Full wwPDB X-ray Structure Validation Report ⓘ

Sep 17, 2023 – 01:25 AM EDT

PDB ID	:	4WGL
Title	:	Crystal structure of a GroEL D83A/R197A double mutant
Authors	:	Yang, D.; Fei, X.; LaRonde, N.A.; Beckett, D.; Lund, P.A.; Lorimer, G.H.
Deposited on	:	2014-09-19
Resolution	:	3.13 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:

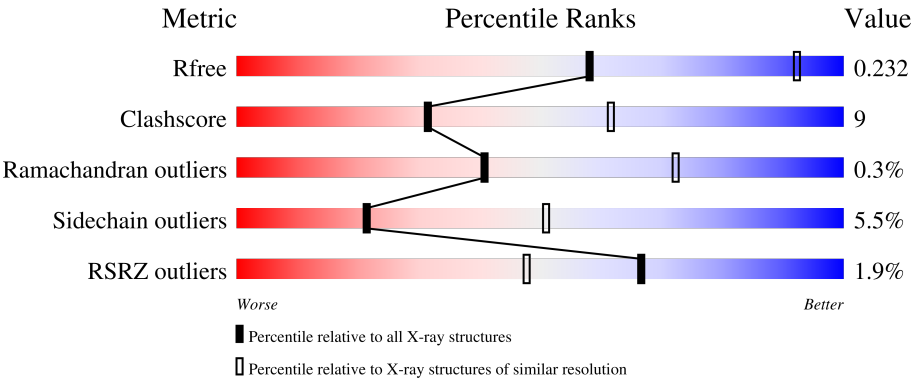
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.13 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1626 (3.18-3.10)
Clashscore	141614	1735 (3.18-3.10)
Ramachandran outliers	138981	1677 (3.18-3.10)
Sidechain outliers	138945	1677 (3.18-3.10)
RSRZ outliers	127900	1588 (3.18-3.10)

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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	548	76% 18%
1	B	548	6% 70% 24%
1	C	548	% 74% 19%
1	D	548	2% 72% 22%
1	E	548	75% 18%

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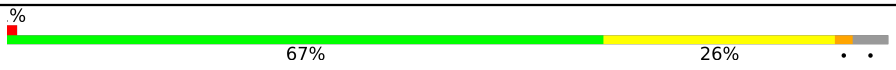
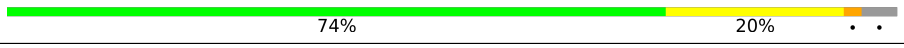
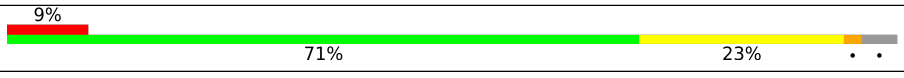
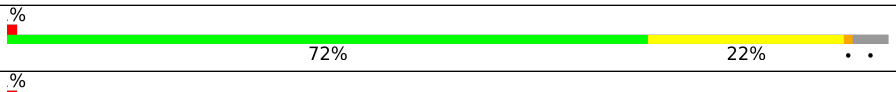
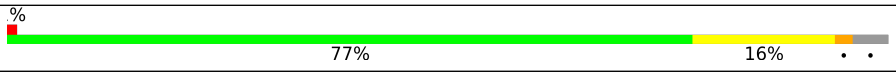
Mol	Chain	Length	Quality of chain
1	F	548	
1	G	548	
1	H	548	
1	I	548	
1	J	548	
1	K	548	
1	L	548	
1	M	548	
1	N	548	

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 53844 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 3846	C 2393	N 662	O 771	S 20	0	0	0
1	B	524	Total 3846	C 2393	N 662	O 771	S 20	0	0	0
1	C	524	Total 3846	C 2393	N 662	O 771	S 20	0	0	0
1	D	524	Total 3846	C 2393	N 662	O 771	S 20	0	0	0
1	E	524	Total 3846	C 2393	N 662	O 771	S 20	0	0	0
1	F	524	Total 3846	C 2393	N 662	O 771	S 20	0	0	0
1	G	524	Total 3846	C 2393	N 662	O 771	S 20	0	0	0
1	H	524	Total 3846	C 2393	N 662	O 771	S 20	0	0	0
1	I	524	Total 3846	C 2393	N 662	O 771	S 20	0	0	0
1	J	524	Total 3846	C 2393	N 662	O 771	S 20	0	0	0
1	K	524	Total 3846	C 2393	N 662	O 771	S 20	0	0	0
1	L	524	Total 3846	C 2393	N 662	O 771	S 20	0	0	0
1	M	524	Total 3846	C 2393	N 662	O 771	S 20	0	0	0
1	N	524	Total 3846	C 2393	N 662	O 771	S 20	0	0	0

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	83	ALA	ASP	engineered mutation	UNP P0A6F5

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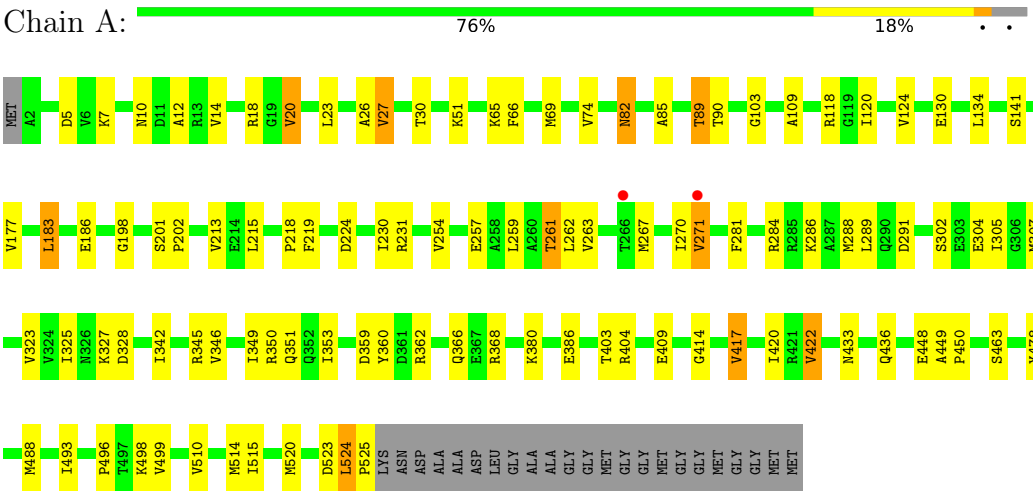
Chain	Residue	Modelled	Actual	Comment	Reference
A	197	ALA	ARG	engineered mutation	UNP P0A6F5
B	83	ALA	ASP	engineered mutation	UNP P0A6F5
B	197	ALA	ARG	engineered mutation	UNP P0A6F5
C	83	ALA	ASP	engineered mutation	UNP P0A6F5
C	197	ALA	ARG	engineered mutation	UNP P0A6F5
D	83	ALA	ASP	engineered mutation	UNP P0A6F5
D	197	ALA	ARG	engineered mutation	UNP P0A6F5
E	83	ALA	ASP	engineered mutation	UNP P0A6F5
E	197	ALA	ARG	engineered mutation	UNP P0A6F5
F	83	ALA	ASP	engineered mutation	UNP P0A6F5
F	197	ALA	ARG	engineered mutation	UNP P0A6F5
G	83	ALA	ASP	engineered mutation	UNP P0A6F5
G	197	ALA	ARG	engineered mutation	UNP P0A6F5
H	83	ALA	ASP	engineered mutation	UNP P0A6F5
H	197	ALA	ARG	engineered mutation	UNP P0A6F5
I	83	ALA	ASP	engineered mutation	UNP P0A6F5
I	197	ALA	ARG	engineered mutation	UNP P0A6F5
J	83	ALA	ASP	engineered mutation	UNP P0A6F5
J	197	ALA	ARG	engineered mutation	UNP P0A6F5
K	83	ALA	ASP	engineered mutation	UNP P0A6F5
K	197	ALA	ARG	engineered mutation	UNP P0A6F5
L	83	ALA	ASP	engineered mutation	UNP P0A6F5
L	197	ALA	ARG	engineered mutation	UNP P0A6F5
M	83	ALA	ASP	engineered mutation	UNP P0A6F5
M	197	ALA	ARG	engineered mutation	UNP P0A6F5
N	83	ALA	ASP	engineered mutation	UNP P0A6F5
N	197	ALA	ARG	engineered mutation	UNP P0A6F5

3 Residue-property plots (i)

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.

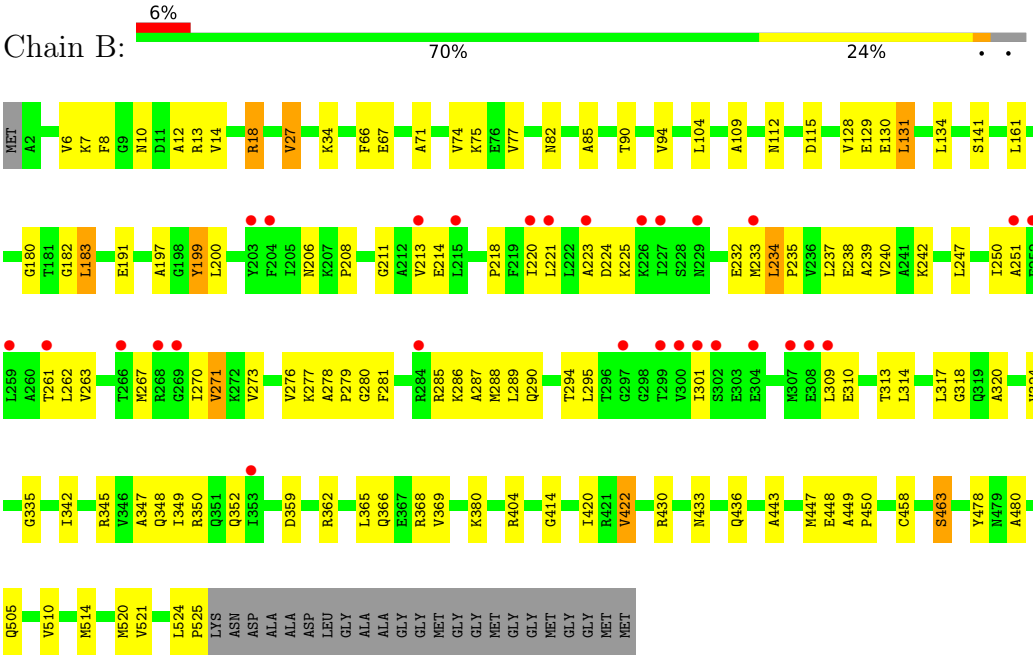
- Molecule 1: 60 kDa chaperonin

Chain A:



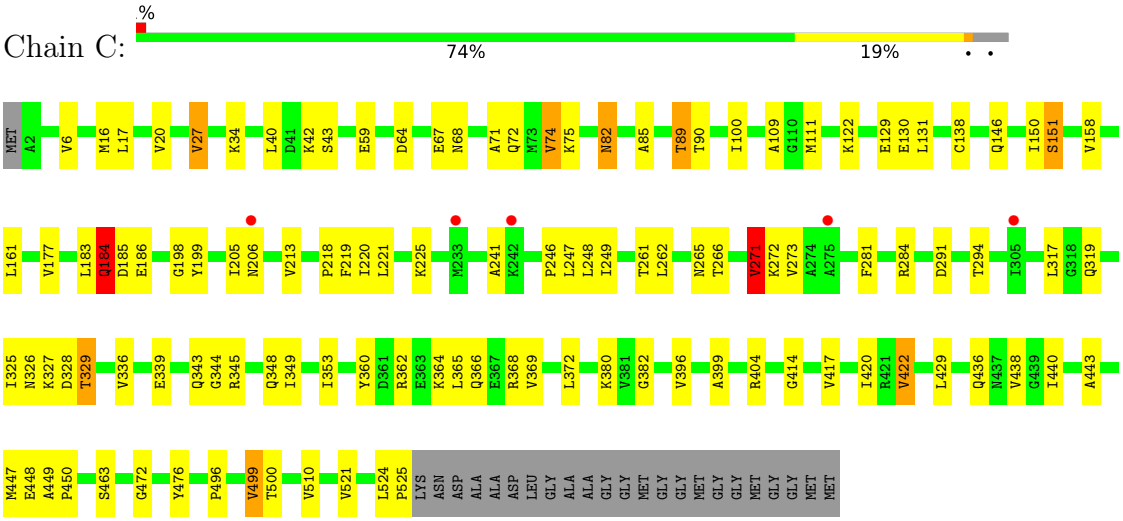
- Molecule 1: 60 kDa chaperonin

Chain B:



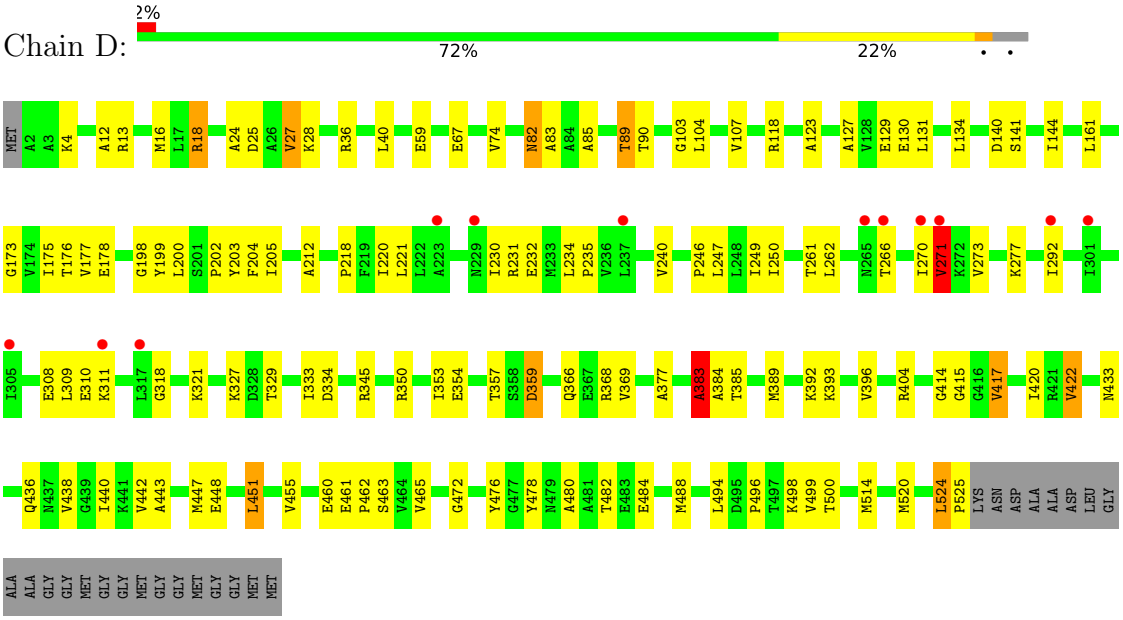
- Molecule 1: 60 kDa chaperonin

Chain C:



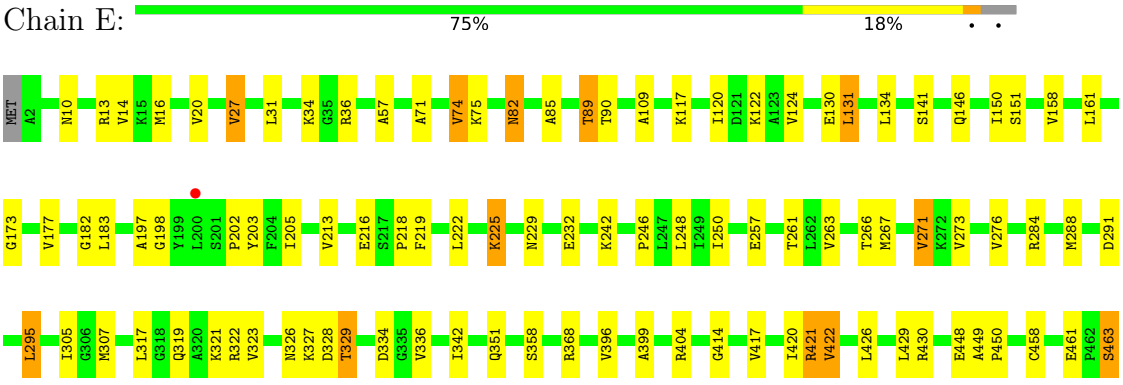
• Molecule 1: 60 kDa chaperonin

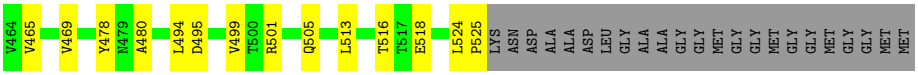
Chain D:



