166:MET:HE2	1:L:171:LYS:HA	1.95	0.48
1:L:221:LEU:HD11	1:L:301:ILE:HD12	1.96	0.48
1:M:479:ASN:ND2	1:M:493:ILE:HD11	2.28	0.48
1:A:381:VAL:HG21	1:A:393:LYS:HA	1.95	0.48
1:C:182:GLY:O	1:C:183:LEU:C	2.55	0.48
1:D:247:LEU:CD2	1:D:249:ILE:HD11	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:217:SER:N	1:H:218:PRO:CD	2.76	0.48
1:I:153:ASN:O	1:I:154:SER:HB2	2.14	0.48
1:I:272:LYS:NZ	1:J:228:SER:HB3	2.29	0.48
1:J:130:GLU:HB3	1:J:422:VAL:HG22	1.96	0.48
1:M:201:SER:C	1:M:202:PRO:O	2.56	0.48
1:A:303:GLU:O	1:A:306:GLY:N	2.41	0.48
1:B:303:GLU:O	1:B:306:GLY:N	2.40	0.48
1:B:494:LEU:C	1:B:494:LEU:HD12	2.38	0.48
1:D:191:GLU:O	1:D:334:ASP:HA	2.13	0.48
1:E:183:LEU:O	1:E:184:GLN:HG3	2.14	0.48
1:F:173:GLY:O	1:F:404:ARG:NH2	2.46	0.48
1:I:314:LEU:HA	1:I:317:LEU:HD22	1.94	0.48
1:I:496:PRO:HB2	1:I:499:VAL:HG13	1.94	0.48
1:L:305:ILE:O	1:L:305:ILE:HG22	2.12	0.48
1:L:344:GLY:O	1:L:347:ALA:HB3	2.14	0.48
1:N:57:ALA:O	1:N:75:LYS:HD2	2.13	0.48
1:N:222:LEU:HD11	1:N:293:ALA:HA	1.96	0.48
1:C:217:SER:N	1:C:218:PRO:CD	2.77	0.48
1:F:71:ALA:O	1:F:75:LYS:HB2	2.14	0.48
1:J:430:ARG:HD2	6:J:3082:HOH:O	2.13	0.48
1:L:153:ASN:O	1:L:154:SER:HB2	2.13	0.48
1:L:381:VAL:HG21	1:L:393:LYS:HA	1.95	0.48
1:M:269:GLY:HA2	1:N:229:ASN:ND2	2.28	0.48
1:A:166:MET:CE	1:A:171:LYS:HA	2.44	0.48
1:C:178:GLU:HA	1:C:393:LYS:HE2	1.95	0.48
1:D:23:LEU:CD2	1:D:74:VAL:HG22	2.44	0.48
1:E:202:PRO:O	1:E:203:TYR:HB2	2.12	0.48
1:E:215:LEU:HB2	1:E:323:VAL:HG22	1.96	0.48
1:E:269:GLY:CA	1:F:229:ASN:ND2	2.76	0.48
1:G:266:THR:CG2	1:G:273:VAL:HB	2.44	0.48
1:I:193:MET:HG2	1:I:194:GLN:N	2.28	0.48
1:J:193:MET:HG2	1:J:194:GLN:N	2.28	0.48
1:K:349:ILE:O	1:K:353:ILE:HG13	2.13	0.48
1:L:144:ILE:HG23	1:L:403:THR:CG2	2.44	0.48
1:N:221:LEU:HD23	1:N:249:ILE:HD12	1.95	0.48
1:B:305:ILE:O	1:B:305:ILE:HG22	2.12	0.48
1:F:383:ALA:HB3	1:F:389:MET:HB2	1.95	0.48
1:F:478:TYR:CE2	1:F:480:ALA:HA	2.49	0.48
1:H:336:VAL:O	1:H:336:VAL:HG12	2.13	0.48
1:I:287:ALA:HB1	1:I:368:ARG:NH1	2.28	0.48
1:J:451:LEU:HD23	1:J:451:LEU:C	2.39	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:220:ILE:HD12	1:L:296:THR:HG21	1.95	0.48
1:L:270:ILE:O	1:L:271:VAL:HB	2.14	0.48
1:N:217:SER:N	1:N:218:PRO:CD	2.76	0.48
1:N:233:MET:HE1	1:N:249:ILE:HD12	1.95	0.48
1:F:197:ARG:HD2	1:F:277:LYS:HB2	1.96	0.48
1:G:166:MET:HE2	1:G:171:LYS:HA	1.94	0.48
1:H:134:LEU:HD11	1:H:475:ASN:ND2	2.28	0.48
1:I:5:ASP:HB2	1:I:524:LEU:CD1	2.44	0.48
1:I:118:ARG:HG3	6:I:3052:HOH:O	2.14	0.48
1:J:478:TYR:CE2	1:J:480:ALA:HA	2.49	0.48
1:K:217:SER:N	1:K:218:PRO:CD	2.76	0.48
1:M:451:LEU:HD23	1:M:455:VAL:HG23	1.96	0.48
1:A:496:PRO:HB2	1:A:499:VAL:HG13	1.96	0.48
1:D:288:MET:HG2	1:D:368:ARG:HD3	1.94	0.48
1:D:359:ASP:HA	1:D:362:ARG:HH12	1.78	0.48
1:E:28:LYS:HD2	1:E:453:GLN:OE1	2.13	0.48
1:G:486:GLY:C	1:G:491:MET:HE2	2.39	0.48
1:H:146:GLN:O	1:H:150:ILE:HG13	2.14	0.48
1:H:231:ARG:NH1	1:N:241:ALA:HB3	2.29	0.48
1:H:460:GLU:O	1:H:462:PRO:HD3	2.13	0.48
1:N:463:SER:O	1:N:467:ASN:HB2	2.14	0.48
1:B:217:SER:N	1:B:218:PRO:CD	2.77	0.47
1:C:455:VAL:CG1	1:C:460:GLU:HB2	2.44	0.47
1:G:266:THR:HG21	1:G:273:VAL:HB	1.96	0.47
1:H:200:LEU:HG	1:H:276:VAL:HA	1.96	0.47
1:I:37:ASN:ND2	1:I:51:LYS:HG3	2.28	0.47
1:J:201:SER:C	1:J:202:PRO:O	2.56	0.47
1:J:272:LYS:NZ	1:K:228:SER:HB3	2.29	0.47
1:J:342:ILE:O	1:J:346:VAL:HG23	2.14	0.47
1:J:438:VAL:O	1:J:442:VAL:HG23	2.14	0.47
4:K:1506:MPD:H53	6:K:3099:HOH:O	2.14	0.47
1:M:345:ARG:HD3	6:M:3113:HOH:O	2.14	0.47
1:N:5:ASP:HB2	1:N:524:LEU:CD1	2.44	0.47
1:N:18:ARG:HG3	1:N:67:GLU:CD	2.39	0.47
1:D:413:ALA:HB2	1:D:475:ASN:HD22	1.79	0.47
1:H:31:LEU:HD13	1:H:90:THR:HG22	1.96	0.47
1:K:37:ASN:ND2	1:K:51:LYS:HG3	2.29	0.47
1:M:217:SER:N	1:M:218:PRO:CD	2.77	0.47
1:N:7:LYS:HG3	1:N:66:PHE:CZ	2.49	0.47
1:F:215:LEU:HB2	1:F:323:VAL:HG22	1.96	0.47
1:F:266:THR:HG21	1:F:273:VAL:HB	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:259:LEU:O	1:G:263:VAL:HG23	2.14	0.47
1:H:228:SER:HB3	1:N:272:LYS:HZ1	1.78	0.47
1:M:18:ARG:HG3	1:M:67:GLU:CD	2.38	0.47
1:N:222:LEU:CD1	1:N:293:ALA:HA	2.44	0.47
1:A:268:ARG:O	1:A:270:ILE:HG13	2.14	0.47
1:A:513:LEU:HD13	1:G:49:ILE:CD1	2.45	0.47
1:C:83:ASP:OD2	1:C:327:LYS:HD3	2.14	0.47
1:C:305:ILE:HG22	1:C:305:ILE:O	2.12	0.47
1:D:220:ILE:HD12	1:D:296:THR:HG21	1.96	0.47
1:E:217:SER:N	1:E:218:PRO:HD3	2.30	0.47
1:H:130:GLU:HB3	1:H:422:VAL:HG22	1.96	0.47
1:M:218:PRO:CB	1:M:246:PRO:HG2	2.41	0.47
1:A:28:LYS:HD2	1:A:453:GLN:OE1	2.15	0.47
1:B:28:LYS:HD2	1:B:453:GLN:OE1	2.15	0.47
1:B:353:ILE:HD13	1:B:366:GLN:HG3	1.97	0.47
1:C:349:ILE:O	1:C:353:ILE:HG13	2.15	0.47
1:D:233:MET:HE1	1:D:249:ILE:CD1	2.43	0.47
1:I:7:LYS:HG3	1:I:66:PHE:CZ	2.49	0.47
1:I:272:LYS:HZ1	1:J:228:SER:HB3	1.80	0.47
1:B:230:ILE:HG22	1:B:257:GLU:OE2	2.14	0.47
1:C:259:LEU:O	1:C:263:VAL:HG23	2.14	0.47
1:I:57:ALA:O	1:I:75:LYS:HD2	2.15	0.47
1:J:68:ASN:O	1:J:72:GLN:HG2	2.14	0.47
1:J:153:ASN:O	1:J:154:SER:HB2	2.13	0.47
1:K:186:GLU:HB2	1:K:380:LYS:HB2	1.97	0.47
1:M:349:ILE:O	1:M:353:ILE:HG13	2.14	0.47
1:N:220:ILE:HD12	1:N:296:THR:HG21	1.96	0.47
1:A:359:ASP:HA	1:A:362:ARG:HH12	1.79	0.47
1:B:272:LYS:HZ1	1:C:229:ASN:HD22	1.58	0.47
1:D:182:GLY:O	1:D:183:LEU:C	2.58	0.47
1:D:472:GLY:HA3	1:D:476:TYR:CD2	2.49	0.47
1:E:40:LEU:HD13	1:E:59:GLU:HG3	1.96	0.47
1:F:191:GLU:O	1:F:334:ASP:HA	2.15	0.47
1:F:217:SER:N	1:F:218:PRO:CD	2.77	0.47
1:G:182:GLY:O	1:G:183:LEU:C	2.57	0.47
1:G:305:ILE:O	1:G:305:ILE:HG22	2.15	0.47
1:H:486:GLY:C	1:H:491:MET:HE2	2.39	0.47
1:I:247:LEU:HD21	1:I:249:ILE:HD11	1.97	0.47
1:J:152:ALA:O	1:J:153:ASN:HB3	2.15	0.47
1:K:486:GLY:C	1:K:491:MET:HE2	2.39	0.47
1:L:302:SER:H	1:L:307:MET:CE	2.26	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:336:VAL:O	1:L:336:VAL:HG12	2.13	0.47
1:M:183:LEU:HD22	1:M:184:GLN:N	2.30	0.47
1:N:451:LEU:HD23	1:N:451:LEU:C	2.40	0.47
1:A:413:ALA:CB	1:A:475:ASN:HD22	2.27	0.47
1:E:200:LEU:HG	1:E:276:VAL:HA	1.95	0.47
1:E:217:SER:N	1:E:218:PRO:CD	2.77	0.47
1:E:263:VAL:O	1:E:267:MET:HB2	2.15	0.47
1:K:199:TYR:C	1:K:201:SER:H	2.21	0.47
1:L:460:GLU:O	1:L:462:PRO:HD3	2.15	0.47
1:L:478:TYR:CE2	1:L:480:ALA:HA	2.50	0.47
1:M:247:LEU:HD21	1:M:249:ILE:HD11	1.97	0.47
1:N:183:LEU:HD22	1:N:184:GLN:H	1.80	0.47
1:B:263:VAL:O	1:B:267:MET:HB2	2.15	0.47
1:C:114:MET:HE3	6:C:3133:HOH:O	2.15	0.47
1:C:383:ALA:O	1:C:384:ALA:CB	2.59	0.47
1:C:472:GLY:HA3	1:C:476:TYR:CD2	2.50	0.47
1:E:524:LEU:HD12	1:E:524:LEU:HA	1.75	0.47
1:G:202:PRO:C	1:G:204:PHE:N	2.73	0.47
1:K:144:ILE:HG23	1:K:403:THR:CG2	2.44	0.47
1:K:220:ILE:CD1	1:K:296:THR:HG21	2.44	0.47
1:K:429:LEU:HG	1:K:440:ILE:HD13	1.96	0.47
1:L:358:SER:HB3	1:L:361:ASP:OD1	2.15	0.47
1:C:28:LYS:HD2	1:C:453:GLN:OE1	2.14	0.47
1:E:23:LEU:CD2	1:E:74:VAL:HG22	2.45	0.47
1:E:386:GLU:HB2	1:F:281:PHE:HB3	1.97	0.47
1:H:39:VAL:CG1	1:I:69:MET:HE2	2.45	0.47
1:H:385:THR:OG1	1:H:388:GLU:HG3	2.15	0.47
1:I:217:SER:N	1:I:218:PRO:HD3	2.30	0.47
1:J:16:MET:SD	1:J:73:MET:HE1	2.54	0.47
1:J:486:GLY:C	1:J:491:MET:HE2	2.40	0.47
1:K:38:VAL:HG13	1:L:519:CYS:HB3	1.95	0.47
1:N:166:MET:HE2	1:N:171:LYS:HA	1.97	0.47
1:N:266:THR:HG21	1:N:273:VAL:HB	1.97	0.47
1:A:326:ASN:HB3	1:A:327:LYS:H	1.61	0.46
1:D:217:SER:N	1:D:218:PRO:CD	2.77	0.46
1:E:166:MET:CE	1:E:171:LYS:HA	2.44	0.46
1:E:269:GLY:HA3	1:F:229:ASN:ND2	2.30	0.46
1:E:472:GLY:HA3	1:E:476:TYR:CD2	2.49	0.46
1:G:344:GLY:O	1:G:347:ALA:HB3	2.14	0.46
1:K:193:MET:HG2	1:K:194:GLN:N	2.29	0.46
1:A:183:LEU:HA	1:A:383:ALA:N	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:362:ARG:HG2	1:A:366:GLN:NE2	2.31	0.46
1:H:201:SER:C	1:H:202:PRO:O	2.55	0.46
1:H:304:GLU:C	1:H:306:GLY:H	2.23	0.46
1:L:319:GLN:O	1:L:336:VAL:HG23	2.16	0.46
1:M:130:GLU:HB3	1:M:422:VAL:HG22	1.96	0.46
1:M:453:GLN:HE22	4:M:1518:MPD:H11	1.80	0.46
1:N:77:VAL:HG21	1:N:510:VAL:HB	1.96	0.46
1:B:496:PRO:HB2	1:B:499:VAL:HG13	1.97	0.46
1:H:26:ALA:HA	1:I:8:PHE:HE1	1.79	0.46
1:H:478:TYR:CE2	1:H:480:ALA:HA	2.50	0.46
1:J:302:SER:H	1:J:307:MET:HE3	1.78	0.46
1:K:16:MET:HB3	1:K:514:MET:CE	2.45	0.46
1:L:259:LEU:O	1:L:263:VAL:HG23	2.16	0.46
1:L:349:ILE:CG2	1:L:369:VAL:HG13	2.45	0.46
1:N:152:ALA:O	1:N:153:ASN:HB3	2.14	0.46
1:N:413:ALA:N	1:N:475:ASN:HD22	2.13	0.46
1:D:478:TYR:CE2	1:D:480:ALA:HA	2.50	0.46
1:G:455:VAL:CG1	1:G:460:GLU:HB2	2.44	0.46
1:H:202:PRO:C	1:H:204:PHE:H	2.23	0.46
1:K:451:LEU:HD23	1:K:451:LEU:C	2.40	0.46
1:N:242:LYS:C	1:N:244:GLY:H	2.22	0.46
1:B:131:LEU:HD21	1:B:500:THR:HG22	1.98	0.46
1:C:202:PRO:C	1:C:204:PHE:N	2.73	0.46
1:C:248:LEU:HD13	1:C:325:ILE:HD11	1.98	0.46
1:F:200:LEU:HG	1:F:276:VAL:HA	1.96	0.46
1:H:152:ALA:O	1:H:153:ASN:HB3	2.16	0.46
1:H:193:MET:CE	1:H:292:ILE:HG12	2.44	0.46
1:H:266:THR:CG2	1:H:273:VAL:HB	2.45	0.46
1:H:413:ALA:N	1:H:475:ASN:HD22	2.14	0.46
1:J:193:MET:CE	1:J:292:ILE:HG12	2.38	0.46
1:J:203:TYR:C	1:J:205:ILE:N	2.73	0.46
1:K:230:ILE:HG21	1:K:261:THR:HG21	1.97	0.46
1:K:266:THR:HG21	1:K:273:VAL:HB	1.97	0.46
1:L:451:LEU:C	1:L:451:LEU:HD23	2.40	0.46
1:N:413:ALA:HB3	1:N:417:VAL:HG22	1.98	0.46
1:D:429:LEU:HD12	6:D:3081:HOH:O	2.15	0.46
1:G:269:GLY:HA2	1:G:272:LYS:HZ2	1.80	0.46
1:H:166:MET:HE2	1:H:171:LYS:HA	1.98	0.46
1:H:381:VAL:HG21	1:H:393:LYS:HA	1.97	0.46
1:I:39:VAL:HG12	1:J:69:MET:HE2	1.98	0.46
1:I:152:ALA:O	1:I:153:ASN:HB3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:314:LEU:HD23	1:I:317:LEU:HD22	1.97	0.46
1:L:25:ASP:OD1	1:L:28:LYS:HE2	2.15	0.46
1:L:173:GLY:O	1:L:404:ARG:NH2	2.48	0.46
1:M:455:VAL:CG1	1:M:460:GLU:HB2	2.44	0.46
1:N:305:ILE:HG22	1:N:305:ILE:O	2.16	0.46
1:N:441:LYS:O	1:N:445:ARG:HB2	2.15	0.46
1:A:217:SER:N	1:A:218:PRO:CD	2.78	0.46
1:B:346:VAL:O	1:B:350:ARG:HB2	2.16	0.46
1:C:353:ILE:HD13	1:C:366:GLN:HG3	1.97	0.46
1:D:349:ILE:O	1:D:353:ILE:HG13	2.16	0.46
1:E:169:VAL:CG1	1:E:377:ALA:HB2	2.46	0.46
1:E:202:PRO:C	1:E:204:PHE:H	2.21	0.46
1:E:369:VAL:HG23	1:E:370:ALA:N	2.29	0.46
1:E:383:ALA:HB3	1:E:389:MET:HB2	1.98	0.46
1:I:16:MET:SD	1:I:73:MET:HE1	2.56	0.46
1:I:429:LEU:HG	1:I:440:ILE:HD13	1.97	0.46
1:I:455:VAL:CG1	1:I:460:GLU:HB2	2.46	0.46
1:K:13:ARG:NH1	1:K:518:GLU:OE2	2.48	0.46
1:K:381:VAL:HG21	1:K:393:LYS:HA	1.98	0.46
1:L:16:MET:HB3	1:L:514:MET:CE	2.45	0.46
1:L:57:ALA:O	1:L:75:LYS:HD2	2.15	0.46
1:L:193:MET:HG2	1:L:194:GLN:N	2.31	0.46
1:M:349:ILE:HA	1:M:352:GLN:CG	2.45	0.46
1:A:247:LEU:CD2	1:A:249:ILE:HD11	2.46	0.46
1:B:134:LEU:HD12	1:B:422:VAL:HG23	1.98	0.46
1:E:203:TYR:C	1:E:205:ILE:N	2.74	0.46
1:H:242:LYS:C	1:H:244:GLY:H	2.24	0.46
1:I:16:MET:HB3	1:I:514:MET:CE	2.46	0.46
1:J:186:GLU:HB2	1:J:380:LYS:HB2	1.98	0.46
1:J:349:ILE:O	1:J:353:ILE:HG13	2.14	0.46
1:M:183:LEU:O	1:M:184:GLN:CB	2.58	0.46
1:M:304:GLU:C	1:M:306:GLY:H	2.23	0.46
1:N:193:MET:HG2	1:N:194:GLN:N	2.31	0.46
1:B:216:GLU:C	1:B:218:PRO:HD3	2.41	0.46
1:C:16:MET:HB3	1:C:514:MET:CE	2.46	0.46
1:C:191:GLU:O	1:C:334:ASP:HA	2.15	0.46
1:E:349:ILE:O	1:E:353:ILE:HG13	2.15	0.46
1:G:77:VAL:HG12	1:G:506:TYR:HB3	1.98	0.46
1:I:144:ILE:HG23	1:I:403:THR:CG2	2.45	0.46
1:I:200:LEU:HG	1:I:276:VAL:HA	1.98	0.46
1:I:204:PHE:O	1:I:213:VAL:HG22	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:381:VAL:HG21	1:I:393:LYS:HA	1.96	0.46
1:K:57:ALA:O	1:K:75:LYS:HD2	2.15	0.46
1:K:413:ALA:N	1:K:475:ASN:HD22	2.14	0.46
1:L:183:LEU:HD22	1:L:184:GLN:H	1.81	0.46
1:L:193:MET:HE1	1:L:292:ILE:CG1	2.36	0.46
1:L:241:ALA:C	1:M:231:ARG:NH1	2.74	0.46
1:L:247:LEU:HD21	1:L:249:ILE:HD11	1.98	0.46
1:N:134:LEU:HD11	1:N:475:ASN:ND2	2.30	0.46
1:A:264:VAL:HG12	1:A:265:ASN:N	2.31	0.46
1:A:273:VAL:HG12	1:A:274:ALA:N	2.30	0.46
1:B:364:LYS:O	1:B:367:GLU:HB2	2.16	0.46
1:D:71:ALA:O	1:D:75:LYS:HB2	2.16	0.46
1:E:289:LEU:HD23	1:E:289:LEU:HA	1.77	0.46
1:E:413:ALA:CB	1:E:417:VAL:HG22	2.46	0.46
1:H:31:LEU:HD13	1:H:90:THR:CG2	2.46	0.46
1:H:257:GLU:HB2	1:N:269:GLY:HA3	1.97	0.46
