Full wwPDB X-ray Structure Validation Report (i)

Feb 21, 2017 – 08:12 PM EST

PDB ID	:	5LOO
Title	:	Structure of full length unliganded CodY from Bacillus subtilis
Authors	:	Wilkinson, A.J.; Levdikov, V.M.; Blagova, E.V.
Deposited on	:	2016-08-09
Resolution	:	4.50 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

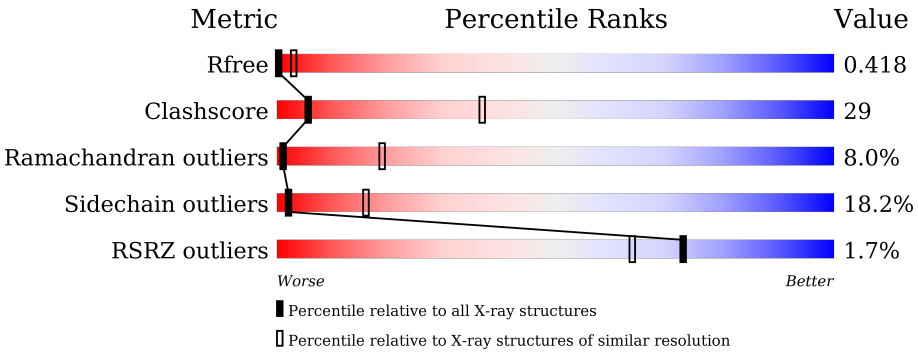
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028442

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 4.50 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}	91344	1071 (5.40-3.60)
Clashscore	102246	1003 (5.30-3.62)
Ramachandran outliers	100387	1117 (5.40-3.60)
Sidechain outliers	100360	1099 (5.40-3.60)
RSRZ outliers	91569	1075 (5.40-3.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	263	30% 49% 17%
1	B	263	38% 44% 14%
1	C	263	32% 50% 16%
1	D	263	34% 49% 13%
1	E	263	% 39% 45% 13%
1	F	263	32% 52% 14%

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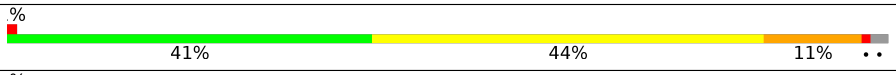
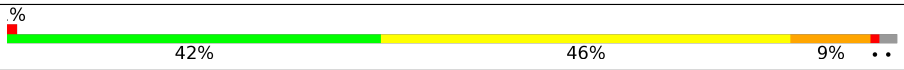
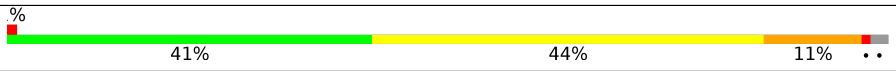
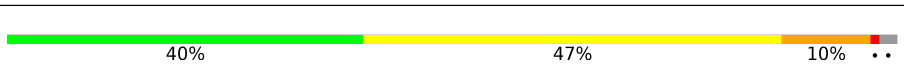
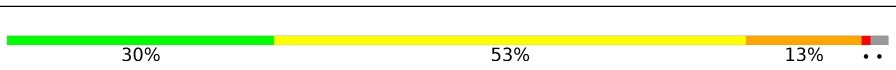
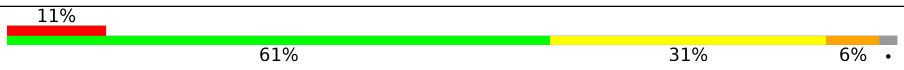
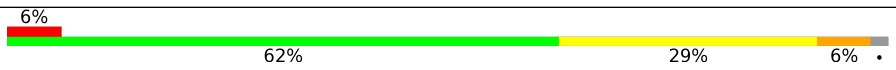
Mol	Chain	Length	Quality of chain
1	G	263	
1	H	263	
1	I	263	
1	J	263	
1	K	263	
1	L	263	
1	M	263	
1	N	263	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 28154 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 GTP-sensing transcriptional pleiotropic repressor CodY.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	257	Total	C	N	O	S	0	0	0
			2011	1265	341	398	7			
1	B	257	Total	C	N	O	S	0	0	0
			2011	1265	341	398	7			
1	C	257	Total	C	N	O	S	0	0	0
			2011	1265	341	398	7			
1	D	257	Total	C	N	O	S	0	0	0
			2011	1265	341	398	7			
1	E	257	Total	C	N	O	S	0	0	0
			2011	1265	341	398	7			
1	F	257	Total	C	N	O	S	0	0	0
			2011	1265	341	398	7			
1	G	257	Total	C	N	O	S	0	0	0
			2011	1265	341	398	7			
1	H	257	Total	C	N	O	S	0	0	0
			2011	1265	341	398	7			
1	I	257	Total	C	N	O	S	0	0	0
			2011	1265	341	398	7			
1	J	257	Total	C	N	O	S	0	0	0
			2011	1265	341	398	7			
1	K	257	Total	C	N	O	S	0	0	0
			2011	1265	341	398	7			
1	L	257	Total	C	N	O	S	0	0	0
			2011	1265	341	398	7			
1	M	257	Total	C	N	O	S	0	0	0
			2011	1265	341	398	7			
1	N	257	Total	C	N	O	S	0	0	0
			2011	1265	341	398	7			