• Molecule 1: 60 kDa chaperonin

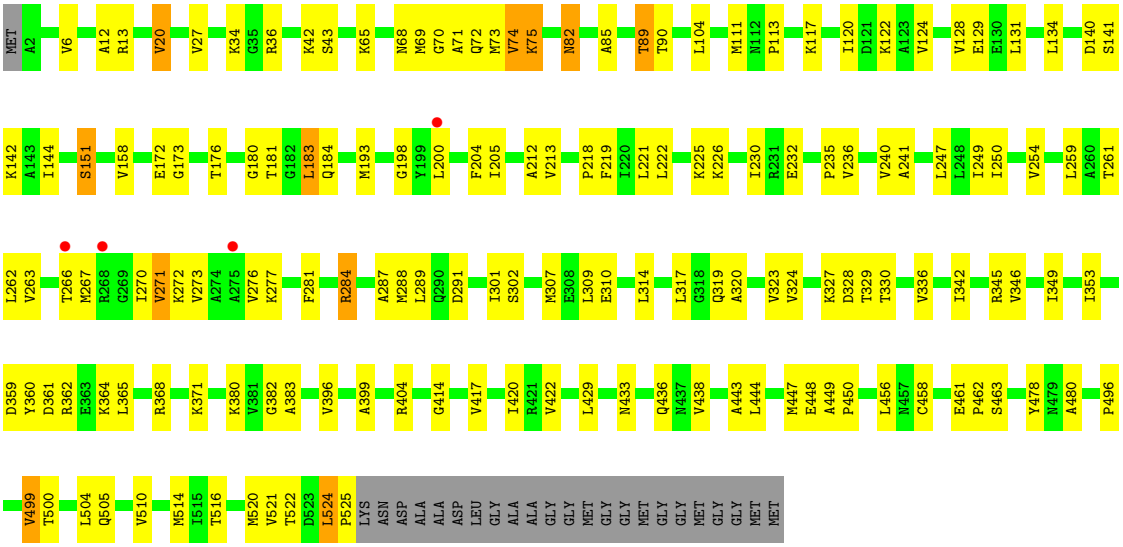
Chain E:





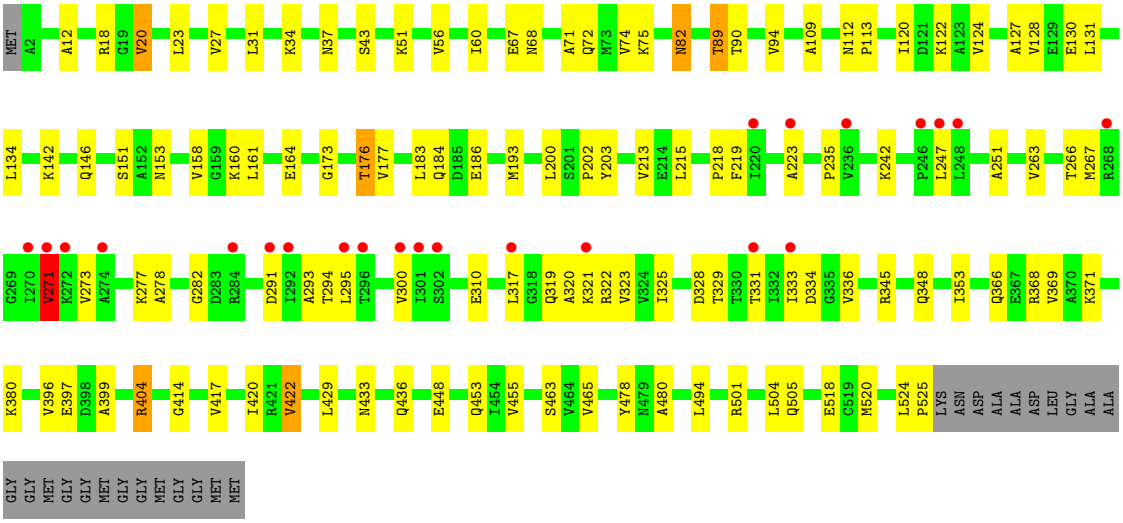
• Molecule 1: 60 kDa chaperonin

Chain F:



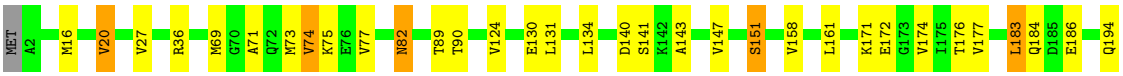
• Molecule 1: 60 kDa chaperonin

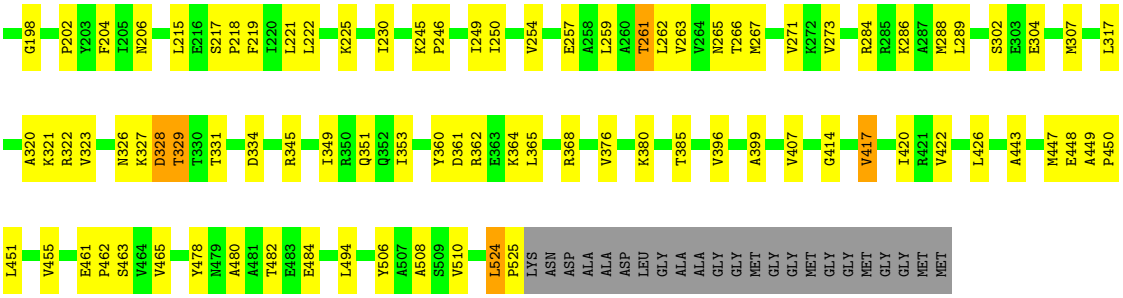
Chain G:



• Molecule 1: 60 kDa chaperonin

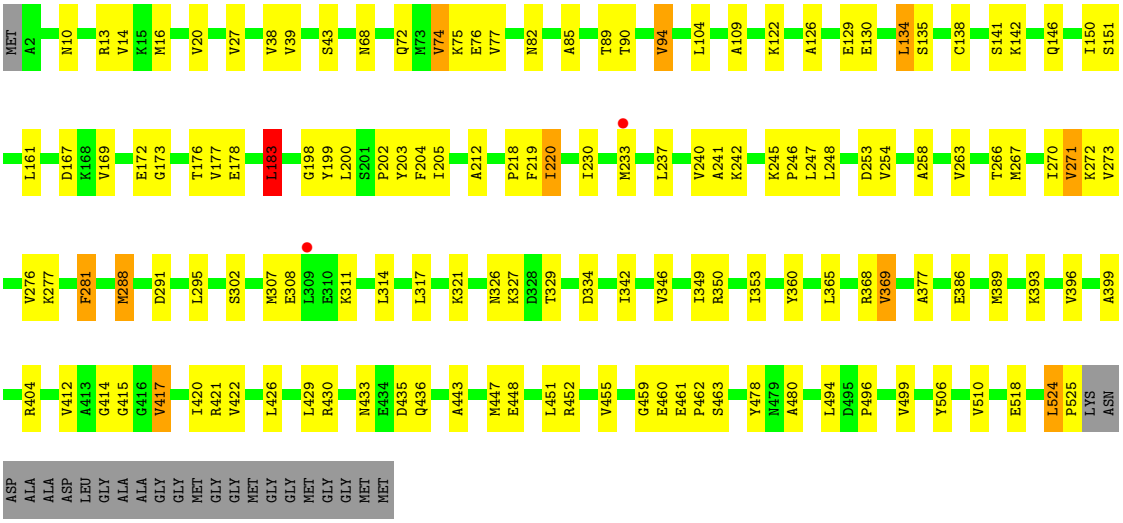
Chain H:





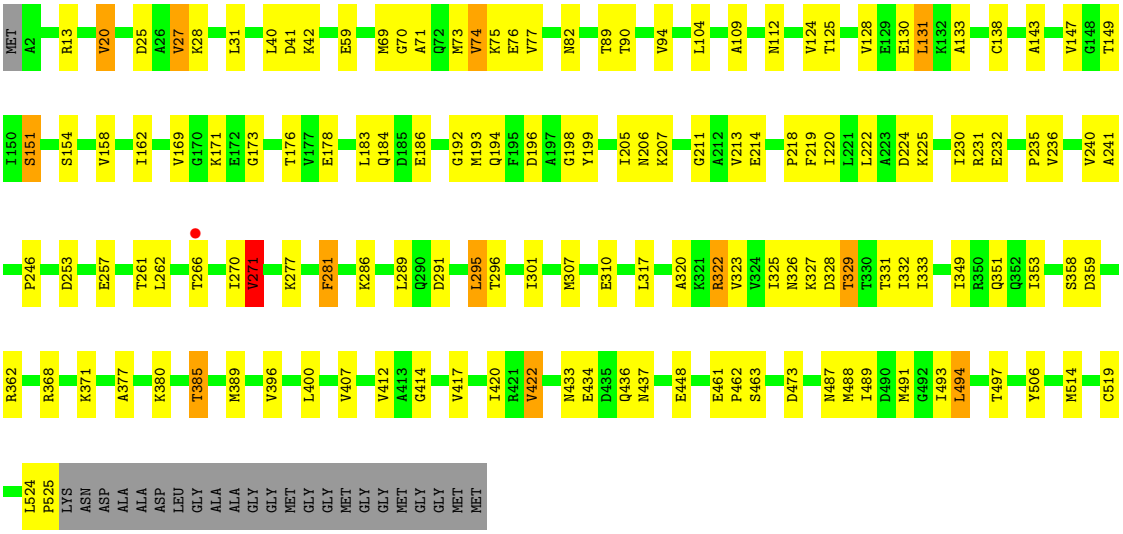
• Molecule 1: 60 kDa chaperonin

Chain I:



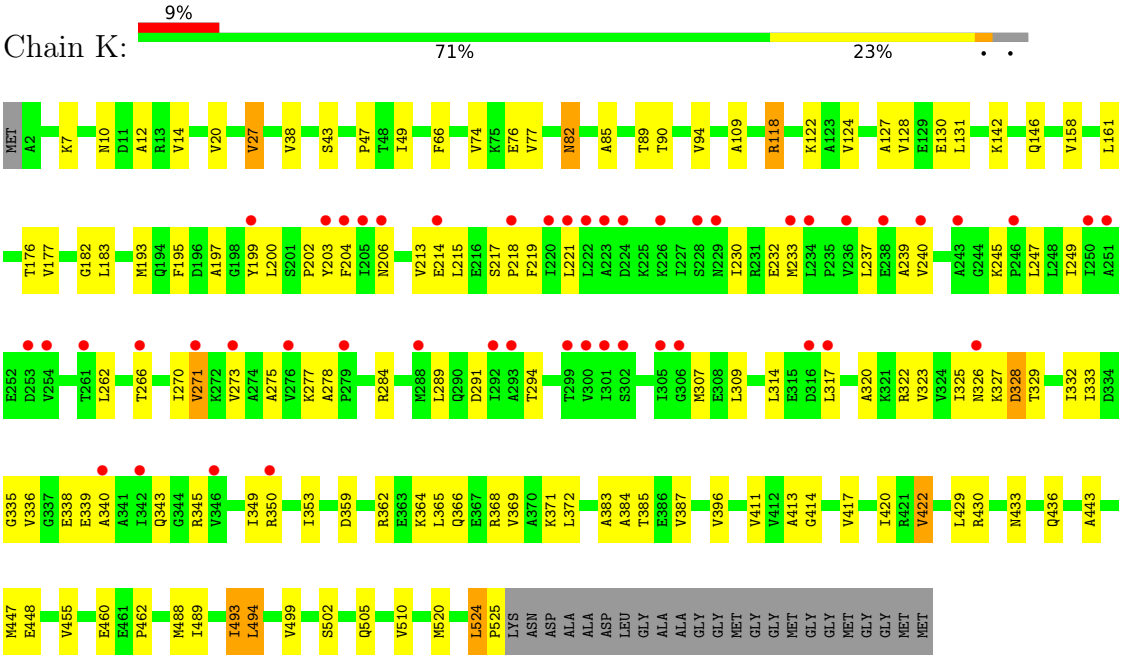
• Molecule 1: 60 kDa chaperonin

Chain J:



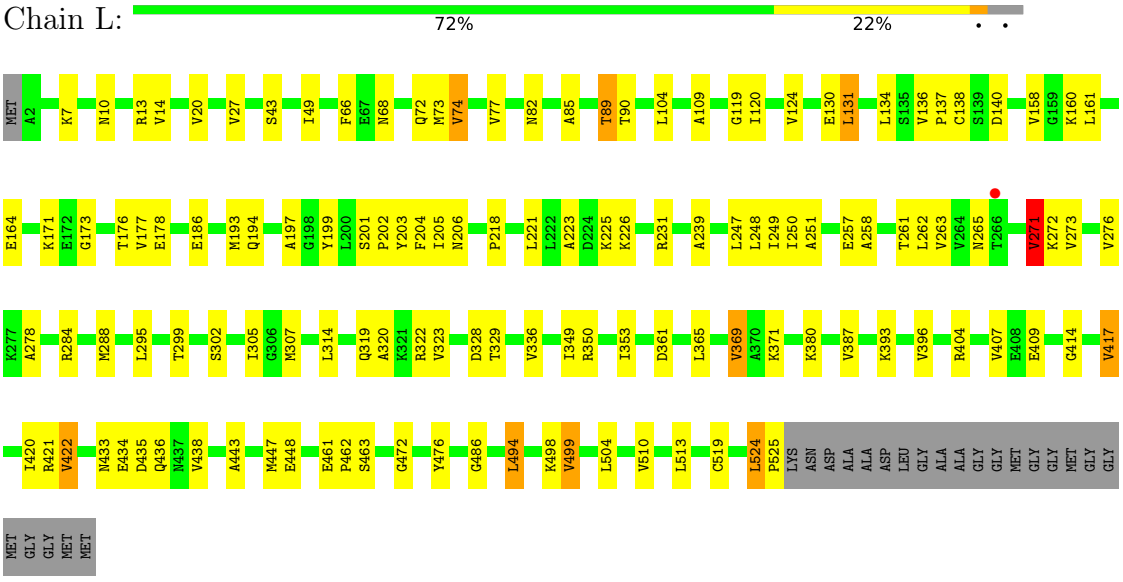
• Molecule 1: 60 kDa chaperonin

Chain K:



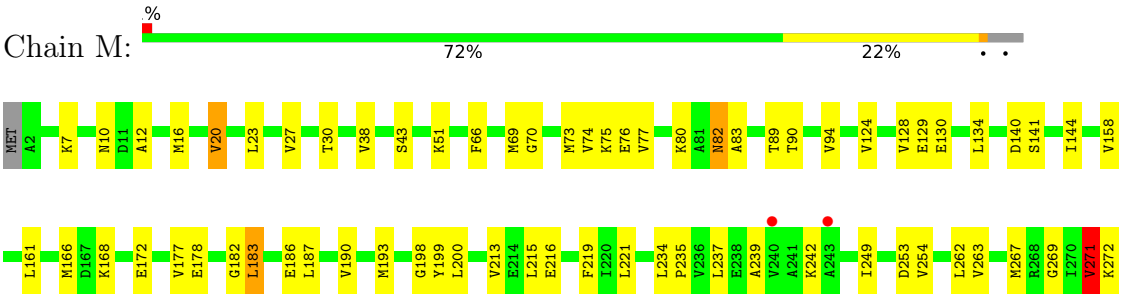
• Molecule 1: 60 kDa chaperonin

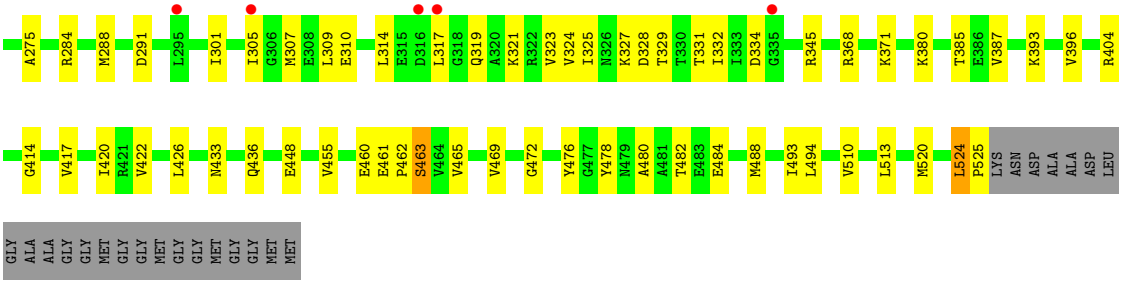
Chain L:



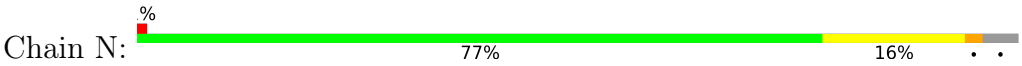
• Molecule 1: 60 kDa chaperonin

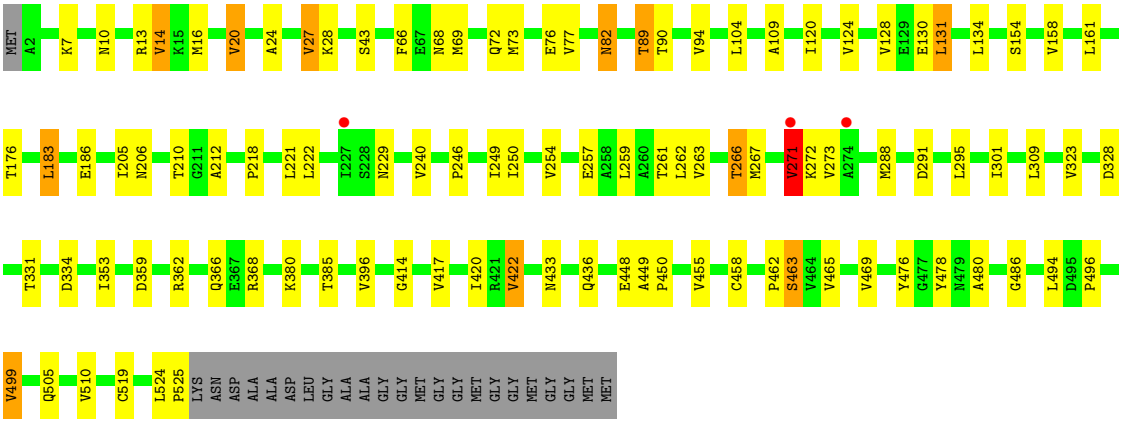
Chain M:





• Molecule 1: 60 kDa chaperonin





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	135.62Å 259.71Å 280.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	123.52 – 3.13 123.52 – 3.13	Depositor EDS
% Data completeness (in resolution range)	99.6 (123.52-3.13) 99.6 (123.52-3.13)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	0.15	Depositor
$< I/\sigma(I) >$ [1]	2.65 (at 3.13Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.166 , 0.233 0.168 , 0.232	Depositor DCC
R_{free} test set	2003 reflections (1.15%)	wwPDB-VP
Wilson B-factor (Å^2)	69.5	Xtriage
Anisotropy	0.402	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 70.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	53844	wwPDB-VP
Average B, all atoms (Å^2)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.62% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.43	0/3874	0.61	0/5232
1	B	0.43	0/3874	0.62	0/5232
1	C	0.42	0/3874	0.60	0/5232
1	D	0.42	0/3874	0.59	1/5232 (0.0%)
1	E	0.42	0/3874	0.61	0/5232
1	F	0.41	0/3874	0.59	0/5232
1	G	0.41	0/3874	0.58	0/5232
1	H	0.45	0/3874	0.62	0/5232
1	I	0.46	0/3874	0.66	1/5232 (0.0%)
1	J	0.46	0/3874	0.63	1/5232 (0.0%)
1	K	0.43	0/3874	0.61	1/5232 (0.0%)
1	L	0.47	0/3874	0.64	0/5232
1	M	0.41	0/3874	0.59	1/5232 (0.0%)
1	N	0.43	0/3874	0.61	0/5232
All	All	0.43	0/54236	0.61	5/73248 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1
1	J	0	1
All	All	0	2

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	I	295	LEU	CA-CB-CG	6.30	129.78	115.30
1	M	183	LEU	CA-CB-CG	5.83	128.70	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	J	131	LEU	CA-CB-CG	5.14	127.11	115.30
1	K	182	GLY	N-CA-C	5.13	125.94	113.10
1	D	383	ALA	N-CA-C	5.11	124.78	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	383	ALA	Peptide
1	J	31	LEU	Peptide

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	3846	0	3969	59	0
1	B	3846	0	3969	83	0
1	C	3846	0	3969	73	0
1	D	3846	0	3969	78	0
1	E	3846	0	3969	64	0
1	F	3846	0	3969	89	0
1	G	3846	0	3969	68	0
1	H	3846	0	3969	71	0
1	I	3846	0	3969	88	0
1	J	3846	0	3969	79	0
1	K	3846	0	3969	87	0
1	L	3846	0	3969	72	0
1	M	3846	0	3969	70	0
1	N	3846	0	3969	54	0
All	All	53844	0	55566	986	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 9.