1:I:13:ARG:NH1	1:I:518:GLU:OE2	2.49	0.46
1:L:354:GLU:C	1:L:356:ALA:H	2.24	0.46
1:N:131:LEU:HD21	1:N:500:THR:HG22	1.99	0.46
1:N:153:ASN:O	1:N:154:SER:HB2	2.16	0.46
1:N:342:ILE:O	1:N:346:VAL:HG23	2.16	0.46
1:N:349:ILE:CG2	1:N:369:VAL:HG13	2.46	0.46
1:B:202:PRO:C	1:B:204:PHE:N	2.73	0.45
1:B:217:SER:N	1:B:218:PRO:HD3	2.32	0.45
1:C:385:THR:OG1	1:C:388:GLU:HG3	2.16	0.45
1:E:290:GLN:O	1:E:293:ALA:HB3	2.16	0.45
1:G:194:GLN:O	1:G:371:LYS:HE3	2.16	0.45
1:H:114:MET:HB3	6:H:3064:HOH:O	2.16	0.45
1:I:266:THR:HG21	1:I:273:VAL:HB	1.98	0.45
1:J:25:ASP:OD1	1:J:28:LYS:HE2	2.17	0.45
1:K:202:PRO:O	1:K:203:TYR:HB2	2.15	0.45
1:A:349:ILE:HG21	1:A:369:VAL:HG13	1.98	0.45
1:B:144:ILE:HG23	1:B:403:THR:CG2	2.46	0.45
1:H:231:ARG:HH12	1:N:241:ALA:HB3	1.82	0.45
1:I:183:LEU:O	1:I:184:GLN:CB	2.54	0.45
1:J:217:SER:N	1:J:218:PRO:HD3	2.32	0.45
1:M:16:MET:HB3	1:M:514:MET:CE	2.46	0.45
1:A:120:ILE:O	1:A:124:VAL:HG23	2.16	0.45
1:F:194:GLN:O	1:F:371:LYS:HE3	2.16	0.45
1:F:202:PRO:O	1:F:203:TYR:CB	2.61	0.45
1:I:291:ASP:OD2	1:I:368:ARG:HD2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:49:ILE:CD1	1:M:513:LEU:HD13	2.46	0.45
1:N:18:ARG:HH12	4:N:1526:MPD:H31	1.80	0.45
1:N:199:TYR:C	1:N:201:SER:H	2.23	0.45
1:A:221:LEU:HD23	1:A:249:ILE:HD12	1.99	0.45
1:B:225:LYS:NZ	1:B:232:GLU:OE2	2.50	0.45
1:D:202:PRO:C	1:D:204:PHE:N	2.74	0.45
1:E:77:VAL:HG21	1:E:510:VAL:HB	1.99	0.45
1:H:39:VAL:HG12	1:I:69:MET:CE	2.47	0.45
1:I:16:MET:O	1:I:20:VAL:HG13	2.16	0.45
1:I:270:ILE:O	1:I:271:VAL:CB	2.61	0.45
1:I:463:SER:O	1:I:467:ASN:HB2	2.16	0.45
1:K:49:ILE:HD12	1:L:513:LEU:HD13	1.98	0.45
1:L:413:ALA:N	1:L:475:ASN:HD22	2.15	0.45
1:N:235:PRO:CG	1:N:310:GLU:HA	2.41	0.45
1:A:351:GLN:O	1:A:354:GLU:HG2	2.17	0.45
1:A:472:GLY:HA3	1:A:476:TYR:CD2	2.51	0.45
1:D:326:ASN:HB3	1:D:327:LYS:H	1.64	0.45
1:F:217:SER:O	1:F:245:LYS:HD3	2.17	0.45
1:F:230:ILE:HD13	1:F:261:THR:HG21	1.98	0.45
1:G:176:THR:HG21	1:G:333:ILE:CD1	2.38	0.45
1:G:303:GLU:O	1:G:306:GLY:N	2.46	0.45
1:H:254:VAL:HG12	1:H:259:LEU:HB2	1.98	0.45
1:K:181:THR:O	1:L:282:GLY:HA3	2.16	0.45
1:K:233:MET:HE1	1:K:249:ILE:HD12	1.96	0.45
1:K:478:TYR:CE2	1:K:480:ALA:HA	2.51	0.45
1:L:201:SER:C	1:L:202:PRO:O	2.60	0.45
1:M:221:LEU:HB3	1:M:249:ILE:HD13	1.98	0.45
1:N:349:ILE:HA	1:N:352:GLN:CG	2.46	0.45
1:N:478:TYR:CE2	1:N:480:ALA:HA	2.52	0.45
1:B:24:ALA:O	1:B:28:LYS:HG2	2.17	0.45
1:B:90:THR:O	1:B:94:VAL:HG13	2.17	0.45
1:B:199:TYR:C	1:B:201:SER:H	2.23	0.45
1:B:301:ILE:HD13	1:B:312:ALA:HB2	1.98	0.45
1:C:23:LEU:CD2	1:C:74:VAL:HG22	2.46	0.45
1:C:494:LEU:C	1:C:494:LEU:HD12	2.41	0.45
1:E:270:ILE:HG12	1:F:231:ARG:HH11	1.82	0.45
1:H:349:ILE:CG2	1:H:369:VAL:HG13	2.47	0.45
1:H:413:ALA:HB1	1:H:488:MET:HG3	1.98	0.45
1:I:221:LEU:HD23	1:I:249:ILE:HD12	1.97	0.45
1:K:413:ALA:HB3	1:K:417:VAL:HG22	1.99	0.45
1:N:16:MET:O	1:N:20:VAL:HG13	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:169:VAL:CG1	1:N:377:ALA:HB2	2.47	0.45
1:B:16:MET:HB3	1:B:514:MET:CE	2.47	0.45
1:B:270:ILE:O	1:B:271:VAL:HB	2.16	0.45
1:B:295:LEU:HA	1:B:342:ILE:CD1	2.47	0.45
1:C:183:LEU:HA	1:C:383:ALA:N	2.31	0.45
1:D:383:ALA:HB3	1:D:389:MET:HB2	1.97	0.45
1:G:40:LEU:HD13	1:G:59:GLU:HG3	1.98	0.45
1:K:183:LEU:HD22	1:K:184:GLN:H	1.81	0.45
1:K:191:GLU:O	1:K:334:ASP:HA	2.17	0.45
1:L:138:CYS:SG	1:L:147:VAL:HG21	2.57	0.45
1:N:304:GLU:C	1:N:306:GLY:H	2.25	0.45
1:N:413:ALA:HB1	1:N:488:MET:HG3	1.99	0.45
1:B:23:LEU:CD2	1:B:74:VAL:HG22	2.47	0.45
1:E:7:LYS:HE3	1:E:15:LYS:HE3	1.99	0.45
1:F:23:LEU:CD2	1:F:74:VAL:HG22	2.46	0.45
1:F:472:GLY:HA3	1:F:476:TYR:CD2	2.51	0.45
1:H:413:ALA:HB3	1:H:417:VAL:HG22	1.99	0.45
1:H:451:LEU:HD23	1:H:451:LEU:O	2.16	0.45
1:I:25:ASP:OD1	1:I:28:LYS:HE2	2.16	0.45
1:K:305:ILE:HB	1:K:307:MET:HE2	1.99	0.45
1:L:339:GLU:O	1:L:343:GLN:HB2	2.17	0.45
1:M:354:GLU:C	1:M:356:ALA:H	2.24	0.45
1:N:203:TYR:C	1:N:205:ILE:N	2.74	0.45
1:N:524:LEU:HD12	1:N:524:LEU:HA	1.81	0.45
1:A:305:ILE:O	1:A:305:ILE:HG22	2.16	0.45
1:A:429:LEU:HG	1:A:440:ILE:HD13	1.99	0.45
1:B:524:LEU:HA	1:B:524:LEU:HD12	1.77	0.45
1:C:478:TYR:CE2	1:C:480:ALA:HA	2.52	0.45
1:G:383:ALA:HB3	1:G:389:MET:HB2	1.99	0.45
1:H:18:ARG:HG3	1:H:67:GLU:CD	2.42	0.45
1:J:193:MET:HE1	1:J:292:ILE:CG1	2.38	0.45
1:J:200:LEU:HG	1:J:276:VAL:HA	1.99	0.45
1:K:18:ARG:HG3	1:K:67:GLU:CD	2.42	0.45
1:L:18:ARG:HG3	1:L:67:GLU:CD	2.42	0.45
1:L:198:GLY:O	1:L:276:VAL:HG12	2.17	0.45
1:L:451:LEU:HD23	1:L:451:LEU:O	2.17	0.45
1:M:478:TYR:CE2	1:M:480:ALA:HA	2.52	0.45
1:N:230:ILE:HB	1:N:258:ALA:HA	1.99	0.45
1:N:413:ALA:CB	1:N:417:VAL:HG22	2.47	0.45
1:A:223:ALA:O	1:A:251:ALA:HA	2.17	0.45
1:D:413:ALA:HB3	1:D:417:VAL:HG22	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:353:ILE:HD13	1:F:366:GLN:HG3	1.99	0.45
1:F:455:VAL:CG1	1:F:460:GLU:HB2	2.46	0.45
1:G:270:ILE:O	1:G:271:VAL:CB	2.64	0.45
1:I:413:ALA:N	1:I:475:ASN:HD22	2.14	0.45
1:J:13:ARG:NH1	1:J:518:GLU:OE2	2.50	0.45
1:J:463:SER:O	1:J:467:ASN:HB2	2.16	0.45
1:K:152:ALA:O	1:K:153:ASN:HB3	2.17	0.45
1:K:252:GLU:O	1:K:253:ASP:HB2	2.16	0.45
1:N:230:ILE:HD13	1:N:261:THR:HG21	1.99	0.45
1:N:247:LEU:HD21	1:N:249:ILE:HD11	1.98	0.45
1:N:310:GLU:OE1	1:N:310:GLU:N	2.47	0.45
1:C:247:LEU:HB3	1:C:273:VAL:HG22	1.98	0.44
1:C:460:GLU:O	1:C:462:PRO:HD3	2.17	0.44
1:E:460:GLU:O	1:E:462:PRO:HD3	2.17	0.44
1:H:229:ASN:C	1:H:231:ARG:H	2.25	0.44
1:H:451:LEU:HD23	1:H:451:LEU:C	2.43	0.44
1:I:176:THR:HG22	1:I:177:VAL:N	2.31	0.44
1:J:219:PHE:HB3	1:J:317:LEU:HD23	1.97	0.44
1:K:112:ASN:HA	1:K:113:PRO:HD3	1.90	0.44
1:K:153:ASN:O	1:K:154:SER:HB2	2.17	0.44
1:L:37:ASN:ND2	1:L:51:LYS:HG3	2.32	0.44
1:M:326:ASN:HB3	1:M:327:LYS:H	1.57	0.44
1:M:392:LYS:O	1:M:396:VAL:HG23	2.17	0.44
1:M:479:ASN:CG	1:M:493:ILE:HD11	2.42	0.44
1:M:486:GLY:C	1:M:491:MET:HE2	2.42	0.44
1:A:524:LEU:HD21	1:G:63:GLU:HB2	1.99	0.44
1:B:82:ASN:HB2	1:B:89:THR:OG1	2.17	0.44
1:D:216:GLU:C	1:D:218:PRO:HD3	2.42	0.44
1:D:305:ILE:O	1:D:305:ILE:HG22	2.16	0.44
1:E:269:GLY:CA	1:F:229:ASN:CG	2.90	0.44
1:E:413:ALA:HB3	1:E:417:VAL:HG22	1.99	0.44
1:G:242:LYS:C	1:G:244:GLY:N	2.67	0.44
1:I:304:GLU:C	1:I:306:GLY:H	2.24	0.44
1:L:5:ASP:HB2	1:L:524:LEU:CD1	2.46	0.44
1:M:252:GLU:O	1:M:253:ASP:HB2	2.17	0.44
1:M:254:VAL:HG12	1:M:259:LEU:HB2	1.99	0.44
1:M:349:ILE:CG2	1:M:369:VAL:HG13	2.48	0.44
1:M:429:LEU:HG	1:M:440:ILE:HD13	1.98	0.44
1:C:496:PRO:HB2	1:C:499:VAL:HG13	1.98	0.44
1:G:273:VAL:CG1	1:G:274:ALA:N	2.80	0.44
1:H:273:VAL:HG12	1:H:274:ALA:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:451:LEU:HD23	1:J:451:LEU:O	2.17	0.44
1:K:100:ILE:O	1:K:104:LEU:HG	2.17	0.44
1:M:144:ILE:HG23	1:M:403:THR:CG2	2.48	0.44
1:M:302:SER:H	1:M:307:MET:HE3	1.83	0.44
1:N:83:ASP:OD2	1:N:327:LYS:CD	2.63	0.44
1:N:144:ILE:HG23	1:N:403:THR:CG2	2.48	0.44
1:A:23:LEU:CD2	1:A:74:VAL:HG22	2.46	0.44
1:B:242:LYS:C	1:B:244:GLY:N	2.75	0.44
1:B:290:GLN:HB3	1:B:345:ARG:NH2	2.33	0.44
1:D:109:ALA:HB2	1:J:109:ALA:HB2	2.00	0.44
1:E:314:LEU:HD23	1:E:317:LEU:CD2	2.45	0.44
1:F:385:THR:OG1	1:F:388:GLU:HG3	2.18	0.44
1:G:413:ALA:HB3	1:G:417:VAL:HG22	1.99	0.44
1:H:114:MET:HE3	6:H:3064:HOH:O	2.17	0.44
1:H:270:ILE:O	1:H:271:VAL:CB	2.66	0.44
1:H:282:GLY:HA3	1:N:181:THR:O	2.17	0.44
1:I:149:THR:HG23	1:I:155:ASP:C	2.42	0.44
1:I:230:ILE:HG21	1:I:261:THR:HG21	1.99	0.44
1:J:38:VAL:HG13	1:K:519:CYS:HB3	2.00	0.44
1:J:233:MET:HE1	1:J:249:ILE:CD1	2.47	0.44
1:J:266:THR:HG21	1:J:273:VAL:HB	1.98	0.44
1:J:344:GLY:O	1:J:347:ALA:HB3	2.17	0.44
1:K:455:VAL:CG1	1:K:460:GLU:HB2	2.45	0.44
1:L:152:ALA:O	1:L:153:ASN:HB3	2.17	0.44
1:M:217:SER:N	1:M:218:PRO:HD3	2.33	0.44
1:N:37:ASN:ND2	1:N:51:LYS:HG3	2.32	0.44
1:A:191:GLU:O	1:A:334:ASP:HA	2.17	0.44
1:E:310:GLU:OE1	1:E:310:GLU:N	2.51	0.44
1:F:359:ASP:HA	1:F:362:ARG:HH12	1.82	0.44
1:F:413:ALA:HB3	1:F:417:VAL:HG22	2.00	0.44
1:F:496:PRO:HB2	1:F:499:VAL:HG13	2.00	0.44
1:H:5:ASP:HB2	1:H:524:LEU:CD1	2.47	0.44
1:I:31:LEU:HD13	1:I:90:THR:HG22	1.99	0.44
1:I:202:PRO:O	1:I:203:TYR:CB	2.62	0.44
1:N:445:ARG:HH22	4:N:1515:MPD:H11	1.81	0.44
1:B:289:LEU:HD23	1:B:289:LEU:HA	1.86	0.44
1:E:242:LYS:C	1:E:244:GLY:N	2.70	0.44
1:F:218:PRO:HD2	1:F:320:ALA:O	2.17	0.44
1:G:183:LEU:HA	1:G:383:ALA:N	2.33	0.44
1:H:262:LEU:O	1:H:266:THR:HG23	2.17	0.44
1:H:272:LYS:NZ	1:I:228:SER:HB3	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:455:VAL:CG1	1:H:460:GLU:HB2	2.48	0.44
1:I:112:ASN:HA	1:I:113:PRO:HD3	1.91	0.44
1:I:194:GLN:O	1:I:371:LYS:HE3	2.18	0.44
1:I:236:VAL:HG22	1:I:312:ALA:O	2.18	0.44
1:I:451:LEU:C	1:I:451:LEU:HD23	2.43	0.44
1:J:202:PRO:C	1:J:204:PHE:H	2.26	0.44
1:J:366:GLN:O	1:J:369:VAL:HG22	2.18	0.44
1:L:25:ASP:HA	1:L:28:LYS:HE2	2.00	0.44
1:L:207:LYS:O	1:L:211:GLY:N	2.50	0.44
1:M:451:LEU:HD23	1:M:451:LEU:O	2.18	0.44
1:N:13:ARG:NH1	1:N:518:GLU:OE2	2.49	0.44
1:A:85:ALA:HB1	1:A:499:VAL:HG12	1.99	0.44
1:A:451:LEU:HD23	1:A:451:LEU:O	2.17	0.44
1:B:202:PRO:O	1:B:203:TYR:HB2	2.18	0.44
1:C:364:LYS:O	1:C:367:GLU:HB2	2.18	0.44
1:C:369:VAL:HG23	1:C:370:ALA:N	2.32	0.44
1:D:460:GLU:O	1:D:462:PRO:HD3	2.18	0.44
1:F:144:ILE:HG23	1:F:403:THR:CG2	2.48	0.44
1:H:118:ARG:HH22	1:N:34:LYS:HE2	1.82	0.44
1:H:219:PHE:HB3	1:H:317:LEU:HD23	2.00	0.44
1:I:242:LYS:O	1:I:243:ALA:CB	2.66	0.44
1:I:329:THR:O	1:I:329:THR:HG22	2.18	0.44
1:J:202:PRO:O	1:J:203:TYR:CB	2.61	0.44
1:J:216:GLU:C	1:J:218:PRO:HD3	2.42	0.44
1:M:303:GLU:HG3	6:M:3108:HOH:O	2.17	0.44
1:B:77:VAL:HG21	1:B:510:VAL:HB	2.00	0.44
1:C:263:VAL:O	1:C:267:MET:HB2	2.18	0.44
1:D:16:MET:HB3	1:D:514:MET:CE	2.48	0.44
1:E:202:PRO:C	1:E:204:PHE:N	2.76	0.44
1:E:429:LEU:HG	1:E:440:ILE:HD13	1.99	0.44
1:F:220:ILE:HD12	1:F:296:THR:HG21	2.00	0.44
1:G:472:GLY:HA3	1:G:476:TYR:CD2	2.53	0.44
1:H:359:ASP:O	1:H:360:TYR:C	2.60	0.44
1:I:23:LEU:CD2	1:I:74:VAL:HG22	2.48	0.44
1:I:201:SER:O	1:I:202:PRO:O	2.36	0.44
1:I:349:ILE:O	1:I:353:ILE:HG13	2.17	0.44
1:J:85:ALA:CB	1:J:499:VAL:HG12	2.42	0.44
1:K:149:THR:HG23	1:K:155:ASP:C	2.42	0.44
1:K:501:ARG:O	1:K:505:GLN:HG3	2.17	0.44
1:L:224:ASP:O	1:L:225:LYS:CB	2.65	0.44
1:L:248:LEU:HD13	1:L:325:ILE:HD11	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:193:MET:CE	1:N:292:ILE:HG12	2.43	0.44
1:B:215:LEU:HB2	1:B:323:VAL:HG22	2.00	0.44
1:C:7:LYS:HG3	1:C:66:PHE:CZ	2.53	0.44
1:E:77:VAL:HG12	1:E:506:TYR:HB3	2.00	0.44
1:E:191:GLU:OE2	4:E:1502:MPD:H53	2.17	0.44
1:E:217:SER:O	1:E:245:LYS:HD3	2.18	0.44
1:G:82:ASN:HB2	1:G:89:THR:OG1	2.18	0.44
1:I:195:PHE:HB2	1:I:279:PRO:HB3	2.00	0.44
1:J:71:ALA:O	1:J:75:LYS:HB2	2.18	0.44
1:J:166:MET:HE2	1:J:171:LYS:HA	2.00	0.44
1:K:217:SER:N	1:K:218:PRO:HD3	2.32	0.44
1:L:455:VAL:CG1	1:L:460:GLU:HB2	2.48	0.44
1:N:146:GLN:O	1:N:150:ILE:HG13	2.18	0.44
1:N:229:ASN:C	1:N:231:ARG:H	2.26	0.44
1:N:381:VAL:HG21	1:N:393:LYS:HA	2.00	0.44
1:N:445:ARG:HG2	2:N:1146:SO4:O2	2.18	0.44
1:A:77:VAL:HG12	1:A:506:TYR:HB3	2.00	0.43
1:A:118:ARG:HD2	1:A:436:GLN:HE22	1.83	0.43
1:A:353:ILE:HG23	1:A:362:ARG:HG3	2.00	0.43
1:B:473:ASP:CG	6:B:3181:HOH:O	2.61	0.43
1:C:38:VAL:HG22	1:D:519:CYS:HB3	2.00	0.43
1:D:85:ALA:HB1	1:D:499:VAL:HG12	1.99	0.43
1:D:132:LYS:O	1:D:135:SER:HB3	2.18	0.43
1:E:149:THR:HG23	1:E:155:ASP:C	2.43	0.43
1:H:49:ILE:HD12	1:I:513:LEU:HD13	1.99	0.43
1:I:486:GLY:C	1:I:491:MET:HE2	2.43	0.43
1:K:219:PHE:CB	1:K:317:LEU:HD23	2.44	0.43
1:K:460:GLU:O	1:K:462:PRO:HD3	2.18	0.43
1:M:234:LEU:O	1:M:238:GLU:HG3	2.18	0.43
1:M:339:GLU:O	1:M:343:GLN:HB2	2.18	0.43
1:M:451:LEU:HD23	1:M:451:LEU:C	2.43	0.43
1:M:456:LEU:HG	4:M:1518:MPD:HM2	2.00	0.43
1:N:486:GLY:C	1:N:491:MET:HE2	2.42	0.43
1:A:263:VAL:O	1:A:267:MET:HB2	2.18	0.43
1:C:230:ILE:HD11	1:C:237:LEU:HD11	2.00	0.43
1:E:169:VAL:HG11	1:E:377:ALA:HB2	2.00	0.43
1:E:416:GLY:HA2	6:E:3146:HOH:O	2.18	0.43
1:H:25:ASP:HA	1:H:28:LYS:HE2	2.01	0.43