There are 70 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	260	HIS	-	expression tag	UNP P39779

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Chain	Residue	Modelled	Actual	Comment	Reference
A	261	HIS	-	expression tag	UNP P39779
A	262	HIS	-	expression tag	UNP P39779
A	263	HIS	-	expression tag	UNP P39779
A	264	HIS	-	expression tag	UNP P39779
B	260	HIS	-	expression tag	UNP P39779
B	261	HIS	-	expression tag	UNP P39779
B	262	HIS	-	expression tag	UNP P39779
B	263	HIS	-	expression tag	UNP P39779
B	264	HIS	-	expression tag	UNP P39779
C	260	HIS	-	expression tag	UNP P39779
C	261	HIS	-	expression tag	UNP P39779
C	262	HIS	-	expression tag	UNP P39779
C	263	HIS	-	expression tag	UNP P39779
C	264	HIS	-	expression tag	UNP P39779
D	260	HIS	-	expression tag	UNP P39779
D	261	HIS	-	expression tag	UNP P39779
D	262	HIS	-	expression tag	UNP P39779
D	263	HIS	-	expression tag	UNP P39779
D	264	HIS	-	expression tag	UNP P39779
E	260	HIS	-	expression tag	UNP P39779
E	261	HIS	-	expression tag	UNP P39779
E	262	HIS	-	expression tag	UNP P39779
E	263	HIS	-	expression tag	UNP P39779
E	264	HIS	-	expression tag	UNP P39779
F	260	HIS	-	expression tag	UNP P39779
F	261	HIS	-	expression tag	UNP P39779
F	262	HIS	-	expression tag	UNP P39779
F	263	HIS	-	expression tag	UNP P39779
F	264	HIS	-	expression tag	UNP P39779
G	260	HIS	-	expression tag	UNP P39779
G	261	HIS	-	expression tag	UNP P39779
G	262	HIS	-	expression tag	UNP P39779
G	263	HIS	-	expression tag	UNP P39779
G	264	HIS	-	expression tag	UNP P39779
H	260	HIS	-	expression tag	UNP P39779
H	261	HIS	-	expression tag	UNP P39779
H	262	HIS	-	expression tag	UNP P39779
H	263	HIS	-	expression tag	UNP P39779
H	264	HIS	-	expression tag	UNP P39779
I	260	HIS	-	expression tag	UNP P39779
I	261	HIS	-	expression tag	UNP P39779
I	262	HIS	-	expression tag	UNP P39779

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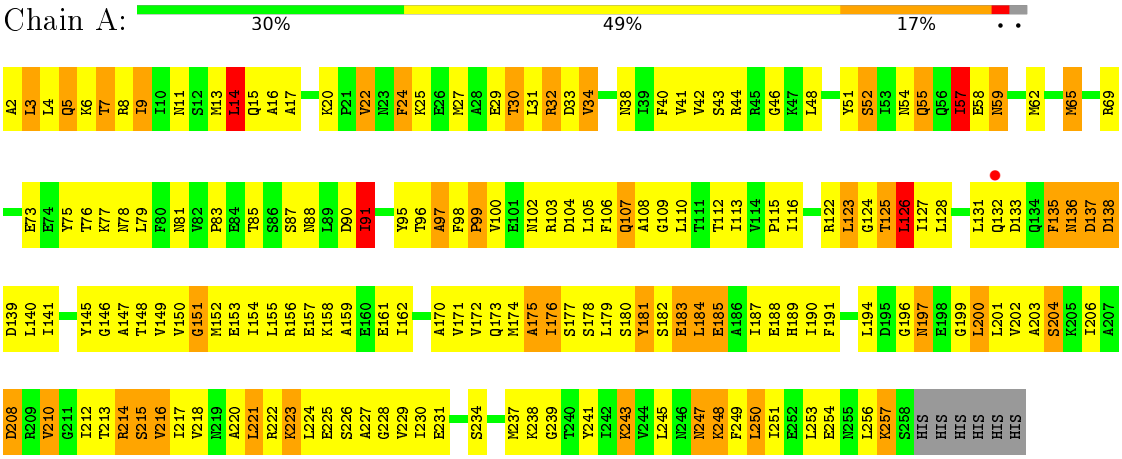
Chain	Residue	Modelled	Actual	Comment	Reference
I	263	HIS	-	expression tag	UNP P39779
I	264	HIS	-	expression tag	UNP P39779
J	260	HIS	-	expression tag	UNP P39779
J	261	HIS	-	expression tag	UNP P39779
J	262	HIS	-	expression tag	UNP P39779
J	263	HIS	-	expression tag	UNP P39779
J	264	HIS	-	expression tag	UNP P39779
K	260	HIS	-	expression tag	UNP P39779
K	261	HIS	-	expression tag	UNP P39779
K	262	HIS	-	expression tag	UNP P39779
K	263	HIS	-	expression tag	UNP P39779
K	264	HIS	-	expression tag	UNP P39779
L	260	HIS	-	expression tag	UNP P39779
L	261	HIS	-	expression tag	UNP P39779
L	262	HIS	-	expression tag	UNP P39779
L	263	HIS	-	expression tag	UNP P39779
L	264	HIS	-	expression tag	UNP P39779
M	260	HIS	-	expression tag	UNP P39779
M	261	HIS	-	expression tag	UNP P39779
M	262	HIS	-	expression tag	UNP P39779
M	263	HIS	-	expression tag	UNP P39779
M	264	HIS	-	expression tag	UNP P39779
N	260	HIS	-	expression tag	UNP P39779
N	261	HIS	-	expression tag	UNP P39779
N	262	HIS	-	expression tag	UNP P39779
N	263	HIS	-	expression tag	UNP P39779
N	264	HIS	-	expression tag	UNP P39779