All (986) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:232:GLU:HB3	1:K:309:LEU:HD11	1.46	0.95
1:F:241:ALA:HA	1:F:271:VAL:HG11	1.51	0.92
1:L:130:GLU:HB3	1:L:422:VAL:HG22	1.51	0.91
1:E:173:GLY:O	1:E:404:ARG:NH2	2.08	0.86
1:E:524:LEU:HD12	1:E:525:PRO:HD2	1.56	0.85
1:J:219:PHE:HB3	1:J:317:LEU:HD23	1.57	0.85
1:F:524:LEU:HD12	1:F:525:PRO:HD2	1.60	0.83
1:G:524:LEU:HD12	1:G:525:PRO:HD2	1.61	0.83
1:A:524:LEU:HD12	1:A:525:PRO:HD2	1.59	0.82
1:J:130:GLU:HB3	1:J:422:VAL:HG22	1.61	0.82
1:A:118:ARG:HH12	1:G:34:LYS:HE2	1.46	0.80
1:H:219:PHE:HB3	1:H:317:LEU:HD23	1.64	0.80
1:D:247:LEU:HB3	1:D:273:VAL:HG22	1.63	0.79
1:B:359:ASP:OD1	1:B:362:ARG:NH1	2.14	0.79
1:B:247:LEU:HB3	1:B:273:VAL:HG22	1.64	0.79
1:H:130:GLU:HB3	1:H:422:VAL:HG22	1.66	0.78
1:I:241:ALA:HA	1:I:271:VAL:HG21	1.66	0.77
1:I:130:GLU:HB3	1:I:422:VAL:HG22	1.65	0.77
1:D:130:GLU:HB3	1:D:422:VAL:HG22	1.67	0.77
1:L:524:LEU:HD12	1:L:525:PRO:HD2	1.67	0.77
1:F:270:ILE:HG22	1:F:271:VAL:HG22	1.66	0.77
1:G:200:LEU:HD21	1:G:277:LYS:HG3	1.66	0.77
1:B:232:GLU:HG2	1:B:309:LEU:HB2	1.68	0.76
1:I:524:LEU:HD12	1:I:525:PRO:HD2	1.68	0.76
1:F:85:ALA:HB1	1:F:499:VAL:HG12	1.69	0.75
1:J:524:LEU:HD12	1:J:525:PRO:HD2	1.68	0.75
1:B:6:VAL:HG22	1:B:521:VAL:HG22	1.69	0.74
1:C:183:LEU:O	1:C:184:GLN:NE2	2.19	0.74
1:C:186:GLU:HB2	1:C:380:LYS:HB2	1.69	0.74
1:M:158:VAL:HG13	1:M:396:VAL:HG22	1.70	0.73
1:A:270:ILE:HG22	1:A:271:VAL:HG23	1.70	0.73
1:H:420:ILE:HG13	1:H:448:GLU:HG2	1.71	0.73
1:K:320:ALA:HA	1:K:335:GLY:HA3	1.72	0.71
1:L:158:VAL:HG13	1:L:396:VAL:HG22	1.72	0.71
1:J:192:GLY:HA2	1:J:295:LEU:HD11	1.72	0.71
1:B:524:LEU:HD12	1:B:525:PRO:HD2	1.72	0.71
1:E:13:ARG:NH2	1:E:518:GLU:OE2	2.23	0.71
1:J:158:VAL:HG13	1:J:396:VAL:HG22	1.72	0.71
1:J:183:LEU:HD23	1:J:184:GLN:HG3	1.73	0.70
1:K:353:ILE:HG23	1:K:362:ARG:HG3	1.72	0.70
1:C:271:VAL:H	1:D:231:ARG:NH1	1.89	0.70
1:H:27:VAL:HG13	1:H:90:THR:HG23	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:173:GLY:O	1:L:404:ARG:NH2	2.24	0.70
1:C:158:VAL:HG13	1:C:396:VAL:HG22	1.72	0.70
1:E:216:GLU:OE1	1:F:226:LYS:NZ	2.25	0.69
1:I:420:ILE:HG13	1:I:448:GLU:HG2	1.74	0.69
1:G:151:SER:HB2	1:G:399:ALA:HA	1.75	0.69
1:F:158:VAL:HG13	1:F:396:VAL:HG22	1.73	0.69
1:G:294:THR:HG21	1:G:345:ARG:HB2	1.75	0.69
1:E:130:GLU:HB3	1:E:422:VAL:HG22	1.75	0.69
1:M:130:GLU:HB3	1:M:422:VAL:HG22	1.74	0.69
1:K:524:LEU:HD12	1:K:525:PRO:HD2	1.75	0.69
1:B:206:ASN:HD22	1:B:214:GLU:H	1.39	0.69
1:M:27:VAL:HG13	1:M:90:THR:HG23	1.74	0.68
1:D:218:PRO:HB3	1:D:246:PRO:HG2	1.75	0.68
1:A:27:VAL:HG13	1:A:90:THR:HG23	1.76	0.68
1:G:293:ALA:HB2	1:G:300:VAL:HG23	1.76	0.68
1:K:420:ILE:HG13	1:K:448:GLU:HG2	1.76	0.68
1:D:173:GLY:O	1:D:404:ARG:NH2	2.27	0.68
1:D:230:ILE:HD12	1:D:261:THR:HG21	1.75	0.67
1:D:420:ILE:HG13	1:D:448:GLU:HG2	1.76	0.67
1:L:27:VAL:HG13	1:L:90:THR:HG23	1.75	0.67
1:K:158:VAL:HG13	1:K:396:VAL:HG22	1.77	0.67
1:N:130:GLU:HB3	1:N:422:VAL:HG22	1.75	0.67
1:I:13:ARG:HD2	1:I:104:LEU:HD22	1.77	0.67
1:K:323:VAL:HG12	1:K:332:ILE:HG12	1.77	0.66
1:N:420:ILE:HG13	1:N:448:GLU:HG2	1.77	0.66
1:F:420:ILE:HG13	1:F:448:GLU:HG2	1.78	0.66
1:C:130:GLU:HB3	1:C:422:VAL:HG22	1.78	0.65
1:G:130:GLU:HB3	1:G:422:VAL:HG22	1.78	0.65
1:B:173:GLY:O	1:B:404:ARG:NH2	2.29	0.65
1:C:40:LEU:HD13	1:C:59:GLU:HG3	1.79	0.65
1:G:353:ILE:HD13	1:G:366:GLN:HG3	1.77	0.65
1:C:85:ALA:HB1	1:C:499:VAL:HG12	1.79	0.65
1:K:278:ALA:HB1	1:K:289:LEU:HD11	1.79	0.65
1:L:13:ARG:HD2	1:L:104:LEU:HD22	1.78	0.64
1:M:38:VAL:HG22	1:N:519:CYS:HB3	1.79	0.64
1:N:218:PRO:HG3	1:N:323:VAL:HG22	1.79	0.64
1:J:489:ILE:HG22	1:J:494:LEU:HD23	1.80	0.64
1:N:353:ILE:HG23	1:N:362:ARG:HG3	1.78	0.64
1:D:200:LEU:HD21	1:D:277:LYS:HG3	1.78	0.64
1:K:130:GLU:HB3	1:K:422:VAL:HG22	1.80	0.64
1:F:200:LEU:HD21	1:F:277:LYS:HG3	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:359:ASP:OD1	1:N:362:ARG:NH1	2.30	0.64
1:F:183:LEU:HD12	1:F:383:ALA:HA	1.79	0.64
1:H:158:VAL:HG13	1:H:396:VAL:HG22	1.79	0.64
1:D:524:LEU:HD12	1:D:525:PRO:HD2	1.80	0.63
1:E:414:GLY:O	1:E:417:VAL:HG13	1.99	0.63
1:B:294:THR:HG22	1:B:342:ILE:HD13	1.80	0.63
1:C:241:ALA:HB1	1:D:231:ARG:HH22	1.63	0.63
1:F:34:LYS:HD2	1:F:458:CYS:HA	1.79	0.63
1:N:27:VAL:HG13	1:N:90:THR:HG23	1.80	0.63
1:B:278:ALA:HB1	1:B:279:PRO:HD2	1.80	0.63
1:F:151:SER:HB2	1:F:399:ALA:HA	1.80	0.63
1:J:359:ASP:OD1	1:J:362:ARG:NH1	2.31	0.63
1:F:6:VAL:HG22	1:F:521:VAL:HG22	1.80	0.62
1:F:122:LYS:HE2	1:F:429:LEU:HD11	1.80	0.62
1:M:186:GLU:HB2	1:M:380:LYS:HB2	1.81	0.62
1:K:338:GLU:HG3	1:K:340:ALA:H	1.64	0.62
1:F:314:LEU:HD23	1:F:317:LEU:HD22	1.80	0.62
1:I:433:ASN:HD21	1:I:436:GLN:HG3	1.64	0.62
1:J:186:GLU:HB2	1:J:380:LYS:HB2	1.81	0.62
1:B:220:ILE:N	1:B:318:GLY:O	2.25	0.62
1:I:126:ALA:HB1	1:I:426:LEU:HD22	1.82	0.62
1:N:229:ASN:ND2	1:N:257:GLU:OE1	2.32	0.62
1:D:366:GLN:HA	1:D:369:VAL:HG22	1.82	0.62
1:K:219:PHE:HB3	1:K:317:LEU:HD23	1.80	0.62
1:C:219:PHE:HB3	1:C:317:LEU:HD23	1.82	0.62
1:H:198:GLY:HA3	1:H:327:LYS:O	1.99	0.62
1:F:12:ALA:HB1	1:F:520:MET:HG3	1.82	0.61
1:M:219:PHE:HB3	1:M:317:LEU:HD23	1.82	0.61
1:M:524:LEU:HD12	1:M:525:PRO:HD2	1.82	0.61
1:H:286:LYS:NZ	1:H:304:GLU:OE2	2.32	0.61
1:A:257:GLU:O	1:A:261:THR:OG1	2.16	0.61
1:I:433:ASN:ND2	1:I:436:GLN:HG3	2.16	0.61
1:C:524:LEU:HD12	1:C:525:PRO:HD2	1.83	0.61
1:L:414:GLY:O	1:L:417:VAL:HG13	2.01	0.61
1:A:386:GLU:HA	1:B:281:PHE:HZ	1.66	0.61
1:D:40:LEU:HD13	1:D:59:GLU:HG3	1.81	0.61
1:E:321:LYS:HB2	1:E:334:ASP:HB3	1.81	0.61
1:G:219:PHE:HB3	1:G:317:LEU:HD23	1.82	0.61
1:N:10:ASN:O	1:N:14:VAL:HG13	2.01	0.61
1:E:288:MET:HG2	1:E:368:ARG:HD3	1.83	0.60
1:G:27:VAL:HG13	1:G:90:THR:HG23	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:199:TYR:CZ	1:B:327:LYS:HA	2.36	0.60
1:I:134:LEU:HD11	1:I:421:ARG:HG2	1.84	0.60
1:N:353:ILE:HD13	1:N:366:GLN:HG3	1.82	0.60
1:A:286:LYS:NZ	1:A:304:GLU:OE2	2.32	0.60
1:G:478:TYR:CE2	1:G:480:ALA:HA	2.35	0.60
1:H:222:LEU:HB3	1:H:289:LEU:HD22	1.84	0.60
1:I:302:SER:H	1:I:307:MET:HE3	1.67	0.60
1:A:305:ILE:HD12	1:A:307:MET:HE2	1.84	0.60
1:J:82:ASN:HB2	1:J:89:THR:OG1	2.01	0.60
1:D:83:ALA:HB2	1:D:327:LYS:HD2	1.83	0.60
1:G:414:GLY:O	1:G:417:VAL:HG13	2.01	0.60
1:H:524:LEU:HD12	1:H:525:PRO:HD2	1.82	0.60
1:B:128:VAL:HG21	1:B:505:GLN:HE21	1.66	0.59
1:L:82:ASN:HB2	1:L:89:THR:OG1	2.02	0.59
1:L:284:ARG:NH2	1:L:361:ASP:OD1	2.36	0.59
1:C:271:VAL:H	1:D:231:ARG:HH12	1.50	0.59
1:C:366:GLN:HA	1:C:369:VAL:HG22	1.84	0.59
1:F:414:GLY:O	1:F:417:VAL:HG13	2.03	0.59
1:J:198:GLY:HA3	1:J:327:LYS:O	2.03	0.59
1:K:291:ASP:OD1	1:K:345:ARG:NE	2.26	0.59
1:F:13:ARG:HD2	1:F:104:LEU:HD22	1.85	0.59
1:J:131:LEU:HD13	1:J:422:VAL:HG21	1.84	0.59
1:G:158:VAL:HG13	1:G:396:VAL:HG22	1.84	0.59
1:H:82:ASN:HB2	1:H:89:THR:OG1	2.03	0.59
1:J:241:ALA:HB2	1:J:271:VAL:HG22	1.83	0.59
1:L:305:ILE:HD12	1:L:307:MET:HE1	1.85	0.59
1:K:213:VAL:HB	1:K:325:ILE:HB	1.85	0.58
1:C:420:ILE:HG13	1:C:448:GLU:HG2	1.86	0.58
1:N:301:ILE:HG21	1:N:309:LEU:HD23	1.85	0.58
1:D:232:GLU:HB3	1:D:309:LEU:HB2	1.85	0.58
1:B:130:GLU:HB3	1:B:422:VAL:HG22	1.86	0.58
1:G:321:LYS:HB2	1:G:334:ASP:HB3	1.85	0.58
1:D:359:ASP:OD1	1:D:359:ASP:N	2.35	0.58
1:E:257:GLU:O	1:E:261:THR:OG1	2.16	0.58
1:E:291:ASP:OD2	1:E:368:ARG:HD2	2.03	0.58
1:N:13:ARG:HD2	1:N:104:LEU:HD22	1.85	0.58
1:H:183:LEU:HD22	1:I:360:TYR:HB2	1.86	0.58
1:E:27:VAL:HG13	1:E:90:THR:HG23	1.86	0.58
1:K:366:GLN:HA	1:K:369:VAL:HG22	1.86	0.58
1:A:414:GLY:O	1:A:417:VAL:HG13	2.03	0.58
1:F:319:GLN:HB3	1:F:336:VAL:HG21	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:147:VAL:O	1:H:151:SER:OG	2.22	0.58
1:J:178:GLU:OE1	1:J:322:ARG:NH1	2.36	0.58
1:G:120:ILE:O	1:G:124:VAL:HG23	2.04	0.57
1:M:219:PHE:HE1	1:M:319:GLN:HE21	1.50	0.57
1:B:250:ILE:HG23	1:B:276:VAL:HG11	1.87	0.57
1:B:270:ILE:HG22	1:B:271:VAL:HG23	1.87	0.57
1:H:328:ASP:OD1	1:H:328:ASP:N	2.38	0.57
1:D:131:LEU:HD21	1:D:500:THR:HG22	1.86	0.57
1:E:225:LYS:NZ	1:E:232:GLU:OE2	2.36	0.57
1:F:266:THR:HB	1:F:272:LYS:HA	1.87	0.57
1:J:291:ASP:OD2	1:J:368:ARG:HD2	2.04	0.57
1:B:18:ARG:HG2	1:B:67:GLU:CD	2.25	0.57
1:I:430:ARG:HG2	1:I:430:ARG:HH11	1.69	0.57
1:N:449:ALA:HB3	1:N:450:PRO:HD3	1.86	0.57
1:D:271:VAL:O	1:D:273:VAL:HG23	2.04	0.57
1:G:124:VAL:HG13	1:G:504:LEU:HG	1.87	0.57
1:H:186:GLU:HB2	1:H:380:LYS:HB2	1.87	0.57
1:K:128:VAL:HG21	1:K:505:GLN:HE21	1.69	0.57
1:B:240:VAL:HG11	1:B:247:LEU:HB2	1.87	0.57
1:D:178:GLU:HA	1:D:393:LYS:HE2	1.86	0.56
1:E:109:ALA:HB2	1:N:109:ALA:HB2	1.86	0.56
1:E:478:TYR:CE2	1:E:480:ALA:HA	2.40	0.56
1:F:496:PRO:HB2	1:F:499:VAL:HG13	1.86	0.56
1:G:176:THR:HG21	1:G:333:ILE:HD11	1.87	0.56
1:I:219:PHE:HB3	1:I:317:LEU:HD23	1.86	0.56
1:C:266:THR:HB	1:C:272:LYS:HA	1.86	0.56
1:C:284:ARG:NH1	1:C:364:LYS:HG3	2.20	0.56
1:M:455:VAL:HG13	1:M:460:GLU:HB2	1.87	0.56
1:J:27:VAL:HG13	1:J:90:THR:HG23	1.87	0.56
1:N:291:ASP:OD2	1:N:368:ARG:HD2	2.05	0.56
1:J:13:ARG:HD2	1:J:104:LEU:HD22	1.87	0.56
1:C:183:LEU:HD12	1:C:184:GLN:H	1.71	0.56
1:F:219:PHE:HB3	1:F:317:LEU:HD23	1.88	0.56
1:I:85:ALA:HB1	1:I:499:VAL:HG12	1.88	0.56
1:M:198:GLY:HA3	1:M:327:LYS:O	2.05	0.56
1:H:414:GLY:O	1:H:417:VAL:HG13	2.06	0.56
1:J:147:VAL:O	1:J:151:SER:OG	2.23	0.56
1:F:82:ASN:HB2	1:F:89:THR:OG1	2.06	0.56
1:G:124:VAL:O	1:G:128:VAL:HG23	2.05	0.56
1:E:198:GLY:HA3	1:E:327:LYS:O	2.06	0.55
1:K:127:ALA:O	1:K:131:LEU:HB2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:254:VAL:HG12	1:F:259:LEU:HB2	1.88	0.55
1:G:177:VAL:HG21	1:G:397:GLU:HG3	1.87	0.55
1:D:27:VAL:HG13	1:D:90:THR:HG23	1.89	0.55
1:I:218:PRO:HB3	1:I:246:PRO:HG2	1.88	0.55
1:F:198:GLY:HA3	1:F:327:LYS:O	2.06	0.55
1:K:489:ILE:HG23	1:K:494:LEU:HD23	1.88	0.55
1:L:85:ALA:HB1	1:L:499:VAL:HG12	1.89	0.55
1:E:219:PHE:HB3	1:E:317:LEU:HD23	1.89	0.55
1:E:501:ARG:NH1	1:E:505:GLN:OE1	2.40	0.55
1:L:134:LEU:HD11	1:L:421:ARG:HG2	1.88	0.55
1:L:247:LEU:HB3	1:L:273:VAL:HG22	1.88	0.55
1:G:433:ASN:ND2	1:G:436:GLN:HG3	2.21	0.55
1:J:224:ASP:OD2	1:J:286:LYS:HG2	2.07	0.55
1:M:269:GLY:HA3	1:N:229:ASN:ND2	2.22	0.55
1:A:130:GLU:HB3	1:A:422:VAL:HG22	1.88	0.55
1:B:250:ILE:HA	1:B:276:VAL:HB	1.89	0.55
1:N:476:TYR:HA	1:N:486:GLY:O	2.06	0.55
1:A:345:ARG:O	1:A:349:ILE:HG13	2.07	0.54
1:C:184:GLN:O	1:C:382:GLY:HA3	2.08	0.54
1:A:186:GLU:HB2	1:A:380:LYS:HB2	1.89	0.54
1:H:284:ARG:O	1:H:288:MET:HG3	2.08	0.54
1:I:200:LEU:HD21	1:I:277:LYS:HG3	1.89	0.54
1:K:291:ASP:OD2	1:K:368:ARG:NH1	2.40	0.54
1:N:128:VAL:HG21	1:N:505:GLN:HE21	1.73	0.54
1:N:222:LEU:HD23	1:N:250:ILE:HB	1.87	0.54
1:A:291:ASP:OD2	1:A:368:ARG:HD2	2.07	0.54
1:C:345:ARG:O	1:C:349:ILE:HG13	2.08	0.54
1:F:124:VAL:HG13	1:F:504:LEU:HG	1.89	0.54
1:J:220:ILE:HD12	1:J:296:THR:HG21	1.89	0.54
1:M:433:ASN:ND2	1:M:436:GLN:HG3	2.23	0.54
1:G:186:GLU:HB2	1:G:380:LYS:HB2	1.89	0.54
1:K:322:ARG:HB3	1:K:333:ILE:HD12	1.88	0.54
1:B:208:PRO:HA	1:B:211:GLY:HA2	1.89	0.54
1:K:74:VAL:HA	1:K:510:VAL:HG21	1.89	0.54
1:I:414:GLY:O	1:I:417:VAL:HG13	2.08	0.54
1:J:323:VAL:HG12	1:J:332:ILE:HG12	1.89	0.54
1:M:77:VAL:HG21	1:M:510:VAL:HB	1.90	0.54
1:M:291:ASP:OD2	1:M:368:ARG:HD2	2.07	0.54
1:K:443:ALA:O	1:K:447:MET:HG3	2.07	0.54
1:D:433:ASN:ND2	1:D:436:GLN:HG3	2.23	0.54