1:I:202:PRO:C	1:I:204:PHE:H	2.25	0.43
1:M:34:LYS:HE2	1:N:118:ARG:NH2	2.25	0.43
1:N:18:ARG:NH1	4:N:1526:MPD:H31	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:202:PRO:O	1:N:204:PHE:N	2.43	0.43
1:B:284:ARG:O	1:B:288:MET:HG3	2.18	0.43
1:D:233:MET:O	1:D:234:LEU:C	2.61	0.43
1:D:266:THR:CG2	1:D:273:VAL:H	2.31	0.43
1:D:301:ILE:HD13	1:D:312:ALA:HB2	2.00	0.43
1:E:16:MET:HB3	1:E:514:MET:CE	2.48	0.43
1:F:460:GLU:O	1:F:462:PRO:HD3	2.18	0.43
1:G:372:LEU:HD12	1:G:372:LEU:HA	1.76	0.43
1:H:518:GLU:HG3	4:N:1517:MPD:H12	2.00	0.43
1:I:451:LEU:HD23	1:I:455:VAL:HG23	1.99	0.43
1:J:247:LEU:HD21	1:J:249:ILE:HD11	2.00	0.43
1:J:353:ILE:HD13	1:J:366:GLN:OE1	2.18	0.43
1:L:417:VAL:O	1:L:420:ILE:HG22	2.18	0.43
1:A:102:GLU:HB2	1:A:442:VAL:HG13	2.00	0.43
1:C:201:SER:O	1:C:202:PRO:O	2.36	0.43
1:E:122:LYS:HE2	1:E:429:LEU:HD11	2.00	0.43
1:E:259:LEU:O	1:E:263:VAL:HG23	2.18	0.43
1:E:478:TYR:CE2	1:E:480:ALA:HA	2.53	0.43
1:H:144:ILE:HG23	1:H:403:THR:CG2	2.48	0.43
1:H:314:LEU:HD23	1:H:317:LEU:HD22	1.99	0.43
1:H:429:LEU:HG	1:H:440:ILE:HD13	2.00	0.43
1:I:34:LYS:HE2	1:J:118:ARG:HH22	1.83	0.43
1:J:183:LEU:HD22	1:J:184:GLN:H	1.82	0.43
1:J:417:VAL:O	1:J:420:ILE:HG22	2.18	0.43
1:M:463:SER:O	1:M:467:ASN:HB2	2.18	0.43
1:C:236:VAL:CG2	1:C:312:ALA:HB3	2.48	0.43
1:D:218:PRO:HB3	1:D:246:PRO:HG2	2.00	0.43
1:F:24:ALA:O	1:F:28:LYS:HG2	2.18	0.43
1:G:369:VAL:HG23	1:G:370:ALA:N	2.33	0.43
1:H:295:LEU:HD13	1:H:295:LEU:C	2.43	0.43
1:I:166:MET:HE2	1:I:171:LYS:HA	2.00	0.43
1:I:266:THR:CG2	1:I:273:VAL:HB	2.48	0.43
1:K:372:LEU:HD12	1:K:372:LEU:HA	1.86	0.43
1:M:32:GLY:C	1:M:34:LYS:H	2.27	0.43
1:M:479:ASN:CG	1:M:493:ILE:CD1	2.92	0.43
1:A:90:THR:O	1:A:94:VAL:HG13	2.18	0.43
1:A:266:THR:CG2	1:A:273:VAL:HB	2.48	0.43
1:A:369:VAL:HG23	1:A:370:ALA:N	2.33	0.43
1:B:200:LEU:CD1	1:B:254:VAL:HB	2.49	0.43
1:C:296:THR:HB	1:C:319:GLN:H	1.83	0.43
1:D:200:LEU:CD1	1:D:254:VAL:HB	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:222:LEU:CD1	1:D:293:ALA:HA	2.49	0.43
1:E:183:LEU:O	1:E:184:GLN:CB	2.66	0.43
1:F:349:ILE:CG2	1:F:369:VAL:HG13	2.48	0.43
1:H:149:THR:HG23	1:H:155:ASP:C	2.44	0.43
1:J:18:ARG:HB2	6:J:3074:HOH:O	2.18	0.43
1:K:266:THR:CG2	1:K:273:VAL:HB	2.48	0.43
1:M:258:ALA:O	1:M:262:LEU:HG	2.18	0.43
1:N:16:MET:HB3	1:N:514:MET:CE	2.49	0.43
1:N:202:PRO:C	1:N:204:PHE:N	2.76	0.43
1:C:213:VAL:HB	1:C:325:ILE:HB	2.00	0.43
1:C:501:ARG:HG2	1:C:501:ARG:HH11	1.84	0.43
1:D:264:VAL:HG12	1:D:265:ASN:N	2.34	0.43
1:D:319:GLN:O	1:D:336:VAL:HG23	2.18	0.43
1:H:218:PRO:HD2	1:H:320:ALA:O	2.18	0.43
1:J:131:LEU:HD21	1:J:500:THR:HG22	2.01	0.43
1:J:242:LYS:C	1:J:244:GLY:H	2.27	0.43
1:M:16:MET:O	1:M:20:VAL:HG13	2.19	0.43
1:A:16:MET:O	1:A:20:VAL:HG13	2.18	0.43
1:A:284:ARG:NH1	1:A:364:LYS:HD2	2.33	0.43
1:A:349:ILE:O	1:A:353:ILE:HG13	2.19	0.43
1:B:49:ILE:HD12	1:C:513:LEU:HD13	2.00	0.43
1:B:77:VAL:HG12	1:B:506:TYR:HB3	2.01	0.43
1:B:183:LEU:O	1:B:184:GLN:CB	2.65	0.43
1:D:10:ASN:HB2	6:D:3029:HOH:O	2.19	0.43
1:E:213:VAL:HB	1:E:325:ILE:HB	2.01	0.43
1:E:326:ASN:HB2	1:E:329:THR:HB	2.01	0.43
1:I:180:GLY:HA3	1:I:381:VAL:O	2.19	0.43
1:L:217:SER:N	1:L:218:PRO:HD3	2.34	0.43
1:M:112:ASN:HA	1:M:113:PRO:HD3	1.90	0.43
1:N:176:THR:HG22	1:N:177:VAL:N	2.32	0.43
1:A:182:GLY:O	1:A:183:LEU:C	2.62	0.43
1:A:303:GLU:O	1:A:304:GLU:C	2.61	0.43
1:B:472:GLY:HA3	1:B:476:TYR:CD2	2.54	0.43
1:C:270:ILE:O	1:C:271:VAL:CB	2.66	0.43
1:F:40:LEU:HD13	1:F:59:GLU:HG3	1.99	0.43
1:G:354:GLU:C	1:G:356:ALA:H	2.26	0.43
1:H:193:MET:HE1	1:H:292:ILE:CG1	2.44	0.43
1:I:123:ALA:HB2	1:I:440:ILE:HG23	2.01	0.43
1:I:413:ALA:CB	1:I:417:VAL:HG22	2.49	0.43
1:L:176:THR:HG22	1:L:177:VAL:N	2.33	0.43
1:M:68:ASN:O	1:M:72:GLN:HG2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:198:GLY:O	1:M:276:VAL:HG12	2.19	0.43
1:M:353:ILE:HG23	1:M:362:ARG:HG3	2.01	0.43
1:C:16:MET:O	1:C:20:VAL:HG13	2.18	0.43
1:D:166:MET:CE	1:D:171:LYS:HA	2.48	0.43
1:H:451:LEU:HD23	1:H:455:VAL:HG23	2.00	0.43
1:I:413:ALA:HB3	1:I:417:VAL:HG22	1.99	0.43
1:J:413:ALA:HB3	1:J:417:VAL:HG22	2.00	0.43
1:K:349:ILE:HA	1:K:352:GLN:CG	2.48	0.43
1:M:176:THR:HG22	1:M:177:VAL:N	2.34	0.43
1:M:201:SER:O	1:M:202:PRO:O	2.37	0.43
1:M:460:GLU:O	1:M:462:PRO:HD3	2.18	0.43
1:N:144:ILE:HD11	1:N:171:LYS:HE2	2.00	0.43
1:B:183:LEU:HG	1:B:384:ALA:HB2	2.01	0.42
1:B:462:PRO:HB2	2:B:1136:SO4:O1	2.19	0.42
1:C:326:ASN:ND2	1:C:329:THR:HB	2.28	0.42
1:H:25:ASP:OD1	1:H:28:LYS:HE2	2.19	0.42
1:J:381:VAL:HG21	1:J:393:LYS:HA	2.01	0.42
1:K:37:ASN:HD21	1:K:51:LYS:HE3	1.83	0.42
1:N:112:ASN:HA	1:N:113:PRO:HD3	1.92	0.42
1:N:195:PHE:HB2	1:N:279:PRO:HB3	2.00	0.42
1:N:290:GLN:HB3	1:N:345:ARG:NH2	2.33	0.42
1:A:202:PRO:C	1:A:204:PHE:H	2.23	0.42
1:A:225:LYS:NZ	1:A:232:GLU:OE2	2.52	0.42
1:B:386:GLU:HB2	1:C:281:PHE:HB3	2.00	0.42
1:C:364:LYS:HA	1:C:364:LYS:HD3	1.88	0.42
1:F:112:ASN:HA	1:F:113:PRO:HD3	1.93	0.42
1:F:202:PRO:C	1:F:204:PHE:N	2.77	0.42
1:I:49:ILE:HD12	1:J:513:LEU:HD13	2.01	0.42
1:I:190:VAL:HB	1:I:334:ASP:OD1	2.19	0.42
1:I:372:LEU:HD12	1:I:372:LEU:HA	1.88	0.42
1:L:158:VAL:HG13	1:L:396:VAL:HG22	2.01	0.42
1:L:242:LYS:O	1:L:243:ALA:CB	2.67	0.42
1:L:345:ARG:HA	1:L:348:GLN:NE2	2.32	0.42
1:M:202:PRO:C	1:M:204:PHE:H	2.27	0.42
1:A:16:MET:HB3	1:A:514:MET:CE	2.49	0.42
1:B:336:VAL:O	1:B:337:GLY:C	2.61	0.42
1:C:169:VAL:CG1	1:C:377:ALA:HB2	2.49	0.42
1:D:494:LEU:C	1:D:494:LEU:HD12	2.44	0.42
1:E:455:VAL:CG1	1:E:460:GLU:HB2	2.49	0.42
1:F:82:ASN:HB2	1:F:89:THR:OG1	2.20	0.42
1:F:242:LYS:O	1:F:243:ALA:CB	2.65	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:383:ALA:O	1:F:384:ALA:CB	2.64	0.42
1:H:186:GLU:HB2	1:H:380:LYS:HB2	2.01	0.42
1:H:413:ALA:H	1:H:475:ASN:HD21	1.67	0.42
1:I:501:ARG:O	1:I:505:GLN:HG3	2.18	0.42
1:J:326:ASN:HB3	1:J:327:LYS:H	1.67	0.42
1:J:472:GLY:HA3	1:J:476:TYR:HD2	1.84	0.42
1:K:16:MET:O	1:K:20:VAL:HG13	2.18	0.42
1:M:230:ILE:HB	1:M:258:ALA:HA	2.00	0.42
1:M:501:ARG:O	1:M:505:GLN:HG3	2.18	0.42
1:B:305:ILE:HB	1:B:307:MET:CE	2.50	0.42
1:C:273:VAL:CG1	1:C:274:ALA:N	2.82	0.42
1:D:252:GLU:O	1:D:253:ASP:HB2	2.20	0.42
1:E:131:LEU:HD21	1:E:500:THR:HG22	2.01	0.42
1:E:216:GLU:C	1:E:218:PRO:HD3	2.44	0.42
1:E:296:THR:HB	1:E:319:GLN:H	1.84	0.42
1:K:218:PRO:CB	1:K:246:PRO:HG2	2.47	0.42
1:K:451:LEU:HD23	1:K:451:LEU:O	2.18	0.42
1:L:223:ALA:O	1:L:251:ALA:HA	2.19	0.42
1:L:524:LEU:HD12	1:L:524:LEU:HA	1.86	0.42
1:M:193:MET:HG2	1:M:194:GLN:H	1.84	0.42
1:M:220:ILE:HD12	1:M:296:THR:HG21	2.00	0.42
1:M:293:ALA:O	1:M:297:GLY:N	2.52	0.42
1:M:499:VAL:CG2	1:M:500:THR:N	2.83	0.42
1:A:118:ARG:HD2	1:A:436:GLN:NE2	2.34	0.42
1:C:359:ASP:HA	1:C:362:ARG:HH12	1.84	0.42
1:D:41:ASP:HB2	1:E:69:MET:SD	2.59	0.42
1:F:326:ASN:HB3	1:F:327:LYS:H	1.66	0.42
1:G:218:PRO:HB3	1:G:246:PRO:HG2	2.01	0.42
1:G:514:MET:HE2	1:G:514:MET:HB3	1.89	0.42
1:H:216:GLU:C	1:H:218:PRO:HD3	2.44	0.42
1:I:262:LEU:O	1:I:266:THR:HG23	2.19	0.42
1:I:353:ILE:HG23	1:I:362:ARG:HG3	2.01	0.42
1:J:39:VAL:HG12	1:K:69:MET:HE2	2.01	0.42
1:J:413:ALA:N	1:J:475:ASN:HD22	2.18	0.42
1:J:441:LYS:HA	1:J:441:LYS:HD3	1.88	0.42
1:K:166:MET:CE	1:K:171:LYS:HA	2.49	0.42
1:K:321:LYS:HD2	1:K:334:ASP:OD2	2.20	0.42
1:L:31:LEU:HD13	1:L:90:THR:HG22	2.00	0.42
1:L:203:TYR:C	1:L:205:ILE:N	2.77	0.42
1:M:372:LEU:HD12	1:M:372:LEU:HA	1.88	0.42
1:B:248:LEU:HD13	1:B:325:ILE:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:364:LYS:O	1:F:367:GLU:HB2	2.20	0.42
1:H:16:MET:O	1:H:20:VAL:HG13	2.19	0.42
1:H:441:LYS:O	1:H:445:ARG:HB2	2.20	0.42
1:K:7:LYS:HG3	1:K:66:PHE:CZ	2.54	0.42
1:M:37:ASN:ND2	1:M:51:LYS:HE3	2.33	0.42
1:M:319:GLN:O	1:M:336:VAL:HG23	2.19	0.42
1:N:123:ALA:HB2	1:N:440:ILE:HG23	2.02	0.42
1:B:353:ILE:HG23	1:B:362:ARG:HG3	2.02	0.42
1:B:413:ALA:CB	1:B:475:ASN:HD22	2.31	0.42
1:E:252:GLU:O	1:E:253:ASP:HB2	2.19	0.42
1:E:436:GLN:O	1:E:440:ILE:HG13	2.20	0.42
1:G:176:THR:HG22	1:G:177:VAL:N	2.34	0.42
1:I:310:GLU:OE1	1:I:310:GLU:N	2.49	0.42
1:J:41:ASP:HB2	1:K:69:MET:HE3	2.01	0.42
1:J:114:MET:HE3	6:J:3085:HOH:O	2.20	0.42
1:J:354:GLU:C	1:J:356:ALA:H	2.28	0.42
1:J:363:GLU:HG2	1:J:363:GLU:H	1.70	0.42
1:A:82:ASN:HB2	1:A:89:THR:OG1	2.19	0.42
1:A:200:LEU:CD1	1:A:254:VAL:HB	2.50	0.42
1:A:236:VAL:CG2	1:A:312:ALA:HB3	2.50	0.42
1:D:303:GLU:O	1:D:306:GLY:N	2.45	0.42
1:E:85:ALA:HB1	1:E:499:VAL:HG12	2.01	0.42
1:E:290:GLN:HB3	1:E:345:ARG:NH2	2.35	0.42
1:G:199:TYR:CD2	1:G:326:ASN:O	2.73	0.42
1:H:358:SER:HB3	1:H:361:ASP:OD1	2.20	0.42
1:I:68:ASN:O	1:I:72:GLN:HG2	2.19	0.42
1:I:221:LEU:HD11	1:I:301:ILE:HD12	2.02	0.42
1:I:234:LEU:O	1:I:238:GLU:HG3	2.20	0.42
1:I:242:LYS:C	1:I:244:GLY:H	2.28	0.42
1:J:16:MET:HB3	1:J:514:MET:CE	2.50	0.42
1:L:199:TYR:C	1:L:201:SER:H	2.27	0.42
1:M:236:VAL:HG22	1:M:312:ALA:O	2.19	0.42
1:M:351:GLN:HE21	1:M:351:GLN:C	2.28	0.42
1:N:186:GLU:HB2	1:N:380:LYS:HB2	2.02	0.42
1:A:233:MET:HE1	1:A:249:ILE:HD12	2.02	0.42
1:B:194:GLN:O	1:B:371:LYS:HE3	2.19	0.42
1:B:247:LEU:HD21	1:B:249:ILE:HD11	2.01	0.42
1:C:239:ALA:O	1:C:314:LEU:HD11	2.19	0.42
1:D:118:ARG:HD2	1:D:436:GLN:HE22	1.84	0.42
1:D:336:VAL:O	1:D:336:VAL:HG12	2.18	0.42
1:D:429:LEU:HG	1:D:440:ILE:HD13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:266:THR:CG2	1:E:273:VAL:HB	2.50	0.42
1:F:166:MET:HE2	1:F:171:LYS:HA	2.01	0.42
1:F:183:LEU:O	1:F:184:GLN:CB	2.68	0.42
1:F:216:GLU:C	1:F:218:PRO:HD3	2.45	0.42
1:F:319:GLN:O	1:F:336:VAL:HG23	2.20	0.42
1:G:354:GLU:C	1:G:356:ALA:N	2.78	0.42
1:H:118:ARG:HD2	1:H:436:GLN:NE2	2.34	0.42
1:I:71:ALA:O	1:I:75:LYS:HB2	2.20	0.42
1:J:270:ILE:O	1:J:271:VAL:CB	2.66	0.42
1:J:353:ILE:HG23	1:J:362:ARG:HG3	2.00	0.42
1:K:220:ILE:HD12	1:K:296:THR:CG2	2.50	0.42
1:M:132:LYS:O	1:M:135:SER:HB3	2.20	0.42
1:M:186:GLU:HB2	1:M:380:LYS:HB2	2.01	0.42
1:N:234:LEU:O	1:N:238:GLU:HG3	2.19	0.42
1:N:449:ALA:HA	6:N:3091:HOH:O	2.19	0.42
1:A:413:ALA:HB3	1:A:417:VAL:HG22	2.02	0.42
1:B:59:GLU:O	1:C:4:LYS:HG3	2.20	0.42
1:B:102:GLU:HB2	1:B:442:VAL:HG13	2.00	0.42
1:C:385:THR:H	1:D:281:PHE:HE1	1.68	0.42
1:E:16:MET:O	1:E:20:VAL:HG13	2.20	0.42
1:E:218:PRO:CB	1:E:246:PRO:HG2	2.46	0.42
1:F:413:ALA:CB	1:F:417:VAL:HG22	2.49	0.42
1:G:7:LYS:HE3	1:G:15:LYS:HE3	2.01	0.42
1:H:16:MET:HB3	1:H:514:MET:CE	2.49	0.42
1:I:349:ILE:HA	1:I:352:GLN:CG	2.49	0.42
1:J:118:ARG:HD2	1:J:436:GLN:NE2	2.34	0.42
1:L:349:ILE:HA	1:L:352:GLN:CG	2.48	0.42
1:L:441:LYS:O	1:L:445:ARG:HB2	2.20	0.42
1:M:198:GLY:HA3	1:M:327:LYS:O	2.20	0.42
1:M:413:ALA:HB1	1:M:488:MET:HG3	2.01	0.42
1:A:270:ILE:O	1:A:271:VAL:HB	2.19	0.41
1:B:169:VAL:CG1	1:B:377:ALA:HB2	2.50	0.41
1:B:239:ALA:O	1:B:314:LEU:HD11	2.20	0.41
1:B:436:GLN:O	1:B:440:ILE:HG13	2.19	0.41
1:B:460:GLU:O	1:B:462:PRO:HD3	2.20	0.41
1:B:478:TYR:CE2	1:B:480:ALA:HA	2.55	0.41
1:B:514:MET:HE2	1:B:514:MET:HB3	1.86	0.41
1:C:269:GLY:O	1:D:229:ASN:OD1	2.38	0.41
1:D:118:ARG:HD2	1:D:436:GLN:NE2	2.35	0.41
1:F:463:SER:HB3	1:N:461:GLU:OE2	2.20	0.41
1:G:501:ARG:HG2	1:G:501:ARG:HH11	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:203:TYR:C	1:H:205:ILE:N	2.77	0.41
1:H:354:GLU:C	1:H:356:ALA:H	2.28	0.41
1:J:455:VAL:CG1	1:J:460:GLU:HB2	2.47	0.41
1:K:242:LYS:O	1:K:243:ALA:CB	2.67	0.41
1:L:273:VAL:HG12	1:L:274:ALA:N	2.35	0.41
1:M:13:ARG:NH1	1:M:518:GLU:OE2	2.50	0.41
1:A:478:TYR:CE2	1:A:480:ALA:HA	2.55	0.41
1:C:40:LEU:HD13	1:C:59:GLU:HG3	2.01	0.41
1:C:457:ASN:OD1	4:C:1514:MPD:H13	2.20	0.41
1:D:254:VAL:HG21	1:D:275:ALA:HB1	2.01	0.41
1:E:305:ILE:HG22	1:E:305:ILE:O	2.18	0.41
1:F:217:SER:N	1:F:218:PRO:HD3	2.35	0.41
1:I:83:ASP:OD2	1:I:327:LYS:HE2	2.19	0.41
1:I:144:ILE:HG23	1:I:403:THR:HG21	2.02	0.41
1:I:236:VAL:O	1:I:240:VAL:HG23	2.20	0.41
1:J:30:THR:HG22	1:J:36:ARG:O	2.19	0.41
1:K:207:LYS:O	1:K:211:GLY:N	2.53	0.41
1:L:202:PRO:C	1:L:204:PHE:N	2.78	0.41
1:L:266:THR:CG2	1:L:273:VAL:HB	2.50	0.41
1:M:218:PRO:HD2	1:M:320:ALA:O	2.20	0.41