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

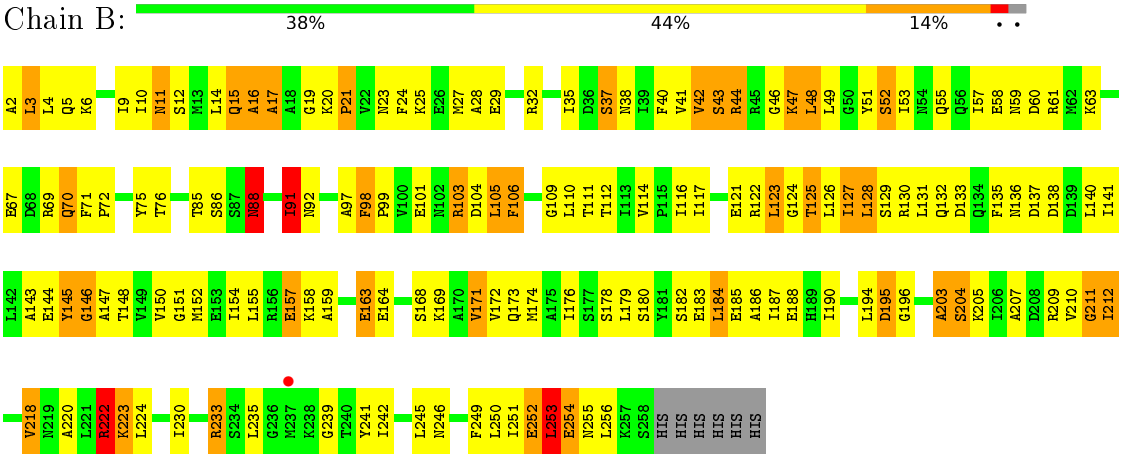
- Molecule 1: GTP-sensing transcriptional pleiotropic repressor CodY

Chain A:



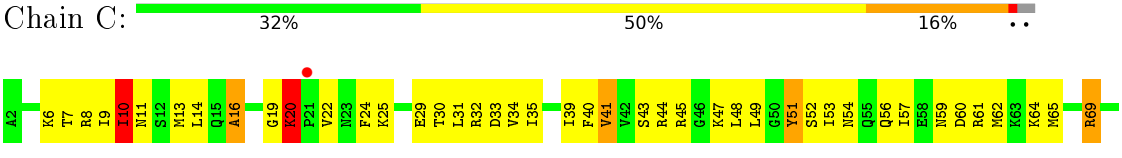
- Molecule 1: GTP-sensing transcriptional pleiotropic repressor CodY

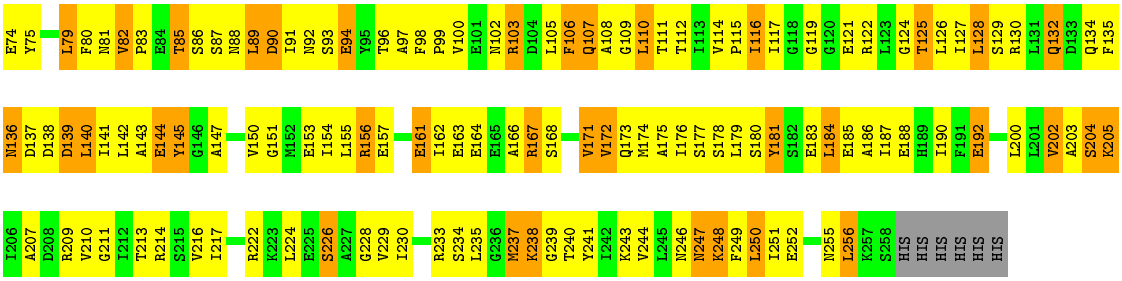
Chain B:



- Molecule 1: GTP-sensing transcriptional pleiotropic repressor CodY

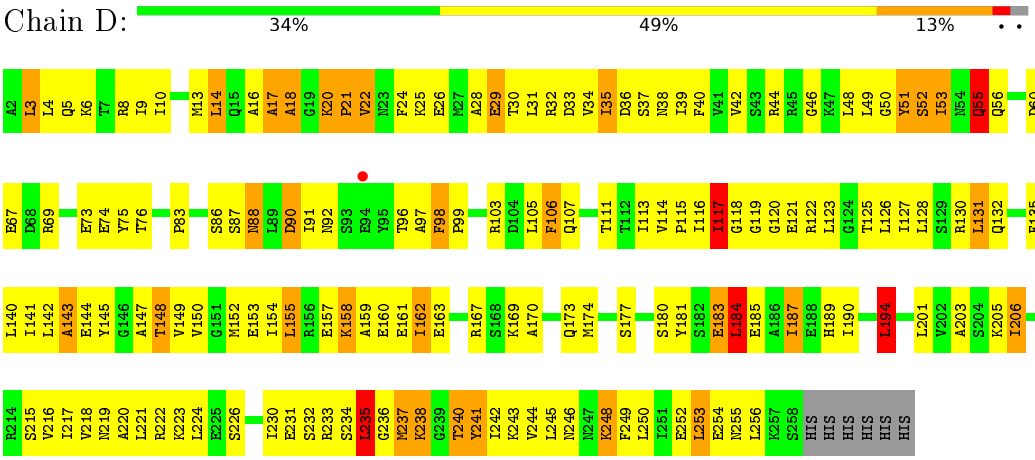
Chain C:





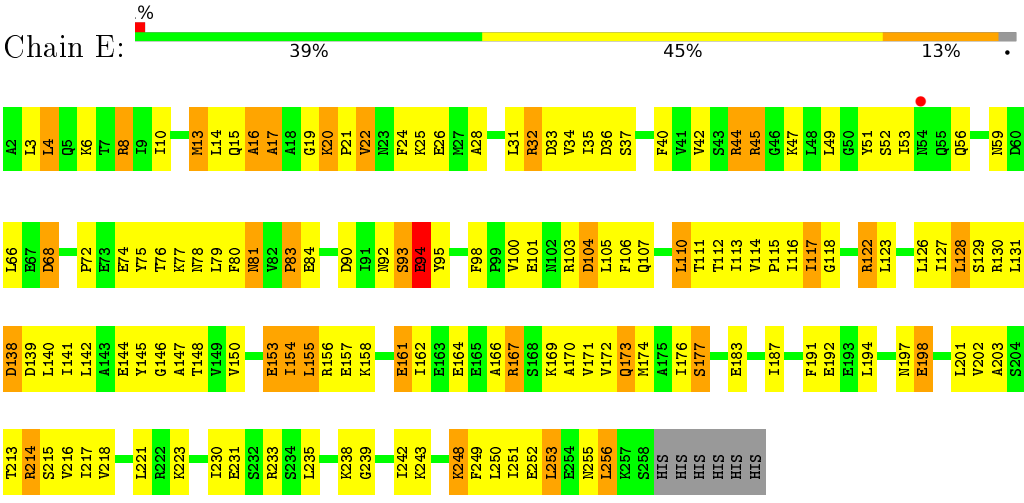
• Molecule 1: GTP-sensing transcriptional pleiotropic repressor CodY

Chain D:



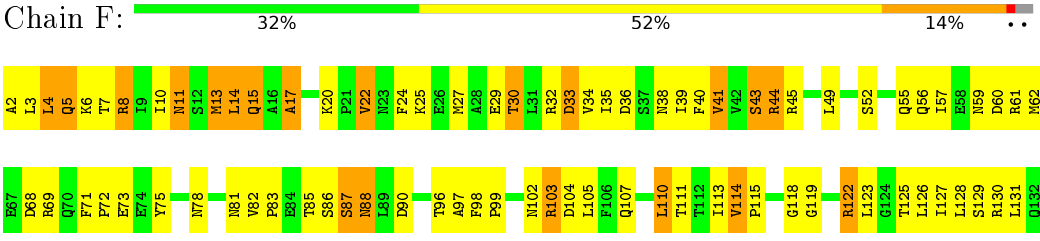
• Molecule 1: GTP-sensing transcriptional pleiotropic repressor CodY

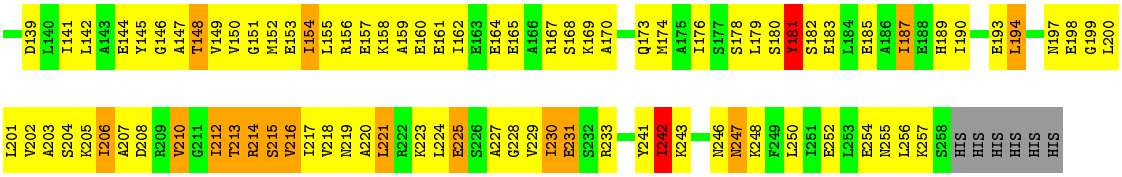
Chain E:



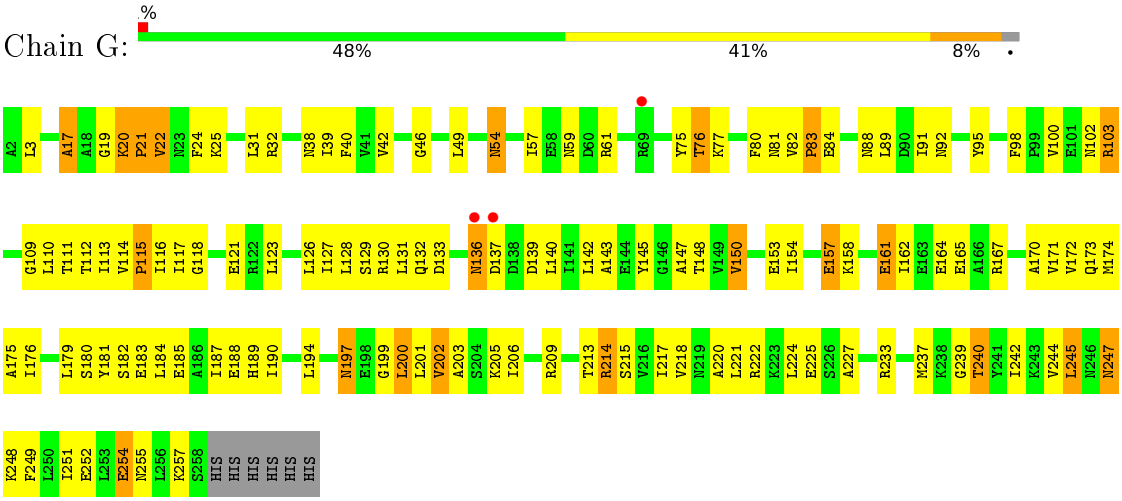
• Molecule 1: GTP-sensing transcriptional pleiotropic repressor CodY

Chain F:

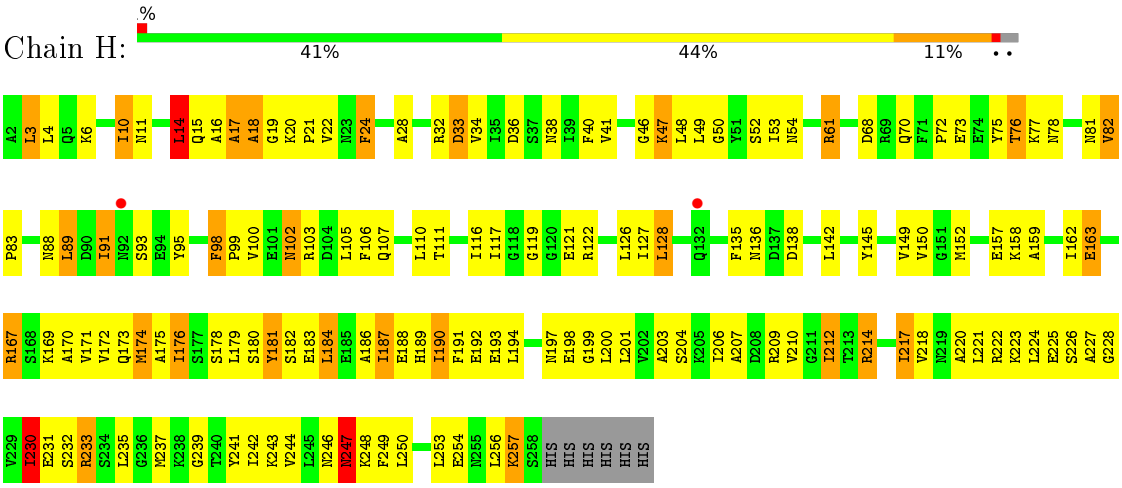




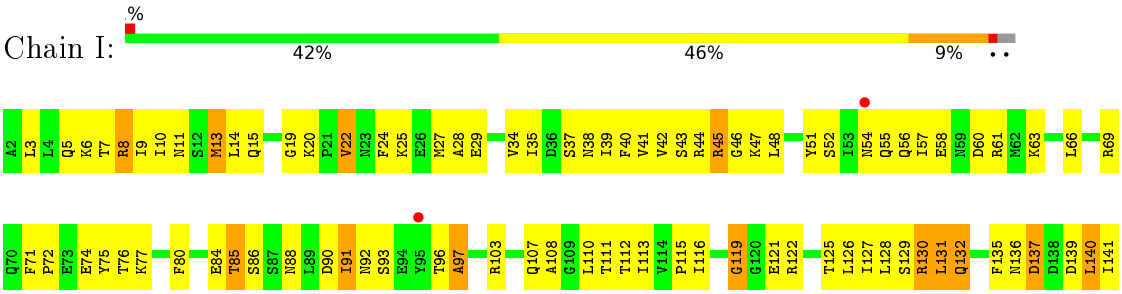
• Molecule 1: GTP-sensing transcriptional pleiotropic repressor CodY