1:G:18:ARG:HD2	1:G:67:GLU:OE2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:131:LEU:HD13	1:B:422:VAL:HG21	1.90	0.53
1:H:266:THR:HG22	1:H:271:VAL:HG23	1.88	0.53
1:A:420:ILE:HG13	1:A:448:GLU:HG2	1.90	0.53
1:B:257:GLU:O	1:B:261:THR:OG1	2.15	0.53
1:I:270:ILE:HG22	1:I:271:VAL:HG23	1.89	0.53
1:K:38:VAL:HG22	1:L:519:CYS:HB3	1.89	0.53
1:K:359:ASP:OD1	1:K:362:ARG:NH1	2.39	0.53
1:C:20:VAL:HB	1:C:74:VAL:HG11	1.90	0.53
1:M:414:GLY:O	1:M:417:VAL:HG13	2.07	0.53
1:B:345:ARG:NH1	1:B:348:GLN:OE1	2.42	0.53
1:D:308:GLU:H	1:D:311:LYS:HD3	1.74	0.53
1:H:151:SER:HB2	1:H:399:ALA:HA	1.89	0.53
1:K:218:PRO:HG3	1:K:323:VAL:HG22	1.91	0.53
1:M:253:ASP:OD1	1:M:254:VAL:N	2.41	0.53
1:M:417:VAL:HA	1:M:420:ILE:HG22	1.91	0.53
1:K:49:ILE:HD12	1:L:513:LEU:HD13	1.90	0.53
1:A:215:LEU:HB2	1:A:323:VAL:HG22	1.90	0.53
1:B:240:VAL:HG21	1:B:247:LEU:HD22	1.91	0.53
1:D:461:GLU:OE2	1:N:463:SER:HB3	2.09	0.53
1:A:478:TYR:CE2	1:A:480:ALA:HA	2.44	0.53
1:C:198:GLY:HA3	1:C:327:LYS:O	2.08	0.52
1:B:263:VAL:O	1:B:267:MET:HB2	2.10	0.52
1:F:131:LEU:HD21	1:F:500:THR:HG22	1.91	0.52
1:H:263:VAL:O	1:H:267:MET:HB2	2.10	0.52
1:J:270:ILE:HG22	1:J:271:VAL:HG23	1.90	0.52
1:N:257:GLU:O	1:N:261:THR:OG1	2.19	0.52
1:E:263:VAL:O	1:E:267:MET:HB2	2.10	0.52
1:L:221:LEU:HB3	1:L:249:ILE:HD13	1.92	0.52
1:B:280:GLY:O	1:B:285:ARG:HB2	2.09	0.52
1:E:463:SER:HB3	1:M:461:GLU:OE2	2.09	0.52
1:H:449:ALA:HB3	1:H:450:PRO:HD3	1.92	0.52
1:I:365:LEU:O	1:I:369:VAL:HG22	2.10	0.52
1:B:213:VAL:O	1:B:324:VAL:HA	2.09	0.52
1:C:109:ALA:HB2	1:I:109:ALA:HB2	1.90	0.52
1:F:247:LEU:HB3	1:F:273:VAL:HG22	1.91	0.52
1:H:321:LYS:HB2	1:H:334:ASP:HB3	1.90	0.52
1:I:39:VAL:HG12	1:J:69:MET:HE2	1.91	0.52
1:N:77:VAL:HG21	1:N:510:VAL:HB	1.91	0.52
1:C:34:LYS:HD3	1:D:118:ARG:HH22	1.75	0.52
1:H:215:LEU:HB2	1:H:323:VAL:HG22	1.90	0.52
1:C:262:LEU:O	1:C:266:THR:HG23	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:434:GLU:O	1:L:438:VAL:HG23	2.09	0.52
1:N:254:VAL:HG12	1:N:259:LEU:HB2	1.92	0.52
1:A:20:VAL:HB	1:A:74:VAL:HG11	1.92	0.52
1:D:24:ALA:O	1:D:28:LYS:HG2	2.10	0.52
1:D:262:LEU:O	1:D:266:THR:HG23	2.09	0.52
1:A:488:MET:HE3	1:A:493:ILE:HB	1.90	0.52
1:B:349:ILE:HA	1:B:352:GLN:HB2	1.92	0.52
1:E:266:THR:HG21	1:E:273:VAL:HB	1.92	0.52
1:J:213:VAL:HB	1:J:325:ILE:HB	1.91	0.52
1:G:23:LEU:HD23	1:G:74:VAL:HG22	1.92	0.52
1:I:27:VAL:HG12	1:I:90:THR:HG23	1.91	0.52
1:I:77:VAL:HG12	1:I:506:TYR:HB3	1.91	0.52
1:B:224:ASP:HB2	1:B:286:LYS:NZ	2.25	0.51
1:E:449:ALA:HB3	1:E:450:PRO:HD3	1.92	0.51
1:I:281:PHE:H	1:I:281:PHE:HD2	1.58	0.51
1:L:206:ASN:HD22	1:L:272:LYS:HE3	1.74	0.51
1:H:262:LEU:O	1:H:266:THR:HG23	2.10	0.51
1:B:27:VAL:HG13	1:B:90:THR:HG23	1.91	0.51
1:D:205:ILE:HG23	1:D:212:ALA:O	2.11	0.51
1:G:12:ALA:HB1	1:G:520:MET:HG3	1.92	0.51
1:I:459:GLY:HA3	1:J:112:ASN:HD22	1.74	0.51
1:N:240:VAL:HG12	1:N:271:VAL:HG11	1.92	0.51
1:B:278:ALA:HB1	1:B:279:PRO:CD	2.40	0.51
1:I:415:GLY:O	1:I:451:LEU:HD23	2.10	0.51
1:J:433:ASN:ND2	1:J:436:GLN:HG3	2.25	0.51
1:K:262:LEU:O	1:K:266:THR:HG23	2.10	0.51
1:G:68:ASN:O	1:G:72:GLN:HG2	2.10	0.51
1:G:501:ARG:NH1	1:G:505:GLN:OE1	2.44	0.51
1:H:230:ILE:HD12	1:H:261:THR:HB	1.92	0.51
1:N:158:VAL:HG13	1:N:396:VAL:HG22	1.91	0.51
1:F:302:SER:H	1:F:307:MET:HE3	1.75	0.51
1:J:225:LYS:NZ	1:J:232:GLU:OE2	2.42	0.51
1:K:47:PRO:HG2	1:L:73:MET:HG3	1.92	0.51
1:M:213:VAL:O	1:M:324:VAL:HA	2.11	0.51
1:M:215:LEU:HB2	1:M:323:VAL:HG22	1.92	0.51
1:N:271:VAL:HG12	1:N:272:LYS:H	1.76	0.51
1:N:455:VAL:HG11	1:N:462:PRO:HA	1.92	0.51
1:B:365:LEU:O	1:B:368:ARG:HG2	2.11	0.51
1:F:342:ILE:O	1:F:346:VAL:HG23	2.11	0.51
1:K:249:ILE:HB	1:K:275:ALA:HA	1.91	0.51
1:L:433:ASN:ND2	1:L:436:GLN:HG3	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:414:GLY:N	1:D:494:LEU:HA	2.26	0.51
1:H:183:LEU:HD13	1:I:360:TYR:CD1	2.46	0.51
1:I:326:ASN:HB2	1:I:329:THR:HB	1.93	0.51
1:K:240:VAL:HG11	1:K:247:LEU:HB2	1.93	0.51
1:D:438:VAL:O	1:D:442:VAL:HG23	2.10	0.51
1:C:291:ASP:OD2	1:C:368:ARG:HD2	2.11	0.51
1:B:206:ASN:HD22	1:B:214:GLU:N	2.08	0.50
1:D:198:GLY:HA3	1:D:327:LYS:O	2.11	0.50
1:D:414:GLY:O	1:D:417:VAL:HG13	2.11	0.50
1:F:266:THR:HG21	1:F:273:VAL:H	1.76	0.50
1:I:178:GLU:HA	1:I:393:LYS:HE2	1.93	0.50
1:K:206:ASN:ND2	1:K:214:GLU:O	2.44	0.50
1:K:433:ASN:ND2	1:K:436:GLN:HG3	2.26	0.50
1:B:27:VAL:CG1	1:B:90:THR:HG23	2.41	0.50
1:H:171:LYS:HB3	1:H:407:VAL:HG11	1.93	0.50
1:B:347:ALA:HA	1:B:350:ARG:HG2	1.92	0.50
1:E:131:LEU:HD13	1:E:422:VAL:HG21	1.92	0.50
1:G:213:VAL:HB	1:G:325:ILE:HB	1.93	0.50
1:I:247:LEU:HB3	1:I:273:VAL:HG22	1.92	0.50
1:A:14:VAL:O	1:A:18:ARG:HG3	2.10	0.50
1:F:184:GLN:H	1:F:382:GLY:HA3	1.76	0.50
1:H:326:ASN:HB2	1:H:329:THR:H	1.76	0.50
1:K:460:GLU:O	1:K:462:PRO:HD3	2.11	0.50
1:L:49:ILE:HD12	1:M:513:LEU:HD13	1.93	0.50
1:L:206:ASN:ND2	1:L:272:LYS:HE3	2.26	0.50
1:I:10:ASN:O	1:I:14:VAL:HG13	2.11	0.50
1:J:218:PRO:HD2	1:J:320:ALA:O	2.11	0.50
1:D:240:VAL:HG12	1:D:271:VAL:HG12	1.93	0.50
1:G:263:VAL:O	1:G:267:MET:HB2	2.11	0.50
1:J:326:ASN:HB2	1:J:329:THR:H	1.77	0.50
1:L:7:LYS:HD2	1:L:66:PHE:CE2	2.47	0.50
1:L:443:ALA:O	1:L:447:MET:HG3	2.12	0.50
1:E:16:MET:O	1:E:20:VAL:HG13	2.12	0.50
1:E:151:SER:HB2	1:E:399:ALA:HA	1.93	0.50
1:H:177:VAL:HG11	1:H:396:VAL:HG12	1.92	0.50
1:J:40:LEU:HD13	1:J:59:GLU:HG3	1.94	0.50
1:L:248:LEU:HD22	1:L:323:VAL:HG21	1.93	0.50
1:C:271:VAL:O	1:C:273:VAL:HG23	2.12	0.50
1:D:232:GLU:HA	1:D:310:GLU:HG3	1.94	0.50
1:J:218:PRO:HG3	1:J:323:VAL:HG22	1.93	0.50
1:G:291:ASP:OD2	1:G:368:ARG:HD2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:266:THR:HB	1:I:272:LYS:HD2	1.94	0.50
1:K:193:MET:HB2	1:K:372:LEU:HD13	1.93	0.50
1:M:321:LYS:HB2	1:M:334:ASP:HB3	1.93	0.50
1:M:433:ASN:HD21	1:M:436:GLN:HG3	1.76	0.50
1:D:414:GLY:H	1:D:494:LEU:HA	1.77	0.49
1:F:433:ASN:ND2	1:F:436:GLN:HG3	2.26	0.49
1:K:85:ALA:HB1	1:K:499:VAL:HG12	1.93	0.49
1:D:478:TYR:CE2	1:D:480:ALA:HA	2.48	0.49
1:G:153:ASN:ND2	1:G:153:ASN:O	2.45	0.49
1:L:203:TYR:HD2	1:L:263:VAL:HG13	1.77	0.49
1:D:270:ILE:HG22	1:D:271:VAL:HG22	1.94	0.49
1:E:27:VAL:CG1	1:E:90:THR:HG23	2.42	0.49
1:F:221:LEU:HD11	1:F:301:ILE:HD12	1.94	0.49
1:G:266:THR:HG21	1:G:273:VAL:HB	1.94	0.49
1:L:247:LEU:HD21	1:L:249:ILE:HD11	1.93	0.49
1:A:7:LYS:HG3	1:A:66:PHE:CZ	2.47	0.49
1:D:25:ASP:HA	1:D:28:LYS:HE2	1.95	0.49
1:F:71:ALA:O	1:F:75:LYS:HB2	2.13	0.49
1:F:205:ILE:HG23	1:F:212:ALA:O	2.12	0.49
1:A:198:GLY:HA3	1:A:327:LYS:O	2.12	0.49
1:I:230:ILE:HB	1:I:258:ALA:HA	1.93	0.49
1:M:269:GLY:HA3	1:N:229:ASN:HD21	1.77	0.49
1:B:109:ALA:HB2	1:J:109:ALA:HB2	1.93	0.49
1:J:218:PRO:HB3	1:J:246:PRO:HG2	1.94	0.49
1:N:131:LEU:HD13	1:N:422:VAL:HG21	1.95	0.49
1:B:295:LEU:HA	1:B:342:ILE:HD11	1.95	0.49
1:J:434:GLU:O	1:J:437:ASN:HB2	2.13	0.49
1:J:487:ASN:O	1:J:491:MET:HG3	2.13	0.49
1:L:194:GLN:O	1:L:371:LYS:HE3	2.12	0.49
1:C:472:GLY:HA3	1:C:476:TYR:CD2	2.47	0.49
1:D:12:ALA:HB1	1:D:520:MET:HG3	1.94	0.49
1:E:34:LYS:HD2	1:E:458:CYS:HA	1.95	0.49
1:I:386:GLU:HA	1:J:281:PHE:HE2	1.78	0.49
1:K:122:LYS:NZ	1:K:430:ARG:O	2.30	0.49
1:M:271:VAL:HG12	1:M:272:LYS:H	1.77	0.49
1:A:263:VAL:O	1:A:267:MET:HB2	2.13	0.49
1:D:18:ARG:HG2	1:D:67:GLU:CD	2.32	0.49
1:I:233:MET:SD	1:I:237:LEU:HD12	2.52	0.49
1:N:263:VAL:O	1:N:267:MET:HB2	2.13	0.49
1:A:359:ASP:OD1	1:A:362:ARG:NH1	2.45	0.49
1:B:478:TYR:CE2	1:B:480:ALA:HA	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:82:ASN:HB2	1:G:89:THR:OG1	2.13	0.49
1:A:26:ALA:HA	1:B:8:PHE:HE1	1.77	0.48
1:C:27:VAL:CG1	1:C:90:THR:HG23	2.43	0.48
1:E:414:GLY:HA2	1:E:495:ASP:OD2	2.13	0.48
1:I:20:VAL:HB	1:I:74:VAL:HG11	1.95	0.48
1:J:149:THR:HG22	1:J:154:SER:HA	1.95	0.48
1:M:16:MET:O	1:M:20:VAL:HG13	2.12	0.48
1:A:109:ALA:HB2	1:K:109:ALA:HB2	1.94	0.48
1:B:183:LEU:O	1:B:183:LEU:HG	2.13	0.48
1:B:218:PRO:HD2	1:B:320:ALA:O	2.13	0.48
1:F:128:VAL:HG21	1:F:505:GLN:HE21	1.79	0.48
1:K:77:VAL:HG21	1:K:510:VAL:HB	1.95	0.48
1:C:436:GLN:O	1:C:440:ILE:HG13	2.14	0.48
1:I:27:VAL:CG1	1:I:90:THR:HG23	2.43	0.48
1:I:135:SER:HA	1:I:412:VAL:HG12	1.96	0.48
1:J:193:MET:HG2	1:J:371:LYS:HB3	1.95	0.48
1:J:301:ILE:HA	1:J:307:MET:HE3	1.94	0.48
1:B:233:MET:SD	1:B:309:LEU:HD13	2.53	0.48
1:K:206:ASN:OD1	1:K:214:GLU:N	2.35	0.48
1:K:414:GLY:O	1:K:417:VAL:HG13	2.13	0.48
1:M:310:GLU:OE1	1:M:310:GLU:N	2.42	0.48
1:K:142:LYS:O	1:K:146:GLN:HG3	2.14	0.48
1:M:193:MET:HG3	1:M:371:LYS:HB3	1.93	0.48
1:C:218:PRO:HB3	1:C:246:PRO:HG2	1.96	0.48
1:E:202:PRO:O	1:E:203:TYR:HB2	2.14	0.48
1:I:38:VAL:HG22	1:J:519:CYS:HB3	1.95	0.48
1:I:177:VAL:HG11	1:I:396:VAL:HG12	1.96	0.48
1:I:240:VAL:HG21	1:I:247:LEU:HD13	1.96	0.48
1:L:124:VAL:HG13	1:L:504:LEU:HG	1.96	0.48
1:N:186:GLU:HB2	1:N:380:LYS:HB2	1.95	0.48
1:B:74:VAL:HA	1:B:510:VAL:HG21	1.96	0.48
1:E:295:LEU:HA	1:E:342:ILE:HD11	1.95	0.48
1:G:417:VAL:HA	1:G:420:ILE:HG22	1.94	0.48
1:I:68:ASN:O	1:I:72:GLN:HG2	2.14	0.48
1:M:213:VAL:HB	1:M:325:ILE:HB	1.95	0.48
1:C:146:GLN:O	1:C:150:ILE:HG13	2.14	0.48
1:C:353:ILE:HG23	1:C:362:ARG:HG3	1.96	0.48
1:D:266:THR:CG2	1:D:273:VAL:H	2.27	0.48
1:D:392:LYS:O	1:D:396:VAL:HG23	2.14	0.48
1:H:259:LEU:O	1:H:263:VAL:HG23	2.13	0.48
1:I:150:ILE:HD12	1:I:494:LEU:HD21	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:198:GLY:HA3	1:I:327:LYS:O	2.14	0.48
1:M:345:ARG:HH21	1:M:368:ARG:HH12	1.62	0.48
1:A:120:ILE:O	1:A:124:VAL:HG23	2.14	0.47
1:A:496:PRO:HB2	1:A:499:VAL:HG13	1.95	0.47
1:C:326:ASN:HB2	1:C:329:THR:HB	1.95	0.47
1:E:426:LEU:HD22	1:E:429:LEU:HD22	1.95	0.47
1:G:235:PRO:HG3	1:G:310:GLU:HA	1.95	0.47
1:M:70:GLY:HA2	1:M:73:MET:HE3	1.95	0.47
1:N:496:PRO:O	1:N:499:VAL:HG13	2.14	0.47
1:B:320:ALA:HA	1:B:335:GLY:HA2	1.97	0.47
1:F:111:MET:SD	1:F:438:VAL:HG11	2.54	0.47
1:F:221:LEU:HB3	1:F:249:ILE:HD13	1.96	0.47
1:H:257:GLU:O	1:H:261:THR:OG1	2.32	0.47
1:K:383:ALA:O	1:K:384:ALA:HB3	2.14	0.47
1:N:68:ASN:O	1:N:72:GLN:HG2	2.14	0.47
1:C:199:TYR:CZ	1:C:327:LYS:HA	2.49	0.47
1:G:247:LEU:HB3	1:G:273:VAL:HG22	1.95	0.47
1:H:218:PRO:HD2	1:H:320:ALA:O	2.14	0.47
1:K:411:VAL:HG21	1:K:494:LEU:HD22	1.96	0.47
1:B:180:GLY:HA2	1:B:380:LYS:HB3	1.97	0.47
1:C:6:VAL:HG22	1:C:521:VAL:HG22	1.95	0.47
1:C:266:THR:HG22	1:C:271:VAL:O	2.14	0.47
1:E:465:VAL:O	1:E:469:VAL:HG23	2.13	0.47
1:F:222:LEU:HD23	1:F:250:ILE:HB	1.96	0.47
1:G:183:LEU:HG	1:G:184:GLN:H	1.79	0.47
1:K:7:LYS:HG3	1:K:66:PHE:CZ	2.49	0.47
1:K:27:VAL:HG13	1:K:90:THR:HG23	1.95	0.47
1:M:124:VAL:O	1:M:128:VAL:HG23	2.14	0.47
1:E:158:VAL:HG13	1:E:396:VAL:HG22	1.97	0.47
1:E:414:GLY:H	1:E:494:LEU:HA	1.80	0.47
1:B:183:LEU:HD22	1:C:360:TYR:CD2	2.50	0.47
1:B:206:ASN:ND2	1:B:214:GLU:O	2.47	0.47
1:C:131:LEU:HD13	1:C:422:VAL:HG21	1.97	0.47
1:I:263:VAL:O	1:I:267:MET:HB2	2.14	0.47
1:I:342:ILE:O	1:I:346:VAL:HG23	2.14	0.47
1:I:448:GLU:O	1:I:452:ARG:HD2	2.14	0.47
1:N:82:ASN:HB2	1:N:89:THR:OG1	2.15	0.47
1:A:342:ILE:O	1:A:346:VAL:HG23	2.14	0.47
1:C:68:ASN:O	1:C:72:GLN:HG2	2.15	0.47
1:D:250:ILE:HD13	1:D:292:ILE:HD13	1.97	0.47
1:E:20:VAL:HB	1:E:74:VAL:HG11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:117:LYS:HD3	1:E:516:THR:HG21	1.95	0.47
1:E:229:ASN:ND2	1:E:257:GLU:OE1	2.32	0.47
1:F:117:LYS:HD3	1:F:516:THR:HG21	1.97	0.47
1:F:236:VAL:O	1:F:240:VAL:HG23	2.14	0.47
1:I:430:ARG:HG2	1:I:430:ARG:NH1	2.30	0.47
1:J:353:ILE:HG23	1:J:362:ARG:HG3	1.97	0.47