1:M:304:GLU:C	1:M:306:GLY:N	2.78	0.41
1:A:122:LYS:HE2	1:A:429:LEU:HD11	2.02	0.41
1:A:289:LEU:HA	1:A:289:LEU:HD23	1.86	0.41
1:B:112:ASN:HA	1:B:113:PRO:HD3	1.93	0.41
1:C:118:ARG:HD2	1:C:436:GLN:HE22	1.85	0.41
1:C:233:MET:C	1:C:235:PRO:HD2	2.45	0.41
1:E:220:ILE:CD1	1:E:296:THR:HG21	2.48	0.41
1:G:217:SER:N	1:G:218:PRO:CD	2.84	0.41
1:I:349:ILE:CG2	1:I:369:VAL:HG13	2.50	0.41
1:J:413:ALA:CB	1:J:417:VAL:HG22	2.50	0.41
1:K:132:LYS:O	1:K:135:SER:HB3	2.20	0.41
1:L:326:ASN:HB3	1:L:327:LYS:H	1.75	0.41
1:N:183:LEU:O	1:N:184:GLN:CB	2.58	0.41
1:N:233:MET:HE1	1:N:249:ILE:CD1	2.50	0.41
1:N:262:LEU:O	1:N:266:THR:HG23	2.19	0.41
1:B:233:MET:HE1	1:B:249:ILE:CD1	2.50	0.41
1:C:218:PRO:HB3	1:C:246:PRO:HG2	2.02	0.41
1:F:130:GLU:HG3	6:F:3137:HOH:O	2.19	0.41
1:F:158:VAL:HG13	1:F:396:VAL:HG22	2.03	0.41
1:G:353:ILE:HD13	1:G:366:GLN:HG3	2.01	0.41
1:H:233:MET:HE1	1:H:249:ILE:CD1	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:438:VAL:O	1:H:442:VAL:HG23	2.19	0.41
1:I:188:ASP:OD1	1:I:188:ASP:N	2.54	0.41
1:I:203:TYR:C	1:I:205:ILE:N	2.76	0.41
1:J:123:ALA:HB2	1:J:440:ILE:HG23	2.01	0.41
1:J:134:LEU:HD13	1:J:134:LEU:O	2.20	0.41
1:J:242:LYS:O	1:J:243:ALA:CB	2.64	0.41
1:J:369:VAL:HG23	1:J:370:ALA:N	2.35	0.41
1:J:460:GLU:O	1:J:462:PRO:HD3	2.20	0.41
1:K:144:ILE:HG23	1:K:403:THR:HG21	2.02	0.41
1:K:413:ALA:CB	1:K:417:VAL:HG22	2.50	0.41
1:M:413:ALA:H	1:M:475:ASN:HD21	1.65	0.41
1:A:269:GLY:O	1:B:229:ASN:OD1	2.39	0.41
1:B:63:GLU:HB2	1:C:524:LEU:HD21	2.03	0.41
1:B:141:SER:HB3	6:B:3163:HOH:O	2.19	0.41
1:C:24:ALA:O	1:C:28:LYS:HG2	2.21	0.41
1:C:193:MET:HG3	1:C:371:LYS:HB3	2.03	0.41
1:D:299:THR:N	1:D:316:ASP:O	2.50	0.41
1:F:225:LYS:HB2	1:F:225:LYS:HE3	1.82	0.41
1:G:193:MET:CE	1:G:292:ILE:HG12	2.51	0.41
1:G:342:ILE:O	1:G:346:VAL:HG23	2.21	0.41
1:H:118:ARG:HD2	1:H:436:GLN:HE22	1.86	0.41
1:H:513:LEU:HD13	1:N:49:ILE:CD1	2.51	0.41
1:I:204:PHE:C	1:I:213:VAL:HG22	2.45	0.41
1:J:203:TYR:C	1:J:205:ILE:H	2.29	0.41
1:L:229:ASN:C	1:L:231:ARG:H	2.29	0.41
1:L:319:GLN:HB3	1:L:336:VAL:CG2	2.49	0.41
1:M:272:LYS:NZ	1:N:229:ASN:HD21	2.16	0.41
1:M:413:ALA:HB3	1:M:417:VAL:HG22	2.03	0.41
1:M:472:GLY:HA3	1:M:476:TYR:HD2	1.85	0.41
1:N:224:ASP:O	1:N:225:LYS:CB	2.65	0.41
1:B:213:VAL:HB	1:B:325:ILE:HB	2.03	0.41
1:B:218:PRO:CB	1:B:246:PRO:HG2	2.44	0.41
1:B:452:ARG:HD3	2:B:1136:SO4:O2	2.20	0.41
1:C:122:LYS:HE2	1:C:429:LEU:HD11	2.02	0.41
1:C:176:THR:HG22	1:C:177:VAL:N	2.35	0.41
1:C:224:ASP:O	1:C:225:LYS:HB3	2.21	0.41
1:C:336:VAL:O	1:C:337:GLY:C	2.64	0.41
1:D:49:ILE:HD12	1:E:513:LEU:HD13	2.01	0.41
1:E:342:ILE:O	1:E:346:VAL:HG23	2.21	0.41
1:F:242:LYS:C	1:F:244:GLY:N	2.74	0.41
1:F:270:ILE:O	1:F:271:VAL:CB	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:364:LYS:O	1:G:367:GLU:HB2	2.20	0.41
1:G:478:TYR:CE2	1:G:480:ALA:HA	2.56	0.41
1:G:524:LEU:HD12	1:G:524:LEU:HA	1.77	0.41
1:I:259:LEU:O	1:I:263:VAL:HG23	2.20	0.41
1:J:429:LEU:HG	1:J:440:ILE:HD13	2.03	0.41
1:K:304:GLU:C	1:K:306:GLY:H	2.28	0.41
1:K:369:VAL:HG23	1:K:370:ALA:N	2.35	0.41
1:L:242:LYS:C	1:L:244:GLY:H	2.28	0.41
1:M:25:ASP:OD1	1:M:28:LYS:HE2	2.21	0.41
1:N:205:ILE:HG23	1:N:212:ALA:O	2.20	0.41
1:A:217:SER:N	1:A:218:PRO:HD3	2.35	0.41
1:B:404:ARG:HH11	1:B:404:ARG:CG	2.30	0.41
1:C:233:MET:O	1:C:234:LEU:C	2.64	0.41
1:E:193:MET:HE1	1:E:292:ILE:CG1	2.46	0.41
1:F:262:LEU:O	1:F:266:THR:HG23	2.20	0.41
1:F:271:VAL:HG12	1:F:273:VAL:HG23	2.02	0.41
1:F:445:ARG:HG2	2:F:1141:SO4:O3	2.20	0.41
1:G:24:ALA:O	1:G:28:LYS:HG2	2.21	0.41
1:G:420:ILE:CG1	1:G:448:GLU:HG2	2.46	0.41
1:H:83:ASP:CG	1:H:327:LYS:HD3	2.45	0.41
1:I:183:LEU:HD22	1:I:184:GLN:H	1.85	0.41
1:I:478:TYR:CE2	1:I:480:ALA:HA	2.54	0.41
1:J:16:MET:O	1:J:20:VAL:HG13	2.21	0.41
1:J:155:ASP:CG	1:J:158:VAL:HG23	2.45	0.41
1:K:183:LEU:HD22	1:K:184:GLN:N	2.36	0.41
1:K:351:GLN:C	1:K:351:GLN:HE21	2.28	0.41
1:L:180:GLY:HA3	1:L:381:VAL:O	2.21	0.41
1:L:230:ILE:HD13	1:L:261:THR:HG22	2.01	0.41
1:N:183:LEU:HD22	1:N:184:GLN:N	2.35	0.41
1:B:38:VAL:HG22	1:C:519:CYS:HB3	2.03	0.41
1:B:385:THR:OG1	1:B:388:GLU:HG3	2.20	0.41
1:C:216:GLU:C	1:C:218:PRO:HD3	2.45	0.41
1:C:242:LYS:O	1:C:243:ALA:HB3	2.20	0.41
1:C:353:ILE:HG23	1:C:362:ARG:HG3	2.03	0.41
1:E:13:ARG:HD3	1:E:104:LEU:HD22	2.02	0.41
1:E:71:ALA:O	1:E:75:LYS:HB2	2.21	0.41
1:G:166:MET:CE	1:G:171:LYS:HA	2.51	0.41
1:H:217:SER:N	1:H:218:PRO:HD3	2.34	0.41
1:J:392:LYS:O	1:J:396:VAL:HG23	2.20	0.41
1:K:224:ASP:O	1:K:225:LYS:CB	2.65	0.41
1:K:353:ILE:HG23	1:K:362:ARG:HG3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:413:ALA:HB3	1:L:417:VAL:HG22	2.02	0.41
1:M:85:ALA:CB	1:M:499:VAL:HG12	2.41	0.41
1:M:152:ALA:O	1:M:153:ASN:HB3	2.21	0.41
1:M:193:MET:CG	1:M:194:GLN:N	2.82	0.41
1:N:218:PRO:CA	1:N:246:PRO:HG2	2.50	0.41
1:N:314:LEU:HA	1:N:317:LEU:HD22	2.03	0.41
1:N:352:GLN:HG2	1:N:352:GLN:H	1.68	0.41
1:N:354:GLU:C	1:N:356:ALA:H	2.29	0.41
1:A:372:LEU:HD12	1:A:372:LEU:HA	1.85	0.41
1:B:349:ILE:CG2	1:B:369:VAL:HG13	2.50	0.41
1:B:384:ALA:C	1:B:385:THR:HG23	2.45	0.41
1:C:31:LEU:HD12	1:C:31:LEU:HA	1.83	0.41
1:C:176:THR:HG21	1:C:333:ILE:CD1	2.34	0.41
1:C:266:THR:CG2	1:C:273:VAL:HB	2.50	0.41
1:C:272:LYS:HZ3	1:D:228:SER:HB3	1.86	0.41
1:C:288:MET:O	1:C:292:ILE:HG13	2.20	0.41
1:D:225:LYS:NZ	1:D:232:GLU:OE2	2.54	0.41
1:D:349:ILE:HG21	1:D:369:VAL:HG13	2.03	0.41
1:D:381:VAL:HG21	1:D:393:LYS:HA	2.03	0.41
1:E:326:ASN:ND2	1:E:329:THR:HB	2.30	0.41
1:E:336:VAL:O	1:E:337:GLY:C	2.62	0.41
1:F:204:PHE:C	1:F:213:VAL:HG22	2.46	0.41
1:F:224:ASP:O	1:F:225:LYS:HB3	2.21	0.41
1:F:381:VAL:HG21	1:F:393:LYS:HA	2.02	0.41
1:G:429:LEU:HG	1:G:440:ILE:HD13	2.02	0.41
1:G:496:PRO:HB2	1:G:499:VAL:HG13	2.02	0.41
1:H:221:LEU:HD11	1:H:301:ILE:HD12	2.03	0.41
1:H:230:ILE:HB	1:H:258:ALA:HA	2.03	0.41
1:I:176:THR:CG2	1:I:177:VAL:N	2.83	0.41
1:I:352:GLN:HG2	1:I:352:GLN:H	1.66	0.41
1:J:5:ASP:HB2	1:J:524:LEU:CD1	2.46	0.41
1:J:339:GLU:O	1:J:343:GLN:HB2	2.20	0.41
1:K:30:THR:HB	1:K:51:LYS:O	2.21	0.41
1:K:183:LEU:O	1:K:184:GLN:CB	2.55	0.41
1:K:413:ALA:H	1:K:475:ASN:HD22	1.64	0.41
1:L:136:VAL:HA	1:L:137:PRO:HD3	1.94	0.41
1:L:413:ALA:CB	1:L:417:VAL:HG22	2.51	0.41
1:L:461:GLU:HB2	6:L:3097:HOH:O	2.21	0.41
1:L:514:MET:HE2	1:L:514:MET:HB3	1.91	0.41
1:M:270:ILE:O	1:M:271:VAL:CB	2.69	0.41
1:N:304:GLU:C	1:N:306:GLY:N	2.79	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:457:ASN:HA	4:N:1517:MPD:HM3	2.03	0.41
1:A:193:MET:HG3	1:A:371:LYS:HB3	2.03	0.41
1:D:16:MET:O	1:D:20:VAL:HG13	2.21	0.41
1:D:219:PHE:HB3	1:D:317:LEU:HD23	2.03	0.41
1:E:344:GLY:O	1:E:348:GLN:HG3	2.21	0.41
1:G:264:VAL:HG12	1:G:265:ASN:N	2.36	0.41
1:I:203:TYR:C	1:I:205:ILE:H	2.27	0.41
1:I:233:MET:O	1:I:234:LEU:C	2.64	0.41
1:J:124:VAL:HG21	1:J:508:ALA:CB	2.51	0.41
1:J:199:TYR:C	1:J:201:SER:H	2.28	0.41
1:K:176:THR:HG22	1:K:177:VAL:N	2.36	0.41
1:K:202:PRO:C	1:K:204:PHE:N	2.76	0.41
1:K:225:LYS:HD2	1:K:226:LYS:O	2.20	0.41
1:L:304:GLU:C	1:L:306:GLY:H	2.29	0.41
1:L:451:LEU:HD23	1:L:455:VAL:HG23	2.02	0.41
1:M:199:TYR:CD2	1:M:326:ASN:O	2.74	0.41
1:M:200:LEU:HG	1:M:276:VAL:HA	2.02	0.41
1:N:24:ALA:O	1:N:28:LYS:HG2	2.21	0.41
1:N:240:VAL:HG11	1:N:247:LEU:HB2	2.03	0.41
1:B:413:ALA:CB	1:B:417:VAL:HG22	2.50	0.40
1:C:199:TYR:C	1:C:201:SER:H	2.28	0.40
1:D:221:LEU:HD23	1:D:249:ILE:HD12	2.03	0.40
1:D:230:ILE:HD13	1:D:261:THR:CG2	2.50	0.40
1:D:247:LEU:HD21	1:D:249:ILE:CD1	2.50	0.40
1:F:16:MET:HB3	1:F:514:MET:CE	2.49	0.40
1:F:384:ALA:O	1:F:385:THR:CG2	2.67	0.40
1:G:385:THR:OG1	1:G:388:GLU:HG3	2.20	0.40
1:K:134:LEU:HD12	1:K:412:VAL:HB	2.03	0.40
1:K:232:GLU:HB3	1:K:309:LEU:HB2	2.03	0.40
1:M:118:ARG:HD2	1:M:436:GLN:NE2	2.37	0.40
1:N:392:LYS:O	1:N:396:VAL:HG23	2.21	0.40
1:N:472:GLY:HA3	1:N:476:TYR:HD2	1.86	0.40
1:A:149:THR:HG23	1:A:155:ASP:C	2.46	0.40
1:A:266:THR:HG21	1:A:273:VAL:HB	2.03	0.40
1:C:90:THR:O	1:C:94:VAL:HG13	2.21	0.40
1:C:183:LEU:O	1:C:184:GLN:CB	2.68	0.40
1:C:217:SER:N	1:C:218:PRO:HD3	2.36	0.40
1:D:203:TYR:C	1:D:205:ILE:N	2.75	0.40
1:E:353:ILE:HD13	1:E:366:GLN:HG3	2.04	0.40
1:F:39:VAL:HG12	1:G:69:MET:CE	2.52	0.40
1:F:144:ILE:HG23	1:F:403:THR:HG21	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:85:ALA:HB1	1:G:499:VAL:HG12	2.02	0.40
1:I:451:LEU:HD23	1:I:451:LEU:O	2.20	0.40
1:J:176:THR:HG22	1:J:177:VAL:N	2.36	0.40
1:J:205:ILE:HG23	1:J:212:ALA:O	2.21	0.40
1:K:284:ARG:NH1	6:K:3077:HOH:O	2.53	0.40
1:L:23:LEU:CD2	1:L:74:VAL:HG22	2.51	0.40
1:M:358:SER:HB3	1:M:361:ASP:OD1	2.20	0.40
1:A:233:MET:O	1:A:234:LEU:C	2.65	0.40
1:B:16:MET:O	1:B:20:VAL:HG13	2.21	0.40
1:C:68:ASN:O	1:C:72:GLN:HG2	2.21	0.40
1:D:102:GLU:HB2	1:D:442:VAL:HG13	2.04	0.40
1:F:7:LYS:HE3	1:F:15:LYS:HE3	2.04	0.40
1:F:233:MET:O	1:F:234:LEU:C	2.64	0.40
1:F:524:LEU:HD12	1:F:524:LEU:HA	1.75	0.40
1:H:23:LEU:CD2	1:H:74:VAL:HG22	2.51	0.40
1:H:501:ARG:O	1:H:505:GLN:HG3	2.21	0.40
1:I:256:GLY:O	1:I:257:GLU:C	2.64	0.40
1:J:100:ILE:O	1:J:104:LEU:HG	2.22	0.40
1:J:501:ARG:O	1:J:505:GLN:HG3	2.21	0.40
1:M:144:ILE:HD11	1:M:171:LYS:HE2	2.02	0.40
1:A:13:ARG:HD3	1:A:104:LEU:HD22	2.02	0.40
1:A:364:LYS:HA	1:A:364:LYS:HD3	1.85	0.40
1:B:247:LEU:HB3	1:B:273:VAL:HG22	2.04	0.40
1:C:169:VAL:HG11	1:C:377:ALA:HB2	2.04	0.40
1:C:229:ASN:C	1:C:231:ARG:H	2.28	0.40
1:D:144:ILE:HG23	1:D:403:THR:HG21	2.03	0.40
1:E:131:LEU:CD1	1:E:422:VAL:HG21	2.46	0.40
1:E:190:VAL:HG21	1:E:333:ILE:HG23	2.03	0.40
1:E:242:LYS:O	1:E:244:GLY:N	2.54	0.40
1:F:77:VAL:HG12	1:F:506:TYR:HB3	2.03	0.40
1:F:429:LEU:HG	1:F:440:ILE:HD13	2.03	0.40
1:G:381:VAL:HG21	1:G:393:LYS:HA	2.04	0.40
1:G:383:ALA:O	1:G:384:ALA:CB	2.69	0.40
1:H:524:LEU:HD12	1:H:524:LEU:HA	1.82	0.40
1:I:216:GLU:C	1:I:218:PRO:HD3	2.45	0.40
1:I:496:PRO:O	1:I:497:THR:C	2.63	0.40
1:K:146:GLN:O	1:K:150:ILE:HG13	2.22	0.40
1:K:230:ILE:HG12	1:K:230:ILE:O	2.21	0.40
1:K:339:GLU:O	1:K:343:GLN:HB2	2.22	0.40
1:L:372:LEU:HD12	1:L:372:LEU:HA	1.92	0.40
1:M:71:ALA:O	1:M:75:LYS:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:344:GLY:O	1:M:347:ALA:HB3	2.21	0.40
1:N:71:ALA:O	1:N:75:LYS:HB2	2.22	0.40
1:A:229:ASN:C	1:A:231:ARG:H	2.28	0.40
1:C:7:LYS:HE3	1:C:15:LYS:HE3	2.03	0.40
1:C:29:VAL:HG12	4:C:1514:MPD:H12	2.03	0.40
1:C:144:ILE:HG23	1:C:403:THR:CG2	2.52	0.40
1:C:451:LEU:HD23	1:C:451:LEU:O	2.22	0.40
1:E:185:ASP:HA	1:E:380:LYS:O	2.21	0.40
1:F:153:ASN:O	1:F:154:SER:HB2	2.22	0.40
1:G:218:PRO:HD2	1:G:320:ALA:O	2.22	0.40
1:G:329:THR:O	1:G:329:THR:HG22	2.19	0.40
1:I:31:LEU:HD13	1:I:90:THR:HG21	2.04	0.40
1:I:282:GLY:O	1:I:285:ARG:HB3	2.21	0.40
1:J:256:GLY:O	1:J:257:GLU:C	2.64	0.40
1:K:290:GLN:O	1:K:293:ALA:HB3	2.22	0.40
1:K:344:GLY:O	1:K:347:ALA:HB3	2.21	0.40
1:L:65:LYS:H	1:L:65:LYS:HG2	1.73	0.40
1:L:287:ALA:HB1	1:L:368:ARG:HH12	1.84	0.40
1:M:25:ASP:HA	1:M:28:LYS:HE2	2.04	0.40
1:M:289:LEU:HD23	1:M:289:LEU:HA	1.85	0.40
1:N:144:ILE:HG23	1:N:403:THR:HG21	2.02	0.40
1:N:239:ALA:HB1	1:N:314:LEU:HG	2.03	0.40
1:N:429:LEU:HG	1:N:440:ILE:HD13	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	522/547 (95%)	488 (94%)	26 (5%)	8 (2%)	8	27
1	B	522/547 (95%)	485 (93%)	28 (5%)	9 (2%)	7	24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	522/547 (95%)	489 (94%)	24 (5%)	9 (2%)	7	24
1	D	522/547 (95%)	488 (94%)	25 (5%)	9 (2%)	7	24
1	E	522/547 (95%)	487 (93%)	28 (5%)	7 (1%)	9	30
1	F	522/547 (95%)	493 (94%)	20 (4%)	9 (2%)	7	24
1	G	522/547 (95%)	488 (94%)	26 (5%)	8 (2%)	8	27
1	H	522/547 (95%)	491 (94%)	23 (4%)	8 (2%)	8	27
1	I	522/547 (95%)	491 (94%)	25 (5%)	6 (1%)	11	35
1	J	522/547 (95%)	490 (94%)	26 (5%)	6 (1%)	11	35
1	K	522/547 (95%)	491 (94%)	23 (4%)	8 (2%)	8	27
1	L	522/547 (95%)	488 (94%)	26 (5%)	8 (2%)	8	27
1	M	522/547 (95%)	492 (94%)	22 (4%)	8 (2%)	8	27
1	N	522/547 (95%)	491 (94%)	23 (4%)	8 (2%)	8	27
All	All	7308/7658 (95%)	6852 (94%)	345 (5%)	111 (2%)	8	27