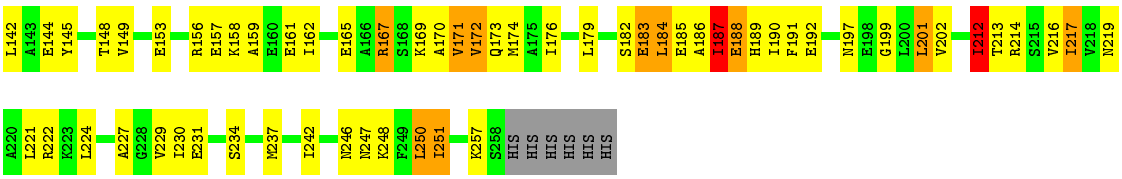


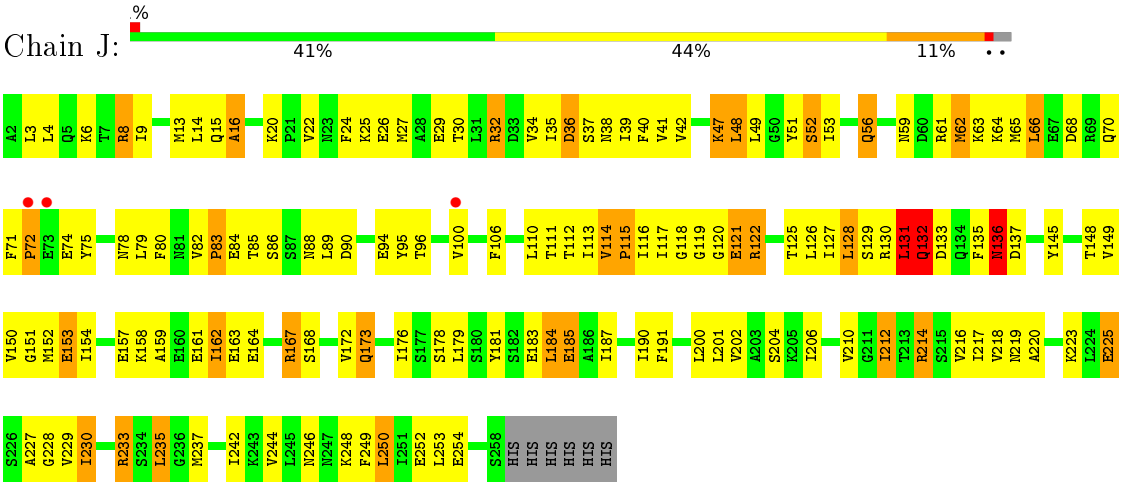
• Molecule 1: GTP-sensing transcriptional pleiotropic repressor CodY



• Molecule 1: GTP-sensing transcriptional pleiotropic repressor CodY





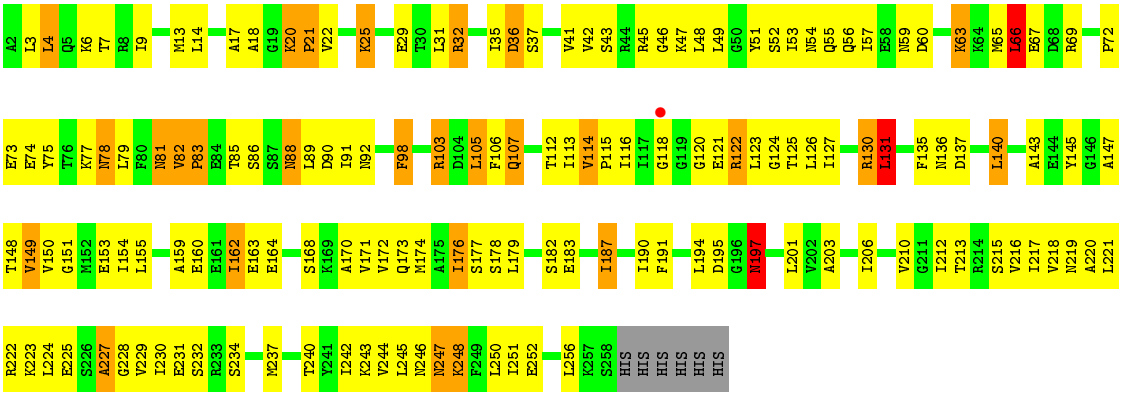


• Molecule 1: GTP-sensing transcriptional pleiotropic repressor CodY

Chain J:

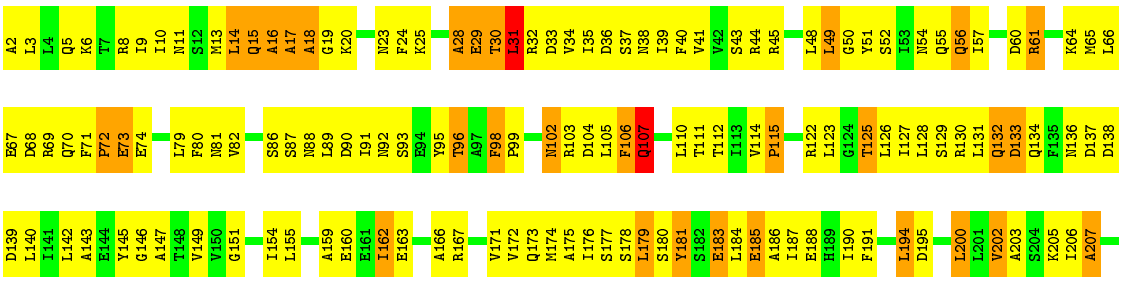
• Molecule 1: GTP-sensing transcriptional pleiotropic repressor CodY