1:L:476:TYR:HA	1:L:486:GLY:O	2.14	0.47
1:F:218:PRO:HG3	1:F:323:VAL:HG22	1.96	0.47
1:I:321:LYS:HB2	1:I:334:ASP:HB3	1.97	0.47
1:J:171:LYS:HB3	1:J:407:VAL:HG11	1.97	0.47
1:K:327:LYS:HG3	1:K:328:ASP:H	1.79	0.47
1:A:118:ARG:NH1	1:G:34:LYS:HE2	2.24	0.47
1:H:221:LEU:HD23	1:H:249:ILE:HG23	1.97	0.47
1:K:326:ASN:N	1:K:329:THR:O	2.42	0.47
1:C:353:ILE:HD13	1:C:366:GLN:HG3	1.97	0.47
1:F:349:ILE:O	1:F:353:ILE:HG13	2.15	0.47
1:I:142:LYS:O	1:I:146:GLN:HG3	2.15	0.47
1:K:118:ARG:HA	1:K:118:ARG:HD2	1.56	0.47
1:K:385:THR:HG22	1:K:387:VAL:H	1.80	0.47
1:L:171:LYS:HB3	1:L:407:VAL:HG11	1.97	0.47
1:L:349:ILE:O	1:L:353:ILE:HG13	2.15	0.47
1:C:82:ASN:OD1	1:C:89:THR:HB	2.15	0.46
1:K:455:VAL:HG13	1:K:460:GLU:HB2	1.97	0.46
1:B:200:LEU:HD23	1:B:200:LEU:HA	1.67	0.46
1:D:496:PRO:O	1:D:499:VAL:HG13	2.15	0.46
1:E:414:GLY:N	1:E:494:LEU:HA	2.30	0.46
1:F:20:VAL:HB	1:F:74:VAL:HG11	1.97	0.46
1:F:184:GLN:O	1:F:382:GLY:N	2.45	0.46
1:H:345:ARG:O	1:H:349:ILE:HG13	2.16	0.46
1:I:241:ALA:CA	1:I:271:VAL:HG21	2.41	0.46
1:K:232:GLU:CD	1:K:309:LEU:HD21	2.36	0.46
1:B:420:ILE:HG13	1:B:448:GLU:HG2	1.98	0.46
1:E:122:LYS:NZ	1:E:430:ARG:O	2.40	0.46
1:E:420:ILE:HG13	1:E:448:GLU:HG2	1.96	0.46
1:J:169:VAL:HG23	1:J:173:GLY:HA3	1.96	0.46
1:K:339:GLU:O	1:K:343:GLN:HB2	2.15	0.46
1:L:225:LYS:HG2	1:L:226:LYS:O	2.15	0.46
1:L:271:VAL:O	1:L:273:VAL:HG23	2.14	0.46
1:M:182:GLY:O	1:M:183:LEU:HG	2.15	0.46
1:B:12:ALA:HB1	1:B:520:MET:HG3	1.95	0.46
1:F:173:GLY:O	1:F:404:ARG:NH2	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:109:ALA:HB2	1:L:109:ALA:HB2	1.96	0.46
1:G:127:ALA:O	1:G:131:LEU:HB2	2.14	0.46
1:J:25:ASP:OD1	1:J:28:LYS:HE2	2.15	0.46
1:J:385:THR:O	1:J:389:MET:HB2	2.15	0.46
1:K:217:SER:HA	1:K:320:ALA:O	2.16	0.46
1:A:218:PRO:HD2	1:A:320:ALA:O	2.15	0.46
1:C:122:LYS:HE2	1:C:429:LEU:HD11	1.96	0.46
1:E:319:GLN:HB3	1:E:336:VAL:HG21	1.97	0.46
1:H:183:LEU:O	1:H:184:GLN:NE2	2.49	0.46
1:I:39:VAL:HG12	1:J:69:MET:CE	2.46	0.46
1:I:349:ILE:O	1:I:353:ILE:HG13	2.15	0.46
1:G:251:ALA:O	1:G:278:ALA:N	2.46	0.46
1:G:319:GLN:HG3	1:G:336:VAL:HG21	1.97	0.46
1:K:230:ILE:HA	1:K:233:MET:HG3	1.97	0.46
1:E:205:ILE:HA	1:E:213:VAL:HG22	1.98	0.46
1:H:194:GLN:HB2	1:H:331:THR:HG23	1.97	0.46
1:H:289:LEU:HD23	1:H:289:LEU:HA	1.76	0.46
1:J:162:ILE:HG12	1:J:400:LEU:HD13	1.97	0.46
1:J:235:PRO:HG3	1:J:310:GLU:HA	1.98	0.46
1:L:349:ILE:CG2	1:L:369:VAL:HG13	2.46	0.46
1:A:360:TYR:CD2	1:G:183:LEU:HD22	2.51	0.46
1:C:74:VAL:HA	1:C:510:VAL:HG21	1.98	0.46
1:D:82:ASN:HB2	1:D:89:THR:OG1	2.16	0.46
1:D:140:ASP:OD1	1:D:140:ASP:N	2.49	0.46
1:F:461:GLU:HA	1:F:462:PRO:HD3	1.85	0.46
1:A:74:VAL:HA	1:A:510:VAL:HG21	1.97	0.46
1:B:13:ARG:HD3	1:B:104:LEU:HD22	1.98	0.46
1:F:70:GLY:HA2	1:F:73:MET:HE3	1.98	0.46
1:I:183:LEU:HD13	1:I:183:LEU:O	2.16	0.46
1:M:284:ARG:O	1:M:288:MET:HG3	2.16	0.46
1:N:262:LEU:O	1:N:266:THR:HG23	2.16	0.46
1:D:127:ALA:O	1:D:131:LEU:HB2	2.16	0.46
1:E:146:GLN:O	1:E:150:ILE:HG13	2.15	0.46
1:G:193:MET:HG3	1:G:371:LYS:HB3	1.97	0.46
1:J:262:LEU:O	1:J:266:THR:HG23	2.16	0.46
1:K:230:ILE:HG12	1:K:233:MET:HB2	1.97	0.46
1:L:20:VAL:HB	1:L:74:VAL:HG11	1.98	0.46
1:H:222:LEU:HD23	1:H:250:ILE:HB	1.98	0.45
1:H:455:VAL:HG11	1:H:462:PRO:HA	1.98	0.45
1:K:294:THR:HG21	1:K:345:ARG:HB3	1.97	0.45
1:L:131:LEU:HD13	1:L:422:VAL:HG21	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:218:PRO:HD2	1:F:320:ALA:O	2.16	0.45
1:I:199:TYR:CZ	1:I:327:LYS:HA	2.50	0.45
1:I:200:LEU:HG	1:I:276:VAL:HA	1.99	0.45
1:M:168:LYS:HG3	1:M:187:LEU:HD21	1.97	0.45
1:A:23:LEU:HD23	1:A:74:VAL:HG22	1.98	0.45
1:C:221:LEU:HB3	1:C:249:ILE:HD13	1.97	0.45
1:G:20:VAL:HB	1:G:74:VAL:HG11	1.98	0.45
1:K:10:ASN:O	1:K:14:VAL:HG13	2.17	0.45
1:K:193:MET:HE2	1:K:195:PHE:HB3	1.98	0.45
1:L:420:ILE:HG13	1:L:448:GLU:HG2	1.97	0.45
1:C:344:GLY:O	1:C:348:GLN:HG3	2.17	0.45
1:M:478:TYR:CE2	1:M:480:ALA:HA	2.51	0.45
1:C:449:ALA:HB3	1:C:450:PRO:HD3	1.97	0.45
1:F:232:GLU:HB3	1:F:309:LEU:HB2	1.97	0.45
1:G:56:VAL:O	1:G:60:ILE:HG12	2.17	0.45
1:J:414:GLY:N	1:J:494:LEU:HA	2.31	0.45
1:M:305:ILE:HD12	1:M:307:MET:HE1	1.97	0.45
1:N:7:LYS:HG3	1:N:66:PHE:CZ	2.51	0.45
1:N:205:ILE:HG23	1:N:212:ALA:O	2.17	0.45
1:B:463:SER:HB3	1:I:461:GLU:OE2	2.17	0.45
1:H:265:ASN:HB3	1:H:271:VAL:HG22	1.99	0.45
1:H:443:ALA:O	1:H:447:MET:HG3	2.16	0.45
1:M:482:THR:O	1:M:484:GLU:HG2	2.16	0.45
1:N:465:VAL:O	1:N:469:VAL:HG23	2.16	0.45
1:D:85:ALA:HB2	1:D:498:LYS:HG2	1.98	0.45
1:D:220:ILE:N	1:D:318:GLY:O	2.41	0.45
1:E:10:ASN:O	1:E:14:VAL:HG13	2.16	0.45
1:H:77:VAL:HG21	1:H:510:VAL:HB	1.99	0.45
1:J:253:ASP:OD2	1:J:277:LYS:HE2	2.16	0.45
1:N:458:CYS:SG	1:N:480:ALA:HB1	2.56	0.45
1:A:254:VAL:HG12	1:A:259:LEU:HB2	1.99	0.45
1:A:433:ASN:HD21	1:A:436:GLN:HG3	1.82	0.45
1:B:34:LYS:HG3	1:B:458:CYS:SG	2.56	0.45
1:B:182:GLY:HA2	1:C:281:PHE:CE2	2.51	0.45
1:F:42:LYS:HE2	1:F:42:LYS:HB3	1.66	0.45
1:G:37:ASN:OD1	1:G:51:LYS:HE3	2.17	0.45
1:G:345:ARG:NH1	1:G:348:GLN:OE1	2.48	0.45
1:H:254:VAL:HG12	1:H:259:LEU:HB2	1.97	0.45
1:I:291:ASP:OD2	1:I:368:ARG:HD2	2.17	0.45
1:M:200:LEU:HG	1:M:275:ALA:O	2.17	0.45
1:N:266:THR:HG21	1:N:273:VAL:H	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:287:ALA:O	1:B:368:ARG:NH2	2.50	0.45
1:F:65:LYS:HB2	1:F:522:THR:HG21	1.99	0.45
1:F:271:VAL:O	1:F:273:VAL:HG23	2.16	0.45
1:H:266:THR:CG2	1:H:273:VAL:H	2.30	0.45
1:J:71:ALA:O	1:J:75:LYS:HB2	2.16	0.45
1:L:250:ILE:HG22	1:L:278:ALA:HB2	1.99	0.45
1:L:261:THR:O	1:L:265:ASN:HB2	2.17	0.45
1:L:414:GLY:N	1:L:494:LEU:HA	2.32	0.45
1:M:488:MET:HE3	1:M:493:ILE:HB	1.98	0.45
1:B:191:GLU:HB3	1:B:295:LEU:HD11	1.99	0.45
1:C:17:LEU:HD13	1:C:100:ILE:HG22	1.99	0.45
1:H:414:GLY:H	1:H:494:LEU:HA	1.82	0.45
1:N:478:TYR:CE2	1:N:480:ALA:HA	2.52	0.45
1:A:219:PHE:HB3	1:A:317:LEU:HD23	1.99	0.44
1:C:151:SER:HB2	1:C:399:ALA:HA	1.98	0.44
1:E:36:ARG:NH1	1:F:113:PRO:HG2	2.32	0.44
1:E:71:ALA:O	1:E:75:LYS:HB2	2.17	0.44
1:E:183:LEU:HD22	1:F:360:TYR:CD2	2.52	0.44
1:F:213:VAL:O	1:F:324:VAL:HA	2.17	0.44
1:G:71:ALA:O	1:G:75:LYS:HB2	2.17	0.44
1:G:202:PRO:O	1:G:203:TYR:HB2	2.17	0.44
1:I:122:LYS:HE2	1:I:429:LEU:HD11	1.99	0.44
1:K:199:TYR:CE2	1:K:327:LYS:HA	2.51	0.44
1:N:16:MET:O	1:N:20:VAL:HG13	2.16	0.44
1:C:284:ARG:HH11	1:C:364:LYS:HG3	1.82	0.44
1:H:36:ARG:HG3	1:I:518:GLU:HG3	1.98	0.44
1:L:160:LYS:NZ	1:L:164:GLU:OE2	2.30	0.44
1:L:218:PRO:HD2	1:L:320:ALA:O	2.18	0.44
1:M:234:LEU:HD23	1:M:237:LEU:HD12	1.99	0.44
1:N:433:ASN:ND2	1:N:436:GLN:HG3	2.32	0.44
1:C:372:LEU:HD12	1:C:372:LEU:HA	1.85	0.44
1:C:496:PRO:HB2	1:C:499:VAL:HG13	1.99	0.44
1:D:13:ARG:HD2	1:D:104:LEU:HD22	2.00	0.44
1:E:248:LEU:HD22	1:E:323:VAL:HG11	1.99	0.44
1:F:193:MET:HG3	1:F:371:LYS:HB3	1.99	0.44
1:H:478:TYR:CE2	1:H:480:ALA:HA	2.53	0.44
1:M:461:GLU:HA	1:M:462:PRO:HD3	1.82	0.44
1:C:59:GLU:O	1:D:4:LYS:HG3	2.16	0.44
1:C:205:ILE:HD12	1:C:205:ILE:H	1.82	0.44
1:J:70:GLY:HA2	1:J:73:MET:HE3	1.99	0.44
1:K:122:LYS:HE2	1:K:429:LEU:HD11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:239:ALA:HB1	1:L:314:LEU:HG	1.99	0.44
1:D:321:LYS:HD2	1:D:334:ASP:OD2	2.18	0.44
1:F:353:ILE:HG23	1:F:362:ARG:HG3	1.98	0.44
1:G:322:ARG:HB3	1:G:333:ILE:HB	1.98	0.44
1:I:77:VAL:HG21	1:I:510:VAL:HB	2.00	0.44
1:I:496:PRO:HB2	1:I:499:VAL:HG13	1.99	0.44
1:K:124:VAL:O	1:K:128:VAL:HG23	2.18	0.44
1:M:178:GLU:HA	1:M:393:LYS:HE2	2.00	0.44
1:A:302:SER:H	1:A:307:MET:CE	2.30	0.44
1:A:409:GLU:OE2	1:A:498:LYS:HG3	2.18	0.44
1:B:221:LEU:HD11	1:B:301:ILE:HD12	1.98	0.44
1:I:478:TYR:CE2	1:I:480:ALA:HA	2.52	0.44
1:J:488:MET:HE3	1:J:493:ILE:HB	1.99	0.44
1:K:197:ALA:HB1	1:K:277:LYS:HB2	1.99	0.44
1:M:323:VAL:HG12	1:M:332:ILE:HG12	1.99	0.44
1:G:112:ASN:HA	1:G:113:PRO:HD3	1.85	0.44
1:G:215:LEU:HB2	1:G:323:VAL:CG2	2.47	0.44
1:G:271:VAL:O	1:G:273:VAL:HG23	2.18	0.44
1:H:69:MET:O	1:H:73:MET:HG3	2.18	0.44
1:I:219:PHE:CE2	1:I:245:LYS:HD2	2.52	0.44
1:K:183:LEU:O	1:K:183:LEU:HG	2.18	0.44
1:A:5:ASP:HB2	1:A:524:LEU:HD13	1.98	0.44
1:B:13:ARG:CD	1:B:104:LEU:HD22	2.47	0.44
1:B:313:THR:O	1:B:317:LEU:HD13	2.17	0.44
1:E:57:ALA:O	1:E:75:LYS:HE3	2.18	0.44
1:F:284:ARG:NH1	1:F:364:LYS:HD2	2.33	0.44
1:F:345:ARG:O	1:F:349:ILE:HG13	2.18	0.44
1:I:281:PHE:N	1:I:281:PHE:CD2	2.86	0.44
1:I:346:VAL:HG13	1:I:369:VAL:HG12	1.98	0.44
1:K:284:ARG:CZ	1:K:364:LYS:HD2	2.48	0.44
1:L:119:GLY:HA3	1:L:436:GLN:O	2.18	0.44
1:A:144:ILE:HG23	1:A:403:THR:CG2	2.48	0.44
1:B:433:ASN:ND2	1:B:436:GLN:HG3	2.33	0.44
1:D:472:GLY:HA3	1:D:476:TYR:CD2	2.53	0.44
1:E:31:LEU:HD12	1:E:31:LEU:HA	1.83	0.44
1:E:461:GLU:OE2	1:M:463:SER:HB3	2.18	0.44
1:H:364:LYS:HA	1:H:364:LYS:HD3	1.64	0.44
1:J:143:ALA:O	1:J:147:VAL:HG23	2.18	0.44
1:A:231:ARG:NH2	1:G:242:LYS:HG3	2.33	0.43
1:E:120:ILE:O	1:E:124:VAL:HG23	2.17	0.43
1:F:230:ILE:HD12	1:F:261:THR:HB	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:420:ILE:HG13	1:G:448:GLU:HG2	2.00	0.43
1:H:451:LEU:HD21	1:H:465:VAL:HG12	2.00	0.43
1:I:173:GLY:O	1:I:404:ARG:NH2	2.49	0.43
1:J:414:GLY:O	1:J:417:VAL:HG13	2.18	0.43
1:C:213:VAL:HB	1:C:325:ILE:HB	1.99	0.43
1:C:294:THR:HG21	1:C:345:ARG:HB2	2.00	0.43
1:C:414:GLY:O	1:C:417:VAL:HG13	2.17	0.43
1:F:120:ILE:O	1:F:124:VAL:HG23	2.18	0.43
1:F:449:ALA:HB3	1:F:450:PRO:HD3	2.00	0.43
1:G:223:ALA:O	1:G:251:ALA:HA	2.18	0.43
1:L:186:GLU:HB2	1:L:380:LYS:HB2	1.99	0.43
1:C:16:MET:O	1:C:20:VAL:HG13	2.18	0.43
1:D:103:GLY:O	1:D:107:VAL:HG23	2.18	0.43
1:F:262:LEU:O	1:F:266:THR:HG23	2.18	0.43
1:H:16:MET:O	1:H:20:VAL:HG13	2.19	0.43
1:H:131:LEU:HD13	1:H:422:VAL:HG21	2.01	0.43
1:H:360:TYR:CZ	1:N:183:LEU:HD13	2.53	0.43
1:J:461:GLU:HA	1:J:462:PRO:HD3	1.75	0.43
1:K:233:MET:HE2	1:K:262:LEU:HD21	2.00	0.43
1:F:291:ASP:OD2	1:F:368:ARG:HD2	2.18	0.43
1:F:443:ALA:O	1:F:447:MET:HG3	2.18	0.43
1:J:257:GLU:O	1:J:261:THR:OG1	2.19	0.43
1:L:193:MET:HG2	1:L:371:LYS:HB3	2.00	0.43
1:D:36:ARG:HG3	1:E:518:GLU:HG3	2.00	0.43
1:D:141:SER:HA	1:D:144:ILE:HB	2.01	0.43
1:K:237:LEU:O	1:K:271:VAL:HG11	2.19	0.43
1:L:77:VAL:HG21	1:L:510:VAL:HB	2.00	0.43
1:L:178:GLU:HA	1:L:393:LYS:HE2	2.01	0.43
1:L:218:PRO:HG3	1:L:323:VAL:HG13	2.01	0.43
1:L:472:GLY:HA3	1:L:476:TYR:CD2	2.53	0.43
1:M:301:ILE:HG21	1:M:309:LEU:HD23	2.00	0.43
1:N:414:GLY:H	1:N:494:LEU:HA	1.84	0.43
1:C:42:LYS:HB3	1:C:42:LYS:HE2	1.71	0.43
1:F:74:VAL:HA	1:F:510:VAL:HG21	2.00	0.43
1:F:417:VAL:HA	1:F:420:ILE:HG22	2.00	0.43
1:H:361:ASP:O	1:H:365:LEU:HG	2.19	0.43
1:I:288:MET:O	1:I:291:ASP:HB2	2.18	0.43
1:J:417:VAL:HA	1:J:420:ILE:HG22	2.00	0.43
1:A:65:LYS:NZ	1:A:523:ASP:HB2	2.34	0.43
1:A:213:VAL:HB	1:A:325:ILE:HB	2.00	0.43
1:B:112:ASN:HB3	1:B:115:ASP:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:202:PRO:O	1:D:203:TYR:HB2	2.19	0.43
1:F:359:ASP:OD1	1:F:362:ARG:NH1	2.52	0.43
1:H:124:VAL:HG21	1:H:508:ALA:HB2	2.01	0.43
1:I:220:ILE:HG23	1:I:248:LEU:HD23	2.00	0.43
1:J:20:VAL:HB	1:J:74:VAL:HG11	2.01	0.43
1:M:465:VAL:O	1:M:469:VAL:HG23	2.18	0.43
1:F:36:ARG:HG3	1:G:518:GLU:HG3	2.01	0.43
1:G:31:LEU:HD23	1:G:453:GLN:HB3	2.00	0.43
1:H:218:PRO:HB3	1:H:246:PRO:HG2	2.01	0.43
1:I:90:THR:O	1:I:94:VAL:HG13	2.18	0.43
1:J:124:VAL:O	1:J:128:VAL:HG23	2.19	0.43
1:K:200:LEU:HD12	1:K:275:ALA:HB1	2.00	0.43
1:A:144:ILE:HG23	1:A:403:THR:HG21	2.01	0.43