All (111) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	184	GLN
1	B	183	LEU
1	B	184	GLN
1	C	183	LEU
1	C	184	GLN
1	D	183	LEU
1	D	184	GLN
1	E	183	LEU
1	E	184	GLN
1	F	183	LEU
1	F	184	GLN
1	G	183	LEU
1	G	184	GLN
1	A	183	LEU
1	A	256	GLY
1	A	385	THR
1	B	202	PRO
1	B	385	THR
1	C	256	GLY
1	C	385	THR
1	D	31	LEU

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Mol	Chain	Res	Type
1	D	202	PRO
1	D	256	GLY
1	D	385	THR
1	E	202	PRO
1	E	385	THR
1	F	256	GLY
1	F	385	THR
1	G	256	GLY
1	G	385	THR
1	H	256	GLY
1	H	271	VAL
1	I	256	GLY
1	J	225	LYS
1	J	256	GLY
1	K	202	PRO
1	K	256	GLY
1	L	225	LYS
1	L	256	GLY
1	M	256	GLY
1	M	271	VAL
1	N	202	PRO
1	N	225	LYS
1	N	256	GLY
1	A	202	PRO
1	A	271	VAL
1	B	256	GLY
1	B	383	ALA
1	C	202	PRO
1	E	271	VAL
1	E	383	ALA
1	F	225	LYS
1	F	271	VAL
1	G	202	PRO
1	G	271	VAL
1	H	184	GLN
1	H	202	PRO
1	I	184	GLN
1	I	271	VAL
1	J	184	GLN
1	J	202	PRO
1	J	271	VAL
1	K	9	GLY