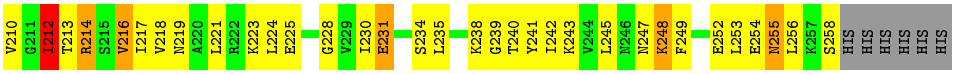
Chain K:



• Molecule 1: GTP-sensing transcriptional pleiotropic repressor CodY

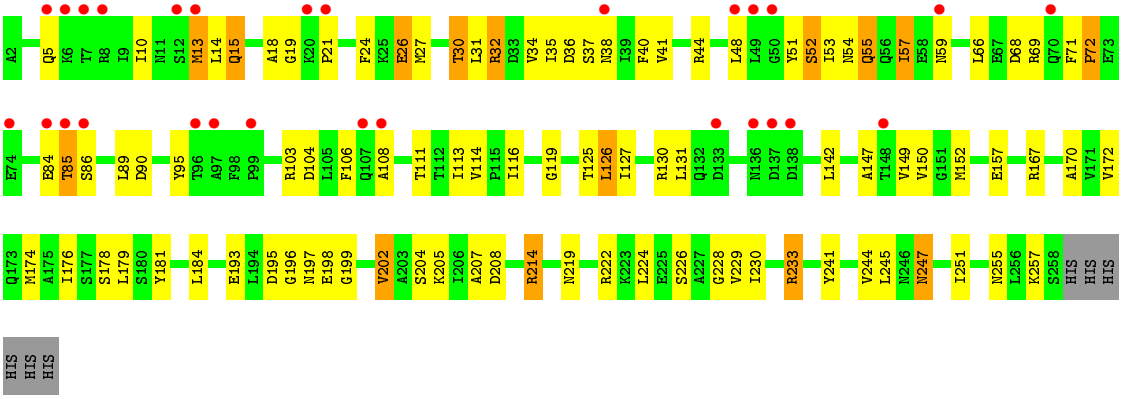
Chain L:





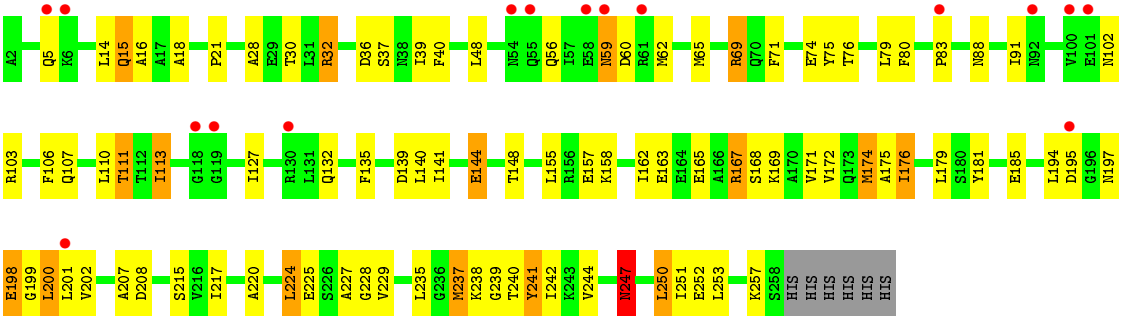
• Molecule 1: GTP-sensing transcriptional pleiotropic repressor CodY

Chain M:



• Molecule 1: GTP-sensing transcriptional pleiotropic repressor CodY

Chain N:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	315.63Å 113.68Å 168.59Å 90.00° 113.23° 90.00°	Depositor
Resolution (Å)	19.88 – 4.50 19.88 – 4.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.88-4.50) 89.7 (19.88-4.50)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.98 (at 4.54Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.251 , 0.430 0.251 , 0.418	Depositor DCC
R_{free} test set	1479 reflections (5.35%)	DCC
Wilson B-factor (Å^2)	199.3	Xtriage
Anisotropy	0.172	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 222.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.36$, $< L^2 > = 0.19$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	28154	wwPDB-VP
Average B, all atoms (Å^2)	234.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.05% 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

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.57	0/2031	0.79	3/2735 (0.1%)
1	B	0.54	0/2031	0.72	1/2735 (0.0%)
1	C	0.57	0/2031	0.75	1/2735 (0.0%)
1	D	0.55	0/2031	0.75	1/2735 (0.0%)
1	E	0.61	2/2031 (0.1%)	0.73	3/2735 (0.1%)
1	F	0.54	0/2031	0.73	0/2735
1	G	0.50	0/2031	0.69	0/2735
1	H	0.53	1/2031 (0.0%)	0.67	0/2735
1	I	0.52	0/2031	0.71	1/2735 (0.0%)
1	J	0.51	0/2031	0.71	1/2735 (0.0%)
1	K	0.49	0/2031	0.68	0/2735
1	L	0.50	0/2031	0.71	1/2735 (0.0%)
1	M	0.42	0/2031	0.56	0/2735
1	N	0.49	2/2031 (0.1%)	0.58	0/2735
All	All	0.53	5/28434 (0.0%)	0.70	12/38290 (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	A	0	1
1	B	0	1
1	D	0	2
1	F	0	2
1	I	0	1
1	J	0	1
1	L	0	1
All	All	0	9