1:F:180:GLY:HA2	1:F:380:LYS:HB3	2.00	0.43
1:F:181:THR:O	1:G:282:GLY:HA3	2.18	0.43
1:F:225:LYS:HB2	1:F:225:LYS:HE3	1.76	0.43
1:G:177:VAL:HG11	1:G:396:VAL:HG12	2.01	0.43
1:H:172:GLU:H	1:H:172:GLU:CD	2.22	0.43
1:M:314:LEU:HD23	1:M:314:LEU:HA	1.87	0.43
1:N:524:LEU:HD12	1:N:525:PRO:HD2	2.00	0.43
1:A:417:VAL:HA	1:A:420:ILE:HG22	2.00	0.43
1:E:182:GLY:HA2	1:F:281:PHE:CE2	2.53	0.43
1:E:222:LEU:HD23	1:E:250:ILE:HB	2.01	0.43
1:E:326:ASN:HB2	1:E:329:THR:H	1.83	0.43
1:G:218:PRO:HD2	1:G:320:ALA:O	2.19	0.43
1:G:266:THR:HG22	1:G:271:VAL:O	2.18	0.43
1:K:314:LEU:HD23	1:K:314:LEU:HA	1.84	0.43
1:L:134:LEU:HD23	1:L:134:LEU:HA	1.86	0.43
1:C:247:LEU:HB3	1:C:273:VAL:HG22	2.00	0.42
1:F:288:MET:HG2	1:F:368:ARG:HD3	2.01	0.42
1:G:173:GLY:O	1:G:404:ARG:NH2	2.51	0.42
1:J:230:ILE:HD12	1:J:261:THR:HB	1.99	0.42
1:L:10:ASN:O	1:L:14:VAL:HG13	2.19	0.42
1:B:449:ALA:HB3	1:B:450:PRO:HD3	2.02	0.42
1:C:71:ALA:O	1:C:75:LYS:HB2	2.20	0.42
1:D:123:ALA:HB2	1:D:440:ILE:HG23	2.00	0.42
1:I:433:ASN:OD1	1:I:435:ASP:HB2	2.19	0.42
1:K:350:ARG:HH21	1:K:369:VAL:HG23	1.84	0.42
1:N:13:ARG:CD	1:N:104:LEU:HD22	2.49	0.42
1:A:449:ALA:HB3	1:A:450:PRO:HD3	2.00	0.42
1:B:223:ALA:O	1:B:251:ALA:HA	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:234:LEU:HA	1:B:237:LEU:HB2	2.01	0.42
1:C:64:ASP:HB3	1:C:67:GLU:HB2	2.01	0.42
1:D:345:ARG:HH21	1:D:368:ARG:HH12	1.68	0.42
1:L:202:PRO:O	1:L:205:ILE:HG13	2.20	0.42
1:M:426:LEU:HA	1:M:426:LEU:HD23	1.75	0.42
1:A:30:THR:HB	1:A:51:LYS:O	2.19	0.42
1:B:349:ILE:HD13	1:B:368:ARG:NE	2.34	0.42
1:C:131:LEU:HD21	1:C:500:THR:HG22	2.01	0.42
1:C:443:ALA:O	1:C:447:MET:HG3	2.18	0.42
1:D:455:VAL:HG13	1:D:460:GLU:HB2	2.00	0.42
1:I:242:LYS:HG2	1:J:231:ARG:NH2	2.34	0.42
1:K:270:ILE:HB	1:L:231:ARG:NH1	2.33	0.42
1:L:225:LYS:HG2	1:L:226:LYS:N	2.34	0.42
1:A:12:ALA:HB1	1:A:520:MET:HG3	2.00	0.42
1:C:345:ARG:HH21	1:C:368:ARG:HH12	1.67	0.42
1:J:207:LYS:HE3	1:J:214:GLU:OE1	2.19	0.42
1:K:204:PHE:O	1:K:213:VAL:HG13	2.19	0.42
1:A:85:ALA:HB1	1:A:499:VAL:HG12	2.02	0.42
1:B:366:GLN:HA	1:B:369:VAL:HG22	2.02	0.42
1:D:455:VAL:HG21	1:D:465:VAL:HG11	2.01	0.42
1:K:488:MET:HE3	1:K:493:ILE:HB	2.01	0.42
1:L:223:ALA:O	1:L:251:ALA:HA	2.20	0.42
1:L:257:GLU:O	1:L:261:THR:OG1	2.28	0.42
1:L:258:ALA:O	1:L:262:LEU:HG	2.20	0.42
1:M:140:ASP:OD1	1:M:140:ASP:N	2.53	0.42
1:M:239:ALA:O	1:M:242:LYS:HB3	2.20	0.42
1:M:472:GLY:HA3	1:M:476:TYR:CD2	2.54	0.42
1:A:82:ASN:HB2	1:A:89:THR:OG1	2.20	0.42
1:A:224:ASP:OD2	1:A:286:LYS:HG2	2.19	0.42
1:B:71:ALA:O	1:B:75:LYS:HB2	2.19	0.42
1:B:262:LEU:HD23	1:B:262:LEU:HA	1.91	0.42
1:D:488:MET:HB3	1:D:488:MET:HE3	1.94	0.42
1:E:197:ALA:HB1	1:E:276:VAL:HB	2.02	0.42
1:F:68:ASN:O	1:F:72:GLN:HG2	2.20	0.42
1:F:69:MET:O	1:F:73:MET:HG3	2.20	0.42
1:I:126:ALA:HB1	1:I:426:LEU:CD2	2.48	0.42
1:I:205:ILE:HG23	1:I:212:ALA:O	2.20	0.42
1:L:68:ASN:O	1:L:72:GLN:HG2	2.20	0.42
1:C:184:GLN:HG2	1:C:185:ASP:N	2.35	0.42
1:F:444:LEU:HD23	1:F:444:LEU:HA	1.83	0.42
1:H:77:VAL:HG12	1:H:506:TYR:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:349:ILE:HB	1:I:369:VAL:HG13	2.00	0.42
1:J:412:VAL:HG13	1:J:497:THR:OG1	2.19	0.42
1:L:197:ALA:HB1	1:L:276:VAL:HB	2.01	0.42
1:M:82:ASN:HB2	1:M:89:THR:OG1	2.20	0.42
1:M:420:ILE:HG13	1:M:448:GLU:HG2	2.01	0.42
1:N:24:ALA:O	1:N:28:LYS:HG2	2.20	0.42
1:N:221:LEU:HD23	1:N:249:ILE:HD12	2.01	0.42
1:A:262:LEU:HD23	1:A:262:LEU:HA	1.79	0.42
1:A:514:MET:HE3	1:A:514:MET:HB3	1.90	0.42
1:B:7:LYS:HG3	1:B:66:PHE:CZ	2.55	0.42
1:B:225:LYS:HE3	1:B:225:LYS:HB2	1.81	0.42
1:B:279:PRO:HG2	1:B:285:ARG:HA	2.02	0.42
1:D:266:THR:HG21	1:D:273:VAL:H	1.85	0.42
1:H:174:VAL:HB	1:H:376:VAL:HG22	2.02	0.42
1:I:455:VAL:HG13	1:I:460:GLU:HB2	2.02	0.42
1:C:339:GLU:O	1:C:343:GLN:HG2	2.20	0.42
1:D:383:ALA:HB2	1:D:389:MET:HA	2.02	0.42
1:F:140:ASP:OD2	1:F:142:LYS:HB3	2.20	0.42
1:M:263:VAL:O	1:M:267:MET:HB2	2.20	0.42
1:A:10:ASN:O	1:A:14:VAL:HG13	2.20	0.41
1:A:284:ARG:O	1:A:288:MET:HG3	2.20	0.41
1:A:433:ASN:ND2	1:A:436:GLN:HG3	2.35	0.41
1:C:151:SER:HB2	1:C:399:ALA:CB	2.50	0.41
1:D:202:PRO:C	1:D:204:PHE:H	2.23	0.41
1:E:305:ILE:HD12	1:E:307:MET:HE2	2.01	0.41
1:H:461:GLU:HA	1:H:462:PRO:HD3	1.84	0.41
1:J:207:LYS:O	1:J:211:GLY:N	2.53	0.41
1:K:193:MET:HG3	1:K:371:LYS:HB3	2.02	0.41
1:N:288:MET:HG2	1:N:368:ARG:HD3	2.02	0.41
1:C:111:MET:SD	1:C:438:VAL:HG21	2.60	0.41
1:D:461:GLU:HA	1:D:462:PRO:HD3	1.85	0.41
1:F:235:PRO:HG3	1:F:310:GLU:HA	2.02	0.41
1:F:263:VAL:O	1:F:267:MET:HB2	2.21	0.41
1:I:169:VAL:HG11	1:I:377:ALA:HB2	2.02	0.41
1:J:176:THR:HG21	1:J:333:ILE:HD13	2.01	0.41
1:K:414:GLY:N	1:K:494:LEU:HA	2.35	0.41
1:L:365:LEU:O	1:L:369:VAL:HG22	2.19	0.41
1:N:414:GLY:N	1:N:494:LEU:HA	2.34	0.41
1:B:197:ALA:HB1	1:B:277:LYS:HB2	2.01	0.41
1:B:234:LEU:N	1:B:235:PRO:HD2	2.35	0.41
1:E:305:ILE:HB	1:E:307:MET:HE2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:160:LYS:O	1:G:164:GLU:HG3	2.20	0.41
1:C:319:GLN:HB3	1:C:336:VAL:HG21	2.02	0.41
1:C:349:ILE:O	1:C:353:ILE:HG13	2.20	0.41
1:D:383:ALA:O	1:D:384:ALA:HB3	2.20	0.41
1:F:478:TYR:CE2	1:F:480:ALA:HA	2.55	0.41
1:H:143:ALA:O	1:H:147:VAL:HG23	2.20	0.41
1:I:202:PRO:C	1:I:204:PHE:H	2.22	0.41
1:K:221:LEU:HB2	1:K:247:LEU:HD11	2.03	0.41
1:L:433:ASN:OD1	1:L:435:ASP:HB2	2.21	0.41
1:M:7:LYS:HD2	1:M:66:PHE:CE2	2.55	0.41
1:B:414:GLY:N	1:B:494:LEU:HA	2.35	0.41
1:E:513:LEU:HD23	1:E:513:LEU:HA	1.89	0.41
1:F:361:ASP:O	1:F:365:LEU:HG	2.20	0.41
1:H:288:MET:HG2	1:H:368:ARG:HD3	2.01	0.41
1:J:27:VAL:CG1	1:J:90:THR:HG23	2.49	0.41
1:K:12:ALA:HB1	1:K:520:MET:HG3	2.02	0.41
1:K:230:ILE:HA	1:K:233:MET:CG	2.51	0.41
1:K:365:LEU:CD2	1:K:368:ARG:HH21	2.33	0.41
1:A:103:GLY:HA3	1:A:515:ILE:HD11	2.02	0.41
1:D:200:LEU:HD23	1:D:200:LEU:HA	1.82	0.41
1:G:366:GLN:HA	1:G:369:VAL:HG22	2.03	0.41
1:I:241:ALA:HA	1:I:271:VAL:CG2	2.44	0.41
1:K:266:THR:HG22	1:K:273:VAL:H	1.85	0.41
1:K:413:ALA:CB	1:K:417:VAL:HG22	2.50	0.41
1:M:262:LEU:HD23	1:M:262:LEU:HA	1.85	0.41
1:M:472:GLY:HA3	1:M:476:TYR:HD2	1.85	0.41
1:D:16:MET:HB3	1:D:514:MET:HE1	2.02	0.41
1:F:27:VAL:CG1	1:F:90:THR:HG23	2.51	0.41
1:H:71:ALA:O	1:H:75:LYS:HB2	2.21	0.41
1:H:353:ILE:HG23	1:H:362:ARG:HG3	2.02	0.41
1:H:482:THR:OG1	1:H:484:GLU:HG2	2.19	0.41
1:I:16:MET:O	1:I:20:VAL:HG13	2.20	0.41
1:K:291:ASP:OD2	1:K:368:ARG:HD2	2.19	0.41
1:K:294:THR:HG21	1:K:345:ARG:CB	2.51	0.41
1:L:201:SER:HB3	1:L:204:PHE:CE2	2.56	0.41
1:L:409:GLU:OE2	1:L:498:LYS:HG3	2.21	0.41
1:M:30:THR:HB	1:M:51:LYS:O	2.21	0.41
1:B:232:GLU:HG3	1:B:310:GLU:CD	2.41	0.41
1:B:430:ARG:HG2	1:B:430:ARG:HH11	1.85	0.41
1:K:239:ALA:O	1:K:314:LEU:HD21	2.20	0.41
1:N:69:MET:O	1:N:73:MET:HE2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:199:TYR:OH	1:D:327:LYS:HG2	2.20	0.41
1:D:234:LEU:N	1:D:235:PRO:HD2	2.35	0.41
1:D:443:ALA:O	1:D:447:MET:HG3	2.20	0.41
1:E:82:ASN:HB2	1:E:89:THR:OG1	2.21	0.41
1:F:141:SER:HA	1:F:144:ILE:HB	2.03	0.41
1:H:302:SER:H	1:H:307:MET:CE	2.33	0.41
1:I:151:SER:HB2	1:I:399:ALA:HA	2.02	0.41
1:I:203:TYR:HB3	1:I:267:MET:HE3	2.03	0.41
1:I:459:GLY:HA3	1:J:112:ASN:ND2	2.36	0.41
1:J:77:VAL:HG12	1:J:506:TYR:HB3	2.02	0.41
1:J:169:VAL:CG1	1:J:377:ALA:HB2	2.51	0.41
1:K:82:ASN:HB2	1:K:89:THR:OG1	2.21	0.41
1:K:270:ILE:HB	1:L:231:ARG:CZ	2.51	0.41
1:M:385:THR:HG22	1:M:387:VAL:H	1.86	0.41
1:B:288:MET:HG3	1:B:368:ARG:NE	2.36	0.41
1:E:13:ARG:HH11	1:E:13:ARG:HD2	1.73	0.41
1:E:85:ALA:HB1	1:E:499:VAL:HG12	2.02	0.41
1:F:247:LEU:HD21	1:F:249:ILE:HD11	2.02	0.41
1:G:122:LYS:HE2	1:G:429:LEU:HD11	2.03	0.41
1:G:142:LYS:O	1:G:146:GLN:HG3	2.21	0.41
1:H:426:LEU:HD23	1:H:426:LEU:HA	1.87	0.41
1:K:202:PRO:O	1:K:203:TYR:HB2	2.21	0.41
1:L:461:GLU:HA	1:L:462:PRO:HD3	1.95	0.41
1:M:12:ALA:HB1	1:M:520:MET:HG3	2.03	0.41
1:M:455:VAL:HG11	1:M:462:PRO:HA	2.03	0.41
1:N:120:ILE:O	1:N:124:VAL:HG23	2.20	0.41
1:A:201:SER:OG	1:A:202:PRO:O	2.31	0.40
1:D:524:LEU:HD12	1:D:524:LEU:HA	1.79	0.40
1:H:20:VAL:HB	1:H:74:VAL:HG11	2.02	0.40
1:I:253:ASP:OD1	1:I:254:VAL:N	2.54	0.40
1:J:130:GLU:O	1:J:133:ALA:HB3	2.22	0.40
1:J:349:ILE:O	1:J:353:ILE:HG13	2.21	0.40
1:M:199:TYR:CZ	1:M:327:LYS:HA	2.56	0.40
1:N:218:PRO:HB3	1:N:246:PRO:HG2	2.03	0.40
1:A:353:ILE:HD13	1:A:366:GLN:HG3	2.02	0.40
1:C:220:ILE:HG23	1:C:248:LEU:HD23	2.02	0.40
1:G:455:VAL:HG21	1:G:465:VAL:HG11	2.03	0.40
1:J:199:TYR:CE2	1:J:205:ILE:HD11	2.56	0.40
1:J:222:LEU:HB3	1:J:289:LEU:HD22	2.03	0.40
1:L:302:SER:H	1:L:307:MET:CE	2.34	0.40
1:L:319:GLN:O	1:L:336:VAL:HG23	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:144:ILE:HD13	1:M:166:MET:SD	2.61	0.40
1:M:288:MET:O	1:M:291:ASP:HB2	2.20	0.40
1:B:10:ASN:O	1:B:14:VAL:HG13	2.21	0.40
1:B:77:VAL:HG21	1:B:510:VAL:HB	2.03	0.40
1:B:238:GLU:O	1:B:242:LYS:HG3	2.21	0.40
1:B:239:ALA:HB1	1:B:314:LEU:HG	2.02	0.40
1:D:175:ILE:HG12	1:D:377:ALA:HB3	2.03	0.40
1:D:350:ARG:HG3	1:D:353:ILE:HD12	2.03	0.40
1:D:415:GLY:O	1:D:451:LEU:HD12	2.21	0.40
1:D:482:THR:O	1:D:484:GLU:HG2	2.21	0.40
1:E:421:ARG:HH11	1:E:421:ARG:HD3	1.76	0.40
1:H:140:ASP:OD1	1:H:140:ASP:N	2.54	0.40
1:H:202:PRO:C	1:H:204:PHE:H	2.25	0.40
1:H:217:SER:O	1:H:245:LYS:HD3	2.21	0.40
1:I:267:MET:HB2	1:I:267:MET:HE2	1.82	0.40
1:J:41:ASP:O	1:J:42:LYS:HD3	2.21	0.40
1:J:194:GLN:O	1:J:371:LYS:HE3	2.22	0.40
1:M:23:LEU:HD23	1:M:74:VAL:HG22	2.02	0.40
1:M:69:MET:O	1:M:73:MET:HG3	2.21	0.40
1:C:365:LEU:O	1:C:369:VAL:HG13	2.22	0.40
1:D:221:LEU:HD23	1:D:249:ILE:HD12	2.03	0.40
1:F:276:VAL:HG11	1:F:330:THR:OG1	2.21	0.40
1:F:287:ALA:HB1	1:F:368:ARG:NH1	2.35	0.40
1:K:128:VAL:HG21	1:K:505:GLN:NE2	2.35	0.40
1:K:349:ILE:HG23	1:K:365:LEU:HD22	2.03	0.40
1:L:120:ILE:O	1:L:124:VAL:HG23	2.21	0.40
1:L:136:VAL:HA	1:L:137:PRO:HD3	1.90	0.40
1:M:80:LYS:HA	1:M:83:ALA:HB3	2.04	0.40
1:M:221:LEU:HB3	1:M:249:ILE:HD13	2.04	0.40
1:M:234:LEU:N	1:M:235:PRO:HD2	2.36	0.40
1:B:85:ALA:HB1	1:B:499:VAL:HG12	2.03	0.40
1:B:443:ALA:O	1:B:447:MET:HG3	2.21	0.40
1:C:261:THR:O	1:C:265:ASN:HB2	2.22	0.40
1:D:451:LEU:HD21	1:D:465:VAL:HG12	2.03	0.40
1:E:218:PRO:HB3	1:E:246:PRO:HG2	2.04	0.40
1:F:131:LEU:HD13	1:F:422:VAL:HG21	2.02	0.40
1:H:225:LYS:HB2	1:H:225:LYS:HE3	1.83	0.40
1:I:308:GLU:HB2	1:I:311:LYS:HG2	2.04	0.40
1:I:443:ALA:O	1:I:447:MET:HG3	2.21	0.40
1:I:461:GLU:HA	1:I:462:PRO:HD3	1.93	0.40
1:J:236:VAL:O	1:J:240:VAL:HG23	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:420:ILE:HG13	1:J:448:GLU:HG2	2.02	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	522/548 (95%)	512 (98%)	8 (2%)	2 (0%)	34	67
1	B	522/548 (95%)	510 (98%)	10 (2%)	2 (0%)	34	67
1	C	522/548 (95%)	510 (98%)	10 (2%)	2 (0%)	34	67
1	D	522/548 (95%)	511 (98%)	10 (2%)	1 (0%)	47	78
1	E	522/548 (95%)	510 (98%)	10 (2%)	2 (0%)	34	67
1	F	522/548 (95%)	511 (98%)	10 (2%)	1 (0%)	47	78
1	G	522/548 (95%)	512 (98%)	9 (2%)	1 (0%)	47	78
1	H	522/548 (95%)	514 (98%)	8 (2%)	0	100	100
1	I	522/548 (95%)	507 (97%)	13 (2%)	2 (0%)	34	67
1	J	522/548 (95%)	514 (98%)	7 (1%)	1 (0%)	47	78
1	K	522/548 (95%)	506 (97%)	14 (3%)	2 (0%)	34	67
1	L	522/548 (95%)	511 (98%)	10 (2%)	1 (0%)	47	78
1	M	522/548 (95%)	507 (97%)	14 (3%)	1 (0%)	47	78
1	N	522/548 (95%)	513 (98%)	8 (2%)	1 (0%)	47	78
All	All	7308/7672 (95%)	7148 (98%)	141 (2%)	19 (0%)	41	72