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Mol	Chain	Res	Type
1	K	184	GLN
1	K	225	LYS
1	K	271	VAL
1	L	184	GLN
1	L	202	PRO
1	L	271	VAL
1	M	202	PRO
1	M	225	LYS
1	N	184	GLN
1	B	225	LYS
1	B	271	VAL
1	C	225	LYS
1	C	271	VAL
1	C	383	ALA
1	D	271	VAL
1	D	383	ALA
1	E	256	GLY
1	F	202	PRO
1	F	383	ALA
1	G	383	ALA
1	I	9	GLY
1	I	202	PRO
1	I	225	LYS
1	M	184	GLN
1	M	201	SER
1	N	271	VAL
1	A	383	ALA
1	H	31	LEU
1	H	225	LYS
1	K	230	ILE
1	M	9	GLY
1	N	230	ILE
1	D	225	LYS
1	H	9	GLY
1	J	9	GLY
1	L	9	GLY
1	N	9	GLY
1	N	201	SER
1	B	234	LEU
1	G	9	GLY
1	L	201	SER
1	A	9	GLY

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Mol	Chain	Res	Type
1	F	9	GLY
1	H	230	ILE
1	K	201	SER
1	L	230	ILE
1	C	9	GLY
1	M	230	ILE

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	404/414 (98%)	383 (95%)	21 (5%)	21	50
1	B	404/414 (98%)	386 (96%)	18 (4%)	24	56
1	C	404/414 (98%)	383 (95%)	21 (5%)	21	50
1	D	404/414 (98%)	384 (95%)	20 (5%)	22	52
1	E	404/414 (98%)	384 (95%)	20 (5%)	22	52
1	F	404/414 (98%)	383 (95%)	21 (5%)	21	50
1	G	404/414 (98%)	384 (95%)	20 (5%)	22	52
1	H	404/414 (98%)	384 (95%)	20 (5%)	22	52
1	I	404/414 (98%)	384 (95%)	20 (5%)	22	52
1	J	404/414 (98%)	385 (95%)	19 (5%)	23	55
1	K	404/414 (98%)	385 (95%)	19 (5%)	23	55
1	L	404/414 (98%)	386 (96%)	18 (4%)	24	56
1	M	404/414 (98%)	383 (95%)	21 (5%)	21	50
1	N	404/414 (98%)	385 (95%)	19 (5%)	23	55
All	All	5656/5796 (98%)	5379 (95%)	277 (5%)	22	52

All (277) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	VAL

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Mol	Chain	Res	Type
1	A	74	VAL
1	A	82	ASN
1	A	89	THR
1	A	94	VAL
1	A	131	LEU
1	A	134	LEU
1	A	177	VAL
1	A	183	LEU
1	A	257	GLU
1	A	284	ARG
1	A	295	LEU
1	A	329	THR
1	A	331	THR
1	A	372	LEU
1	A	398	ASP
1	A	404	ARG
1	A	417	VAL
1	A	422	VAL
1	A	499	VAL
1	A	524	LEU
1	B	20	VAL
1	B	74	VAL
1	B	82	ASN
1	B	89	THR
1	B	94	VAL
1	B	129	GLU
1	B	131	LEU
1	B	134	LEU
1	B	177	VAL
1	B	183	LEU
1	B	257	GLU
1	B	284	ARG
1	B	372	LEU
1	B	404	ARG
1	B	417	VAL
1	B	422	VAL
1	B	499	VAL
1	B	524	LEU
1	C	20	VAL
1	C	74	VAL
1	C	82	ASN
1	C	89	THR

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Mol	Chain	Res	Type
1	C	94	VAL
1	C	129	GLU
1	C	131	LEU
1	C	134	LEU
1	C	177	VAL
1	C	183	LEU
1	C	257	GLU
1	C	284	ARG
1	C	329	THR
1	C	331	THR
1	C	372	LEU
1	C	398	ASP
1	C	404	ARG
1	C	417	VAL
1	C	422	VAL
1	C	499	VAL
1	C	524	LEU
1	D	20	VAL
1	D	74	VAL
1	D	82	ASN
1	D	89	THR
1	D	94	VAL
1	D	131	LEU
1	D	134	LEU
1	D	177	VAL
1	D	183	LEU
1	D	257	GLU
1	D	284	ARG
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	524	LEU
1	E	20	VAL
1	E	74	VAL
1	E	82	ASN
1	E	89	THR
1	E	94	VAL

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Mol	Chain	Res	Type
1	E	131	LEU
1	E	134	LEU
1	E	177	VAL
1	E	183	LEU
1	E	218	PRO
1	E	284	ARG
1	E	329	THR
1	E	331	THR
1	E	372	LEU
1	E	398	ASP
1	E	404	ARG
1	E	417	VAL
1	E	422	VAL
1	E	499	VAL
1	E	524	LEU
1	F	20	VAL
1	F	74	VAL
1	F	82	ASN
1	F	89	THR
1	F	94	VAL
1	F	131	LEU
1	F	134	LEU
1	F	177	VAL
1	F	183	LEU
1	F	257	GLU
1	F	284	ARG
1	F	295	LEU
1	F	329	THR
1	F	331	THR
1	F	372	LEU
1	F	398	ASP
1	F	404	ARG
1	F	417	VAL
1	F	422	VAL
1	F	499	VAL
1	F	524	LEU
1	G	20	VAL
1	G	74	VAL
1	G	82	ASN
1	G	89	THR
1	G	94	VAL
1	G	131	LEU

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Mol	Chain	Res	Type
1	G	134	LEU
1	G	177	VAL
1	G	183	LEU
1	G	257	GLU
1	G	284	ARG
1	G	329	THR
1	G	331	THR
1	G	372	LEU
1	G	398	ASP
1	G	404	ARG
1	G	417	VAL
1	G	422	VAL
1	G	499	VAL
1	G	524	LEU
1	H	20	VAL
1	H	74	VAL
1	H	76	GLU
1	H	77	VAL
1	H	82	ASN
1	H	89	THR
1	H	94	VAL
1	H	183	LEU
1	H	209	GLU
1	H	328	ASP
1	H	329	THR
1	H	331	THR
1	H	351	GLN
1	H	372	LEU
1	H	398	ASP
1	H	404	ARG
1	H	417	VAL
1	H	422	VAL
1	H	499	VAL
1	H	524	LEU
1	I	20	VAL
1	I	74	VAL
1	I	76	GLU
1	I	77	VAL
1	I	82	ASN
1	I	89	THR
1	I	94	VAL
1	I	183	LEU