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	271	VAL

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Mol	Chain	Res	Type
1	J	271	VAL
1	M	271	VAL
1	N	271	VAL
1	A	183	LEU
1	K	336	VAL
1	L	271	VAL
1	E	225	LYS
1	F	271	VAL
1	I	183	LEU
1	B	183	LEU
1	C	184	GLN
1	D	271	VAL
1	C	271	VAL
1	G	271	VAL
1	B	271	VAL
1	K	271	VAL
1	A	271	VAL
1	I	271	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	402/413 (97%)	379 (94%)	23 (6%)	20 49
1	B	402/413 (97%)	382 (95%)	20 (5%)	24 55
1	C	402/413 (97%)	382 (95%)	20 (5%)	24 55
1	D	402/413 (97%)	380 (94%)	22 (6%)	21 51
1	E	402/413 (97%)	381 (95%)	21 (5%)	23 53
1	F	402/413 (97%)	380 (94%)	22 (6%)	21 51
1	G	402/413 (97%)	385 (96%)	17 (4%)	30 60
1	H	402/413 (97%)	383 (95%)	19 (5%)	26 57
1	I	402/413 (97%)	376 (94%)	26 (6%)	17 45
1	J	402/413 (97%)	377 (94%)	25 (6%)	18 47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	K	402/413 (97%)	383 (95%)	19 (5%)	26	57
1	L	402/413 (97%)	376 (94%)	26 (6%)	17	45
1	M	402/413 (97%)	379 (94%)	23 (6%)	20	49
1	N	402/413 (97%)	375 (93%)	27 (7%)	16	44
All	All	5628/5782 (97%)	5318 (94%)	310 (6%)	21	51

All (310) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	VAL
1	A	27	VAL
1	A	69	MET
1	A	82	ASN
1	A	89	THR
1	A	134	LEU
1	A	141	SER
1	A	161	LEU
1	A	177	VAL
1	A	183	LEU
1	A	230	ILE
1	A	261	THR
1	A	281	PHE
1	A	289	LEU
1	A	328	ASP
1	A	350	ARG
1	A	351	GLN
1	A	404	ARG
1	A	417	VAL
1	A	422	VAL
1	A	463	SER
1	A	483	GLU
1	A	524	LEU
1	B	18	ARG
1	B	27	VAL
1	B	82	ASN
1	B	94	VAL
1	B	129	GLU
1	B	131	LEU
1	B	134	LEU
1	B	141	SER
1	B	161	LEU

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Mol	Chain	Res	Type
1	B	176	THR
1	B	177	VAL
1	B	199	TYR
1	B	234	LEU
1	B	289	LEU
1	B	290	GLN
1	B	328	ASP
1	B	329	THR
1	B	422	VAL
1	B	463	SER
1	B	514	MET
1	C	27	VAL
1	C	43	SER
1	C	74	VAL
1	C	82	ASN
1	C	89	THR
1	C	129	GLU
1	C	138	CYS
1	C	151	SER
1	C	161	LEU
1	C	177	VAL
1	C	184	GLN
1	C	206	ASN
1	C	225	LYS
1	C	271	VAL
1	C	328	ASP
1	C	329	THR
1	C	404	ARG
1	C	422	VAL
1	C	463	SER
1	C	499	VAL
1	D	18	ARG
1	D	27	VAL
1	D	74	VAL
1	D	82	ASN
1	D	89	THR
1	D	129	GLU
1	D	134	LEU
1	D	161	LEU
1	D	176	THR
1	D	177	VAL
1	D	271	VAL

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Mol	Chain	Res	Type
1	D	329	THR
1	D	333	ILE
1	D	354	GLU
1	D	357	THR
1	D	359	ASP
1	D	385	THR
1	D	417	VAL
1	D	422	VAL
1	D	451	LEU
1	D	463	SER
1	D	524	LEU
1	E	27	VAL
1	E	74	VAL
1	E	82	ASN
1	E	89	THR
1	E	131	LEU
1	E	134	LEU
1	E	141	SER
1	E	161	LEU
1	E	177	VAL
1	E	242	LYS
1	E	271	VAL
1	E	284	ARG
1	E	295	LEU
1	E	322	ARG
1	E	328	ASP
1	E	329	THR
1	E	351	GLN
1	E	358	SER
1	E	421	ARG
1	E	422	VAL
1	E	463	SER
1	F	20	VAL
1	F	43	SER
1	F	74	VAL
1	F	75	LYS
1	F	82	ASN
1	F	89	THR
1	F	129	GLU
1	F	134	LEU
1	F	151	SER
1	F	172	GLU

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Mol	Chain	Res	Type
1	F	176	THR
1	F	183	LEU
1	F	204	PHE
1	F	284	ARG
1	F	289	LEU
1	F	328	ASP
1	F	329	THR
1	F	456	LEU
1	F	463	SER
1	F	499	VAL
1	F	514	MET
1	F	524	LEU
1	G	20	VAL
1	G	43	SER
1	G	82	ASN
1	G	89	THR
1	G	94	VAL
1	G	134	LEU
1	G	161	LEU
1	G	176	THR
1	G	271	VAL
1	G	295	LEU
1	G	328	ASP
1	G	329	THR
1	G	331	THR
1	G	404	ARG
1	G	422	VAL
1	G	463	SER
1	G	494	LEU
1	H	20	VAL
1	H	74	VAL
1	H	82	ASN
1	H	134	LEU
1	H	141	SER
1	H	151	SER
1	H	161	LEU
1	H	176	THR
1	H	183	LEU
1	H	206	ASN
1	H	261	THR
1	H	322	ARG
1	H	328	ASP

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Mol	Chain	Res	Type
1	H	329	THR
1	H	351	GLN
1	H	385	THR
1	H	417	VAL
1	H	463	SER
1	H	524	LEU
1	I	43	SER
1	I	74	VAL
1	I	75	LYS
1	I	76	GLU
1	I	82	ASN
1	I	89	THR
1	I	94	VAL
1	I	129	GLU
1	I	134	LEU
1	I	138	CYS
1	I	141	SER
1	I	161	LEU
1	I	167	ASP
1	I	172	GLU
1	I	176	THR
1	I	183	LEU
1	I	220	ILE
1	I	281	PHE
1	I	288	MET
1	I	314	LEU
1	I	350	ARG
1	I	369	VAL
1	I	389	MET
1	I	417	VAL
1	I	463	SER
1	I	524	LEU
1	J	20	VAL
1	J	27	VAL
1	J	74	VAL
1	J	76	GLU
1	J	94	VAL
1	J	125	THR
1	J	138	CYS
1	J	151	SER
1	J	196	ASP
1	J	206	ASN

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Mol	Chain	Res	Type
1	J	271	VAL
1	J	281	PHE
1	J	295	LEU
1	J	322	ARG
1	J	328	ASP
1	J	329	THR
1	J	331	THR
1	J	351	GLN
1	J	358	SER
1	J	385	THR
1	J	422	VAL
1	J	463	SER
1	J	473	ASP
1	J	494	LEU
1	J	514	MET
1	K	20	VAL
1	K	27	VAL
1	K	43	SER
1	K	76	GLU
1	K	82	ASN
1	K	94	VAL
1	K	118	ARG
1	K	161	LEU
1	K	176	THR
1	K	177	VAL
1	K	215	LEU
1	K	245	LYS
1	K	307	MET
1	K	328	ASP
1	K	422	VAL
1	K	493	ILE
1	K	494	LEU
1	K	502	SER
1	K	524	LEU
1	L	43	SER
1	L	74	VAL
1	L	89	THR
1	L	131	LEU
1	L	138	CYS
1	L	140	ASP
1	L	161	LEU
1	L	176	THR

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Mol	Chain	Res	Type
1	L	177	VAL
1	L	199	TYR
1	L	271	VAL
1	L	288	MET
1	L	295	LEU
1	L	299	THR
1	L	322	ARG
1	L	328	ASP
1	L	329	THR
1	L	350	ARG
1	L	369	VAL
1	L	387	VAL
1	L	417	VAL
1	L	422	VAL
1	L	463	SER
1	L	494	LEU
1	L	499	VAL
1	L	524	LEU
1	M	10	ASN
1	M	20	VAL
1	M	43	SER
1	M	75	LYS
1	M	76	GLU
1	M	82	ASN
1	M	94	VAL
1	M	129	GLU
1	M	134	LEU
1	M	141	SER
1	M	161	LEU
1	M	172	GLU
1	M	177	VAL
1	M	190	VAL
1	M	216	GLU
1	M	271	VAL
1	M	328	ASP
1	M	329	THR
1	M	331	THR
1	M	404	ARG
1	M	463	SER
1	M	494	LEU
1	M	524	LEU
1	N	14	VAL

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Mol	Chain	Res	Type
1	N	20	VAL
1	N	27	VAL
1	N	43	SER
1	N	76	GLU
1	N	82	ASN
1	N	89	THR
1	N	94	VAL
1	N	131	LEU
1	N	134	LEU
1	N	154	SER
1	N	161	LEU
1	N	176	THR
1	N	183	LEU
1	N	206	ASN
1	N	210	THR
1	N	266	THR
1	N	271	VAL
1	N	295	LEU
1	N	328	ASP
1	N	331	THR
1	N	334	ASP
1	N	385	THR
1	N	417	VAL
1	N	422	VAL
1	N	463	SER
1	N	499	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	326	ASN
1	B	206	ASN
1	H	184	GLN
1	H	326	ASN
1	H	479	ASN
1	J	146	GLN
1	M	433	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	524/548 (95%)	-0.18	2 (0%) 92 86	22, 60, 120, 174	0
1	B	524/548 (95%)	0.17	31 (5%) 22 10	24, 65, 207, 301	0
1	C	524/548 (95%)	-0.12	5 (0%) 82 70	25, 70, 166, 204	0
1	D	524/548 (95%)	-0.02	12 (2%) 60 40	28, 73, 161, 232	0
1	E	524/548 (95%)	-0.15	1 (0%) 95 91	28, 69, 136, 190	0
1	F	524/548 (95%)	-0.07	4 (0%) 86 74	31, 77, 135, 190	0
1	G	524/548 (95%)	0.09	23 (4%) 34 17	27, 80, 167, 208	0
1	H	524/548 (95%)	-0.25	0 100 100	25, 63, 118, 168	0
1	I	524/548 (95%)	-0.13	2 (0%) 92 86	21, 54, 146, 227	0
1	J	524/548 (95%)	-0.16	1 (0%) 95 91	18, 63, 134, 189	0
1	K	524/548 (95%)	0.29	48 (9%) 9 3	22, 66, 239, 292	0
1	L	524/548 (95%)	-0.23	1 (0%) 95 91	25, 58, 125, 177	0
1	M	524/548 (95%)	-0.04	7 (1%) 77 61	28, 77, 172, 233	0
1	N	524/548 (95%)	-0.12	3 (0%) 89 80	22, 64, 152, 206	0
All	All	7336/7672 (95%)	-0.07	140 (1%) 66 48	18, 66, 167, 301	0

All (140) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	223	ALA	12.0
1	B	251	ALA	8.8
1	K	301	ILE	7.6
1	K	203	TYR	7.2
1	K	251	ALA	7.2
1	K	316	ASP	7.0
1	B	302	SER	6.3
1	G	301	ILE	6.3

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Mol	Chain	Res	Type	RSRZ
1	K	302	SER	5.5
1	K	317	LEU	5.2
1	B	223	ALA	5.1
1	B	301	ILE	4.9
1	D	223	ALA	4.6
1	B	203	TYR	4.2
1	K	342	ILE	4.1
1	G	247	LEU	4.0
1	B	204	PHE	3.9
1	K	226	LYS	3.9
1	B	353	ILE	3.9
1	K	236	VAL	3.8
1	G	300	VAL	3.8
1	B	307	MET	3.8
1	D	317	LEU	3.7
1	B	252	GLU	3.7
1	B	269	GLY	3.7
1	K	233	MET	3.6
1	K	350	ARG	3.6
1	B	309	LEU	3.6
1	K	292	ILE	3.5
1	M	305	ILE	3.3
1	F	268	ARG	3.3
1	K	279	PRO	3.2
1	B	257	GLU	3.2
1	B	266	THR	3.2
1	F	200	LEU	3.2
1	B	300	VAL	3.1
1	K	204	PHE	3.1
1	K	326	ASN	3.1
1	N	227	ILE	3.1
1	K	240	VAL	3.1
1	C	305	ILE	3.0
1	K	299	THR	3.0
1	M	335	GLY	3.0
1	K	250	ILE	3.0
1	I	233	MET	3.0
1	D	292	ILE	2.9
1	G	295	LEU	2.9
1	K	228	SER	2.9
1	K	206	ASN	2.9
1	K	273	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	K	234	LEU	2.9
1	B	268	ARG	2.9
1	G	220	ILE	2.8
1	B	284	ARG	2.8
1	K	340	ALA	2.8
1	B	256	GLY	2.7
1	K	214	GLU	2.7
1	D	271	VAL	2.7
1	D	311	LYS	2.7
1	G	272	LYS	2.7
1	G	292	ILE	2.7
1	L	266	THR	2.7
1	G	302	SER	2.7
1	K	224	ASP	2.7
1	E	200	LEU	2.6
1	D	266	THR	2.6
1	G	296	THR	2.6
1	K	271	VAL	2.6
1	G	248	LEU	2.6
1	B	261	THR	2.6
1	K	254	VAL	2.5
1	B	227	ILE	2.5
1	A	266	THR	2.5
1	I	309	LEU	2.5
1	K	222	LEU	2.5
1	J	266	THR	2.5
1	A	271	VAL	2.5
1	K	300	VAL	2.5
1	K	253	ASP	2.5
1	K	346	VAL	2.5
1	B	220	ILE	2.5
1	K	238	GLU	2.5
1	M	317	LEU	2.5
1	G	246	PRO	2.4
1	B	221	LEU	2.4
1	M	316	ASP	2.4
1	B	229	ASN	2.4
1	B	304	GLU	2.4
1	K	293	ALA	2.4
1	G	268	ARG	2.4
1	G	291	ASP	2.4
1	K	220	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	265	ASN	2.4
1	M	243	ALA	2.3
1	B	259	LEU	2.3
1	D	301	ILE	2.3
1	B	213	VAL	2.3
1	G	333	ILE	2.3
1	G	270	ILE	2.3
1	K	229	ASN	2.3
1	D	237	LEU	2.3
1	K	218	PRO	2.3
1	C	206	ASN	2.2
1	D	305	ILE	2.2
1	N	271	VAL	2.2
1	C	275	ALA	2.2
1	B	215	LEU	2.2
1	M	240	VAL	2.2
1	G	223	ALA	2.2
1	G	284	ARG	2.2
1	B	308	GLU	2.2
1	G	271	VAL	2.2
1	B	226	LYS	2.2
1	G	331	THR	2.2
1	K	266	THR	2.2
1	K	243	ALA	2.2
1	K	205	ILE	2.2
1	K	261	THR	2.2
1	C	242	LYS	2.2
1	B	297	GLY	2.1
1	D	229	ASN	2.1
1	B	233	MET	2.1
1	D	270	ILE	2.1
1	K	276	VAL	2.1
1	K	306	GLY	2.1
1	K	246	PRO	2.1
1	G	236	VAL	2.1
1	C	233	MET	2.1
1	K	221	LEU	2.1
1	F	275	ALA	2.1
1	G	274	ALA	2.1
1	F	266	THR	2.1
1	M	295	LEU	2.1
1	K	288	MET	2.1

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Mol	Chain	Res	Type	RSRZ
1	K	305	ILE	2.0
1	N	274	ALA	2.0
1	K	199	TYR	2.0
1	G	317	LEU	2.0
1	B	299	THR	2.0
1	G	321	LYS	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 monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.