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Mol	Chain	Res	Type
1	I	209	GLU
1	I	328	ASP
1	I	329	THR
1	I	331	THR
1	I	351	GLN
1	I	372	LEU
1	I	398	ASP
1	I	404	ARG
1	I	417	VAL
1	I	422	VAL
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	82	ASN
1	J	89	THR
1	J	94	VAL
1	J	289	LEU
1	J	328	ASP
1	J	329	THR
1	J	331	THR
1	J	351	GLN
1	J	372	LEU
1	J	398	ASP
1	J	404	ARG
1	J	417	VAL
1	J	422	VAL
1	J	499	VAL
1	J	524	LEU
1	K	20	VAL
1	K	74	VAL
1	K	76	GLU
1	K	77	VAL
1	K	82	ASN
1	K	89	THR
1	K	94	VAL
1	K	183	LEU
1	K	209	GLU
1	K	328	ASP
1	K	329	THR

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Mol	Chain	Res	Type
1	K	331	THR
1	K	351	GLN
1	K	398	ASP
1	K	404	ARG
1	K	417	VAL
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	77	VAL
1	L	82	ASN
1	L	89	THR
1	L	94	VAL
1	L	328	ASP
1	L	329	THR
1	L	331	THR
1	L	351	GLN
1	L	372	LEU
1	L	398	ASP
1	L	404	ARG
1	L	417	VAL
1	L	422	VAL
1	L	499	VAL
1	L	524	LEU
1	M	20	VAL
1	M	74	VAL
1	M	76	GLU
1	M	77	VAL
1	M	82	ASN
1	M	89	THR
1	M	94	VAL
1	M	183	LEU
1	M	209	GLU
1	M	284	ARG
1	M	328	ASP
1	M	329	THR
1	M	331	THR
1	M	351	GLN
1	M	372	LEU
1	M	398	ASP

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Mol	Chain	Res	Type
1	M	404	ARG
1	M	417	VAL
1	M	422	VAL
1	M	499	VAL
1	M	524	LEU
1	N	20	VAL
1	N	74	VAL
1	N	76	GLU
1	N	77	VAL
1	N	82	ASN
1	N	89	THR
1	N	94	VAL
1	N	183	LEU
1	N	209	GLU
1	N	328	ASP
1	N	329	THR
1	N	331	THR
1	N	351	GLN
1	N	398	ASP
1	N	404	ARG
1	N	417	VAL
1	N	422	VAL
1	N	499	VAL
1	N	524	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (107) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	ASN
1	A	146	GLN
1	A	229	ASN
1	A	265	ASN
1	A	319	GLN
1	A	326	ASN
1	A	366	GLN
1	A	401	HIS
1	A	475	ASN
1	B	10	ASN
1	B	37	ASN
1	B	82	ASN
1	B	146	GLN
1	B	265	ASN

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Mol	Chain	Res	Type
1	B	326	ASN
1	B	366	GLN
1	B	401	HIS
1	B	475	ASN
1	C	37	ASN
1	C	146	GLN
1	C	229	ASN
1	C	265	ASN
1	C	326	ASN
1	C	475	ASN
1	D	10	ASN
1	D	146	GLN
1	D	265	ASN
1	D	290	GLN
1	D	326	ASN
1	D	366	GLN
1	D	475	ASN
1	E	37	ASN
1	E	146	GLN
1	E	265	ASN
1	E	319	GLN
1	E	326	ASN
1	E	366	GLN
1	E	401	HIS
1	E	475	ASN
1	F	10	ASN
1	F	37	ASN
1	F	146	GLN
1	F	229	ASN
1	F	265	ASN
1	F	326	ASN
1	F	366	GLN
1	F	475	ASN
1	G	37	ASN
1	G	146	GLN
1	G	265	ASN
1	G	326	ASN
1	G	351	GLN
1	G	366	GLN
1	G	475	ASN
1	H	37	ASN
1	H	82	ASN

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Mol	Chain	Res	Type
1	H	146	GLN
1	H	265	ASN
1	H	319	GLN
1	H	351	GLN
1	H	475	ASN
1	I	37	ASN
1	I	146	GLN
1	I	265	ASN
1	I	343	GLN
1	I	348	GLN
1	I	351	GLN
1	I	475	ASN
1	J	37	ASN
1	J	82	ASN
1	J	146	GLN
1	J	265	ASN
1	J	319	GLN
1	J	351	GLN
1	J	475	ASN
1	K	37	ASN
1	K	82	ASN
1	K	146	GLN
1	K	153	ASN
1	K	229	ASN
1	K	265	ASN
1	K	348	GLN
1	K	351	GLN
1	K	475	ASN
1	L	37	ASN
1	L	82	ASN
1	L	146	GLN
1	L	229	ASN
1	L	265	ASN
1	L	348	GLN
1	L	351	GLN
1	L	475	ASN
1	M	37	ASN
1	M	82	ASN
1	M	146	GLN
1	M	265	ASN
1	M	319	GLN
1	M	351	GLN

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Mol	Chain	Res	Type
1	M	475	ASN
1	N	37	ASN
1	N	82	ASN
1	N	146	GLN
1	N	229	ASN
1	N	265	ASN
1	N	326	ASN
1	N	351	GLN
1	N	475	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 89 ligands modelled in this entry, 14 are monoatomic - leaving 75 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	MPD	E	1528	-	7,7,7	0.53	0	9,10,10	0.85	0
2	SO4	D	1129	-	4,4,4	0.37	0	6,6,6	0.11	0
2	SO4	J	1127	-	4,4,4	0.38	0	6,6,6	0.05	0
2	SO4	G	1109	-	4,4,4	0.37	0	6,6,6	0.07	0
4	MPD	C	1514	-	7,7,7	0.36	0	9,10,10	0.74	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	A	1107	-	4,4,4	0.38	0	6,6,6	0.11	0
4	MPD	E	1521	-	7,7,7	0.52	0	9,10,10	0.86	0
2	SO4	H	1103	-	4,4,4	0.41	0	6,6,6	0.09	0
2	SO4	I	1119	-	4,4,4	0.39	0	6,6,6	0.07	0
4	MPD	A	1511	-	7,7,7	0.53	0	9,10,10	0.85	0
2	SO4	M	1105	-	4,4,4	0.39	0	6,6,6	0.12	0
2	SO4	C	1101	-	4,4,4	0.40	0	6,6,6	0.06	0
4	MPD	F	1520	-	7,7,7	0.46	0	9,10,10	0.86	0
2	SO4	G	1132	-	4,4,4	0.38	0	6,6,6	0.09	0
2	SO4	D	1110	-	4,4,4	0.39	0	6,6,6	0.07	0
4	MPD	I	1505	-	7,7,7	0.49	0	9,10,10	0.91	1 (11%)
4	MPD	L	1500	-	7,7,7	0.55	0	9,10,10	0.93	1 (11%)
2	SO4	C	1137	-	4,4,4	0.38	0	6,6,6	0.11	0
5	PEG	E	2100	-	6,6,6	0.81	0	5,5,5	1.62	1 (20%)
4	MPD	N	1517	-	7,7,7	0.52	0	9,10,10	0.79	0
2	SO4	F	1141	-	4,4,4	0.41	0	6,6,6	0.07	0
4	MPD	B	1512	-	7,7,7	0.47	0	9,10,10	0.79	0
2	SO4	B	1114	-	4,4,4	0.38	0	6,6,6	0.05	0
2	SO4	B	1130	-	4,4,4	0.38	0	6,6,6	0.12	0
2	SO4	N	1146	-	4,4,4	0.39	0	6,6,6	0.12	0
2	SO4	K	1134	-	4,4,4	0.40	0	6,6,6	0.11	0
4	MPD	E	1504	-	7,7,7	0.47	0	9,10,10	0.90	0
2	SO4	L	1116	-	4,4,4	0.39	0	6,6,6	0.05	0
4	MPD	F	1501	-	7,7,7	0.51	0	9,10,10	0.72	0
4	MPD	E	1502	-	7,7,7	0.47	0	9,10,10	0.79	0
4	MPD	B	1513	-	7,7,7	0.55	0	9,10,10	0.86	1 (11%)
2	SO4	D	1112	-	4,4,4	0.41	0	6,6,6	0.12	0
4	MPD	H	1516	-	7,7,7	0.44	0	9,10,10	0.84	0
2	SO4	F	1125	-	4,4,4	0.39	0	6,6,6	0.10	0
4	MPD	F	1522	-	7,7,7	0.38	0	9,10,10	0.73	0
2	SO4	E	1140	-	4,4,4	0.39	0	6,6,6	0.13	0
2	SO4	M	1126	-	4,4,4	0.35	0	6,6,6	0.12	0
2	SO4	K	1145	-	4,4,4	0.39	0	6,6,6	0.09	0
2	SO4	M	1106	-	4,4,4	0.37	0	6,6,6	0.06	0
4	MPD	G	1509	-	7,7,7	0.51	0	9,10,10	0.82	0
4	MPD	I	1524	-	7,7,7	0.46	0	9,10,10	0.83	0
4	MPD	I	1530	-	7,7,7	0.51	0	9,10,10	0.93	0
2	SO4	L	1117	-	4,4,4	0.38	0	6,6,6	0.10	0
4	MPD	B	1510	-	7,7,7	0.34	0	9,10,10	0.84	0
4	MPD	K	1506	-	7,7,7	0.60	0	9,10,10	0.74	0
4	MPD	M	1518	-	7,7,7	0.56	0	9,10,10	0.69	0
2	SO4	J	1118	-	4,4,4	0.37	0	6,6,6	0.10	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	MPD	N	1526	-	7,7,7	0.47	0	9,10,10	0.79	0
2	SO4	B	1136	-	4,4,4	0.37	0	6,6,6	0.11	0
4	MPD	N	1515	-	7,7,7	0.60	0	9,10,10	0.90	1 (11%)
2	SO4	H	1120	-	4,4,4	0.38	0	6,6,6	0.09	0
2	SO4	D	1138	-	4,4,4	0.40	0	6,6,6	0.06	0
4	MPD	K	1527	-	7,7,7	0.43	0	9,10,10	0.79	0
2	SO4	G	1108	-	4,4,4	0.38	0	6,6,6	0.12	0
2	SO4	I	1143	-	4,4,4	0.38	0	6,6,6	0.09	0
2	SO4	H	1142	-	4,4,4	0.39	0	6,6,6	0.10	0
4	MPD	B	1523	-	7,7,7	0.56	0	9,10,10	0.81	0
4	MPD	E	1503	-	7,7,7	0.48	0	9,10,10	0.84	1 (11%)
4	MPD	A	1507	-	7,7,7	0.53	0	9,10,10	0.85	1 (11%)
4	MPD	H	1525	-	7,7,7	0.52	0	9,10,10	0.86	1 (11%)
2	SO4	B	1135	-	4,4,4	0.38	0	6,6,6	0.08	0
2	SO4	J	1111	-	4,4,4	0.37	0	6,6,6	0.06	0
4	MPD	D	1508	-	7,7,7	0.46	0	9,10,10	0.75	0
4	MPD	J	1529	-	7,7,7	0.46	0	9,10,10	0.75	0
2	SO4	C	1124	-	4,4,4	0.39	0	6,6,6	0.10	0
2	SO4	J	1144	-	4,4,4	0.38	0	6,6,6	0.09	0
2	SO4	D	1128	-	4,4,4	0.38	0	6,6,6	0.13	0
2	SO4	E	1123	-	4,4,4	0.37	0	6,6,6	0.07	0
2	SO4	A	1115	-	4,4,4	0.36	0	6,6,6	0.09	0
2	SO4	A	1121	-	4,4,4	0.40	0	6,6,6	0.12	0
2	SO4	A	1139	-	4,4,4	0.36	0	6,6,6	0.10	0
2	SO4	N	1104	-	4,4,4	0.40	0	6,6,6	0.15	0
2	SO4	C	1133	-	4,4,4	0.37	0	6,6,6	0.13	0
2	SO4	B	1113	-	4,4,4	0.37	0	6,6,6	0.11	0
4	MPD	G	1519	-	7,7,7	0.45	0	9,10,10	0.78	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MPD	E	1528	-	-	2/5/5/5	-
4	MPD	E	1521	-	-	0/5/5/5	-
4	MPD	C	1514	-	-	0/5/5/5	-
4	MPD	A	1511	-	-	1/5/5/5	-
4	MPD	F	1520	-	-	3/5/5/5	-
4	MPD	I	1505	-	-	1/5/5/5	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MPD	L	1500	-	-	0/5/5/5	-
5	PEG	E	2100	-	-	1/4/4/4	-
4	MPD	N	1517	-	-	2/5/5/5	-
4	MPD	B	1512	-	-	0/5/5/5	-
4	MPD	F	1501	-	-	2/5/5/5	-
4	MPD	E	1504	-	-	1/5/5/5	-
4	MPD	E	1502	-	-	2/5/5/5	-
4	MPD	B	1513	-	-	2/5/5/5	-
4	MPD	H	1516	-	-	0/5/5/5	-
4	MPD	F	1522	-	-	2/5/5/5	-
4	MPD	I	1524	-	-	0/5/5/5	-
4	MPD	G	1509	-	-	0/5/5/5	-
4	MPD	I	1530	-	-	1/5/5/5	-
4	MPD	K	1506	-	-	2/5/5/5	-
4	MPD	B	1510	-	-	0/5/5/5	-
4	MPD	M	1518	-	-	1/5/5/5	-
4	MPD	N	1526	-	-	0/5/5/5	-
4	MPD	K	1527	-	-	3/5/5/5	-
4	MPD	B	1523	-	-	0/5/5/5	-
4	MPD	E	1503	-	-	0/5/5/5	-
4	MPD	A	1507	-	-	2/5/5/5	-
4	MPD	H	1525	-	-	0/5/5/5	-
4	MPD	D	1508	-	-	2/5/5/5	-
4	MPD	J	1529	-	-	2/5/5/5	-
4	MPD	N	1515	-	-	0/5/5/5	-
4	MPD	G	1519	-	-	2/5/5/5	-

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	2100	PEG	O2-C2-C1	2.59	121.54	110.11
4	I	1505	MPD	O4-C4-C3	2.14	119.88	111.35
4	B	1513	MPD	O4-C4-C3	2.05	119.52	111.35
4	L	1500	MPD	O4-C4-C3	2.05	119.49	111.35
4	H	1525	MPD	O4-C4-C3	2.02	119.38	111.35
4	N	1515	MPD	O4-C4-C3	2.02	119.38	111.35
4	A	1507	MPD	O4-C4-C3	2.01	119.37	111.35
4	E	1503	MPD	O4-C4-C3	2.00	119.32	111.35

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	F	1520	MPD	C1-C2-C3-C4
4	F	1520	MPD	O2-C2-C3-C4
5	E	2100	PEG	O1-C1-C2-O2
4	A	1511	MPD	O2-C2-C3-C4
4	E	1504	MPD	O2-C2-C3-C4
4	I	1530	MPD	O2-C2-C3-C4
4	B	1513	MPD	C1-C2-C3-C4
4	F	1501	MPD	C1-C2-C3-C4
4	F	1522	MPD	CM-C2-C3-C4
4	K	1527	MPD	C1-C2-C3-C4
4	M	1518	MPD	C1-C2-C3-C4
4	N	1517	MPD	CM-C2-C3-C4
4	E	1528	MPD	O2-C2-C3-C4
4	K	1506	MPD	O2-C2-C3-C4
4	K	1527	MPD	O2-C2-C3-C4
4	A	1507	MPD	C1-C2-C3-C4
4	A	1507	MPD	CM-C2-C3-C4
4	B	1513	MPD	CM-C2-C3-C4
4	D	1508	MPD	C1-C2-C3-C4
4	D	1508	MPD	CM-C2-C3-C4
4	E	1502	MPD	C1-C2-C3-C4
4	E	1502	MPD	CM-C2-C3-C4
4	E	1528	MPD	C1-C2-C3-C4
4	F	1501	MPD	CM-C2-C3-C4
4	F	1520	MPD	CM-C2-C3-C4
4	F	1522	MPD	C1-C2-C3-C4
4	G	1519	MPD	C1-C2-C3-C4
4	G	1519	MPD	CM-C2-C3-C4
4	I	1505	MPD	CM-C2-C3-C4
4	J	1529	MPD	C1-C2-C3-C4
4	J	1529	MPD	CM-C2-C3-C4
4	K	1506	MPD	CM-C2-C3-C4
4	K	1527	MPD	CM-C2-C3-C4
4	N	1517	MPD	C1-C2-C3-C4

There are no ring outliers.

14 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	1514	MPD	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	N	1517	MPD	2	0
2	F	1141	SO4	1	0
2	N	1146	SO4	1	0
4	E	1502	MPD	1	0
4	H	1516	MPD	2	0
4	F	1522	MPD	1	0
4	G	1509	MPD	1	0
4	B	1510	MPD	2	0
4	K	1506	MPD	2	0
4	M	1518	MPD	3	0
4	N	1526	MPD	2	0
2	B	1136	SO4	2	0
4	N	1515	MPD	5	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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	524/547 (95%)	-0.11	8 (1%) 72 64	15, 40, 73, 90	0
1	B	524/547 (95%)	0.04	15 (2%) 53 44	15, 43, 75, 91	0
1	C	524/547 (95%)	-0.14	11 (2%) 63 54	17, 43, 75, 90	0
1	D	524/547 (95%)	-0.10	7 (1%) 75 67	15, 41, 73, 90	0
1	E	524/547 (95%)	-0.13	8 (1%) 72 64	17, 42, 74, 90	0
1	F	524/547 (95%)	-0.16	6 (1%) 78 71	16, 40, 75, 90	0
1	G	524/547 (95%)	-0.16	8 (1%) 72 64	16, 40, 73, 88	0
1	H	524/547 (95%)	0.09	23 (4%) 39 30	20, 48, 89, 101	0
1	I	524/547 (95%)	0.11	16 (3%) 51 41	21, 49, 89, 101	0
1	J	524/547 (95%)	0.05	10 (1%) 66 58	19, 48, 89, 102	0
1	K	524/547 (95%)	0.01	6 (1%) 78 71	20, 48, 89, 102	0
1	L	524/547 (95%)	0.26	48 (9%) 14 12	19, 49, 91, 103	0
1	M	524/547 (95%)	0.08	17 (3%) 50 40	20, 49, 90, 103	0
1	N	524/547 (95%)	0.03	11 (2%) 63 54	21, 49, 89, 102	0
All	All	7336/7658 (95%)	-0.01	194 (2%) 57 47	15, 45, 84, 103	0

All (194) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	271	VAL	5.0
1	I	284	ARG	4.4
1	B	489	ILE	4.3
1	M	271	VAL	4.3
1	L	275	ALA	4.1
1	M	270	ILE	4.1
1	E	271	VAL	4.0
1	C	243	ALA	3.7

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Mol	Chain	Res	Type	RSRZ
1	L	236	VAL	3.7
1	B	266	THR	3.7
1	J	284	ARG	3.6
1	L	272	LYS	3.5
1	L	309	LEU	3.5
1	B	271	VAL	3.5
1	L	270	ILE	3.5
1	L	201	SER	3.5
1	J	243	ALA	3.4
1	L	266	THR	3.4
1	L	274	ALA	3.3
1	E	272	LYS	3.3
1	L	234	LEU	3.3
1	H	244	GLY	3.3
1	N	243	ALA	3.3
1	L	210	THR	3.2
1	L	269	GLY	3.2
1	L	200	LEU	3.2
1	B	272	LYS	3.2
1	L	313	THR	3.2
1	M	44	PHE	3.1
1	M	243	ALA	3.1
1	N	271	VAL	3.1
1	A	354	GLU	3.1
1	L	243	ALA	3.0
1	F	284	ARG	3.0
1	N	311	LYS	3.0
1	C	203	TYR	2.9
1	K	270	ILE	2.9
1	L	341	ALA	2.9
1	L	233	MET	2.9
1	L	219	PHE	2.9
1	L	255	GLU	2.9
1	L	229	ASN	2.9
1	H	44	PHE	2.9
1	M	266	THR	2.9
1	L	301	ILE	2.9
1	B	284	ARG	2.8
1	H	362	ARG	2.8
1	L	239	ALA	2.8
1	B	44	PHE	2.8
1	J	314	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	L	259	LEU	2.8
1	A	271	VAL	2.8
1	H	360	TYR	2.8
1	L	264	VAL	2.8
1	H	210	THR	2.8
1	L	202	PRO	2.8
1	L	312	ALA	2.8
1	M	203	TYR	2.8
1	H	209	GLU	2.7
1	N	284	ARG	2.7
1	C	272	LYS	2.7
1	J	44	PHE	2.7
1	H	266	THR	2.7
1	D	284	ARG	2.7
1	K	284	ARG	2.7
1	M	310	GLU	2.7
1	D	44	PHE	2.7
1	M	284	ARG	2.7
1	D	280	GLY	2.7
1	N	360	TYR	2.6
1	H	284	ARG	2.6
1	N	266	THR	2.6
1	K	271	VAL	2.6
1	E	525	PRO	2.6
1	F	44	PHE	2.6
1	I	44	PHE	2.6
1	C	271	VAL	2.6
1	L	300	VAL	2.6
1	B	490	ASP	2.6
1	H	356	ALA	2.6
1	I	271	VAL	2.6
1	H	359	ASP	2.6
1	N	272	LYS	2.5
1	I	266	THR	2.5
1	F	272	LYS	2.5
1	L	302	SER	2.5
1	G	44	PHE	2.5
1	I	314	LEU	2.5
1	K	44	PHE	2.5
1	L	231	ARG	2.5
1	M	272	LYS	2.5
1	B	270	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	44	PHE	2.4
1	I	360	TYR	2.4
1	L	203	TYR	2.4
1	L	260	ALA	2.4
1	E	270	ILE	2.4
1	H	305	ILE	2.4
1	H	349	ILE	2.4
1	L	205	ILE	2.4
1	L	303	GLU	2.4
1	E	184	GLN	2.4
1	K	266	THR	2.4
1	N	210	THR	2.4
1	B	301	ILE	2.4
1	H	230	ILE	2.4
1	L	249	ILE	2.4
1	L	263	VAL	2.4
1	L	267	MET	2.4
1	J	272	LYS	2.3
1	M	204	PHE	2.3
1	N	44	PHE	2.3
1	I	205	ILE	2.3
1	I	230	ILE	2.3
1	M	202	PRO	2.3
1	J	271	VAL	2.3
1	H	184	GLN	2.3
1	H	357	THR	2.3
1	H	272	LYS	2.3
1	G	366	GLN	2.3
1	I	366	GLN	2.3
1	C	305	ILE	2.3
1	G	284	ARG	2.3
1	I	268	ARG	2.3
1	J	484	GLU	2.3
1	B	473	ASP	2.3
1	E	262	LEU	2.3
1	I	272	LYS	2.3
1	I	358	SER	2.3
1	D	242	LYS	2.2
1	H	361	ASP	2.2
1	A	270	ILE	2.2
1	I	349	ILE	2.2
1	N	270	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	L	299	THR	2.2
1	A	358	SER	2.2
1	H	43	SER	2.2
1	L	276	VAL	2.2
1	G	384	ALA	2.2
1	L	241	ALA	2.2
1	D	305	ILE	2.2
1	M	268	ARG	2.2
1	J	266	THR	2.2
1	A	139	SER	2.2
1	G	315	GLU	2.2
1	L	214	GLU	2.2
1	F	271	VAL	2.2
1	E	44	PHE	2.2
1	C	384	ALA	2.2
1	D	354	GLU	2.2
1	I	243	ALA	2.2
1	C	256	GLY	2.2
1	B	302	SER	2.2
1	G	243	ALA	2.2
1	H	339	GLU	2.2
1	I	274	ALA	2.2
1	F	270	ILE	2.1
1	H	301	ILE	2.1
1	L	256	GLY	2.1
1	N	244	GLY	2.1
1	M	360	TYR	2.1
1	F	184	GLN	2.1
1	B	525	PRO	2.1
1	J	230	ILE	2.1
1	L	230	ILE	2.1
1	G	401	HIS	2.1
1	K	272	LYS	2.1
1	I	181	THR	2.1
1	C	284	ARG	2.1
1	B	203	TYR	2.1
1	H	353	ILE	2.1
1	M	239	ALA	2.1
1	M	241	ALA	2.1
1	H	355	GLU	2.1
1	M	267	MET	2.1
1	L	254	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	L	273	VAL	2.1
1	C	525	PRO	2.1
1	J	256	GLY	2.1
1	D	270	ILE	2.1
1	L	305	ILE	2.1
1	L	242	LYS	2.0
1	L	245	LYS	2.0
1	A	401	HIS	2.0
1	H	240	VAL	2.0
1	L	235	PRO	2.0
1	G	314	LEU	2.0
1	B	265	ASN	2.0
1	A	44	PHE	2.0
1	B	280	GLY	2.0
1	E	244	GLY	2.0
1	M	320	ALA	2.0
1	A	172	GLU	2.0
1	C	484	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	A	1115	5/5	0.54	0.16	157,157,158,158	0
4	MPD	I	1524	8/8	0.56	0.26	75,80,83,83	0
4	MPD	E	1521	8/8	0.57	0.21	80,81,84,84	0
3	K	F	3120	1/1	0.62	0.15	81,81,81,81	0
2	SO4	A	1107	5/5	0.65	0.12	128,129,129,129	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	K	I	3040	1/1	0.66	0.15	94,94,94,94	0
3	K	M	3080	1/1	0.69	0.14	87,87,87,87	0
3	K	K	3050	1/1	0.73	0.13	91,91,91,91	0
2	SO4	K	1145	5/5	0.73	0.23	127,127,128,128	0
2	SO4	C	1124	5/5	0.77	0.17	133,133,134,134	0
3	K	C	3100	1/1	0.77	0.14	78,78,78,78	0
2	SO4	E	1140	5/5	0.78	0.22	135,135,136,136	0
5	PEG	E	2100	7/7	0.78	0.28	83,86,88,89	0
2	SO4	N	1146	5/5	0.79	0.21	135,135,136,136	0
4	MPD	N	1526	8/8	0.79	0.26	85,86,87,87	0
3	K	H	3030	1/1	0.79	0.16	86,86,86,86	0
2	SO4	B	1136	5/5	0.80	0.33	130,130,130,130	0
4	MPD	B	1512	8/8	0.80	0.24	69,72,73,74	0
3	K	A	3010	1/1	0.81	0.14	88,88,88,88	0
4	MPD	E	1502	8/8	0.81	0.20	73,75,79,81	0
3	K	G	3130	1/1	0.81	0.14	79,79,79,79	0
3	K	L	3070	1/1	0.81	0.08	71,71,71,71	0
2	SO4	M	1106	5/5	0.81	0.12	147,147,147,147	0
3	K	N	3090	1/1	0.81	0.10	67,67,67,67	0
2	SO4	E	1123	5/5	0.82	0.14	137,137,137,137	0
3	K	D	3020	1/1	0.82	0.09	65,65,65,65	0
3	K	E	3110	1/1	0.82	0.09	80,80,80,80	0
4	MPD	A	1507	8/8	0.82	0.19	56,59,60,62	0
2	SO4	H	1142	5/5	0.82	0.20	120,120,121,121	0
2	SO4	B	1130	5/5	0.83	0.19	132,133,133,133	0
2	SO4	L	1117	5/5	0.83	0.13	146,146,147,147	0
2	SO4	J	1127	5/5	0.83	0.15	137,137,137,138	0
2	SO4	J	1144	5/5	0.83	0.22	129,129,130,131	0
3	K	J	3060	1/1	0.83	0.10	78,78,78,78	0
4	MPD	B	1510	8/8	0.83	0.20	76,76,77,77	0
4	MPD	D	1508	8/8	0.84	0.21	78,80,81,81	0
2	SO4	F	1141	5/5	0.84	0.23	103,104,104,104	0
2	SO4	H	1103	5/5	0.84	0.13	116,116,117,117	0
2	SO4	D	1128	5/5	0.84	0.28	118,118,118,119	0
4	MPD	K	1527	8/8	0.84	0.20	99,101,102,102	0
2	SO4	B	1135	5/5	0.84	0.19	137,138,139,139	0
2	SO4	C	1137	5/5	0.84	0.14	139,140,140,140	0
4	MPD	F	1522	8/8	0.85	0.19	70,73,74,75	0
4	MPD	H	1525	8/8	0.85	0.18	74,75,75,75	0
4	MPD	C	1514	8/8	0.85	0.23	59,60,66,66	0
2	SO4	I	1143	5/5	0.85	0.20	120,121,121,121	0
2	SO4	A	1139	5/5	0.85	0.20	124,124,125,125	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	K	B	3140	1/1	0.85	0.13	70,70,70,70	0
4	MPD	B	1513	8/8	0.86	0.17	45,51,55,56	0
4	MPD	I	1505	8/8	0.86	0.18	63,66,68,68	0
2	SO4	G	1132	5/5	0.86	0.15	145,146,146,146	0
4	MPD	F	1501	8/8	0.87	0.19	54,59,66,68	0
4	MPD	L	1500	8/8	0.87	0.16	43,46,49,49	0
4	MPD	F	1520	8/8	0.87	0.18	41,47,56,57	0
4	MPD	B	1523	8/8	0.87	0.20	77,77,79,79	0
2	SO4	B	1114	5/5	0.88	0.10	130,130,131,132	0
2	SO4	B	1113	5/5	0.88	0.17	112,113,114,114	0
4	MPD	I	1530	8/8	0.88	0.18	58,59,62,62	0
2	SO4	C	1101	5/5	0.88	0.22	101,102,103,103	0
4	MPD	G	1509	8/8	0.88	0.19	55,57,62,65	0
4	MPD	G	1519	8/8	0.88	0.18	57,59,60,60	0
2	SO4	D	1138	5/5	0.88	0.24	134,134,134,135	0
4	MPD	E	1504	8/8	0.89	0.18	52,53,57,59	0
2	SO4	M	1126	5/5	0.89	0.18	115,115,116,116	0
2	SO4	D	1129	5/5	0.89	0.16	144,144,144,144	0
2	SO4	G	1109	5/5	0.89	0.09	85,85,86,86	0
2	SO4	K	1134	5/5	0.89	0.16	109,109,109,110	0
2	SO4	G	1108	5/5	0.90	0.18	116,117,117,118	0
2	SO4	N	1104	5/5	0.90	0.17	108,108,108,108	0
4	MPD	M	1518	8/8	0.90	0.19	64,65,65,66	0
2	SO4	M	1105	5/5	0.90	0.23	124,125,125,125	0
2	SO4	D	1110	5/5	0.90	0.18	113,114,115,115	0
2	SO4	J	1111	5/5	0.91	0.13	111,112,112,112	0
2	SO4	F	1125	5/5	0.91	0.10	110,111,111,111	0
4	MPD	N	1515	8/8	0.91	0.16	67,69,70,70	0
4	MPD	N	1517	8/8	0.91	0.19	67,69,70,71	0
4	MPD	K	1506	8/8	0.91	0.14	46,50,50,51	0
2	SO4	C	1133	5/5	0.91	0.16	139,139,140,140	0
4	MPD	A	1511	8/8	0.92	0.13	42,43,45,45	0
2	SO4	H	1120	5/5	0.92	0.20	107,108,109,109	0
4	MPD	E	1528	8/8	0.92	0.16	63,65,69,70	0
4	MPD	E	1503	8/8	0.92	0.12	56,56,59,59	0
2	SO4	J	1118	5/5	0.93	0.22	104,104,104,105	0
2	SO4	L	1116	5/5	0.94	0.17	114,115,115,115	0
2	SO4	I	1119	5/5	0.94	0.20	105,106,106,107	0
2	SO4	D	1112	5/5	0.94	0.11	88,90,90,90	0
4	MPD	J	1529	8/8	0.95	0.14	55,56,57,57	0
2	SO4	A	1121	5/5	0.95	0.15	98,98,99,99	0
4	MPD	H	1516	8/8	0.95	0.11	48,49,49,49	0

6.5 Other polymers [i](#)

There are no such residues in this entry.