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	20	LYS	CE-NZ	13.13	1.81	1.49
1	H	257	LYS	CE-NZ	9.42	1.72	1.49
1	N	144	GLU	CD-OE1	7.69	1.34	1.25
1	N	144	GLU	CD-OE2	7.13	1.33	1.25
1	E	20	LYS	CD-CE	5.13	1.64	1.51

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	110	LEU	CA-CB-CG	7.05	131.52	115.30
1	E	20	LYS	CD-CE-NZ	-6.61	96.51	111.70
1	A	14	LEU	CA-CB-CG	5.96	129.01	115.30
1	A	200	LEU	CA-CB-CG	5.77	128.56	115.30
1	A	126	LEU	CA-CB-CG	5.72	128.46	115.30
1	D	194	LEU	CA-CB-CG	5.35	127.61	115.30
1	J	66	LEU	CA-CB-CG	5.35	127.60	115.30
1	E	221	LEU	CA-CB-CG	5.31	127.50	115.30
1	L	200	LEU	CA-CB-CG	5.24	127.35	115.30
1	C	79	LEU	CA-CB-CG	5.12	127.07	115.30
1	I	250	LEU	CA-CB-CG	5.09	127.01	115.30
1	B	253	LEU	CA-CB-CG	5.02	126.84	115.30

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	15	GLN	Peptide
1	B	222	ARG	Peptide
1	D	14	LEU	Peptide
1	D	16	ALA	Peptide
1	F	144	GLU	Peptide
1	F	60	ASP	Peptide
1	I	148	THR	Peptide
1	J	132	GLN	Peptide
1	L	132	GLN	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	2011	0	2048	216	0
1	B	2011	0	2048	159	0
1	C	2011	0	2048	174	0
1	D	2011	0	2048	152	0
1	E	2011	0	2048	129	0
1	F	2011	0	2048	155	0
1	G	2011	0	2047	117	0
1	H	2011	0	2047	129	0
1	I	2011	0	2048	107	0
1	J	2011	0	2048	128	0
1	K	2011	0	2047	118	0
1	L	2011	0	2048	154	0
1	M	2011	0	2048	57	0
1	N	2011	0	2048	49	0
All	All	28154	0	28669	1672	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 29.

All (1672) 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:H:257:LYS:CE	1:H:257:LYS:NZ	1.72	1.47
1:E:20:LYS:CE	1:E:20:LYS:NZ	1.81	1.41
1:G:145:TYR:HA	1:H:145:TYR:CZ	1.63	1.31
1:K:145:TYR:CZ	1:L:145:TYR:CA	2.12	1.27
1:K:145:TYR:CZ	1:L:145:TYR:HA	1.67	1.20
1:K:145:TYR:CE2	1:L:145:TYR:HA	1.79	1.16
1:A:98:PHE:HB3	1:A:106:PHE:HZ	1.08	1.12
1:G:145:TYR:O	1:H:145:TYR:CE1	2.01	1.12
1:B:60:ASP:HB3	1:B:104:ASP:HB2	1.19	1.11
1:J:212:ILE:HG12	1:K:121:GLU:HB3	1.38	1.02
1:E:173:GLN:HG2	1:H:169:LYS:HB3	1.41	1.02
1:A:250:LEU:HD23	1:A:250:LEU:H	1.25	1.01
1:J:187:ILE:HD11	1:J:220:ALA:HB1	1.43	1.00
1:I:187:ILE:HD12	1:I:191:PHE:CE2	1.96	1.00
1:B:106:PHE:CD2	1:B:111:THR:HB	1.97	1.00
1:A:223:LYS:HA	1:A:226:SER:HB3	1.40	0.99
1:K:130:ARG:HH11	1:K:130:ARG:HG3	1.22	0.99
1:A:98:PHE:HB3	1:A:106:PHE:CZ	1.99	0.97
1:C:59:ASN:HB3	1:C:62:MET:HB2	1.47	0.97
1:B:158:LYS:HD3	1:C:181:TYR:HE2	1.24	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:106:PHE:HD2	1:B:111:THR:HB	1.30	0.96
1:C:183:GLU:O	1:C:187:ILE:HG12	1.66	0.96
1:A:98:PHE:CB	1:A:106:PHE:HZ	1.79	0.96
1:J:117:ILE:HG22	1:J:118:GLY:H	1.27	0.96
1:B:135:PHE:HB3	1:B:140:LEU:HD21	1.48	0.95
1:A:22:VAL:HG11	1:A:157:GLU:HB2	1.48	0.95
1:A:2:ALA:HB1	1:A:6:LYS:HG3	1.47	0.94
1:G:150:VAL:HA	1:G:153:GLU:HB2	1.50	0.93
1:E:4:LEU:HD11	1:F:141:ILE:HA	1.51	0.93
1:B:203:ALA:H	1:B:239:GLY:HA3	1.34	0.92
1:G:145:TYR:O	1:H:145:TYR:HE1	1.52	0.92
1:D:28:ALA:HB1	1:D:52:SER:HB2	1.49	0.92
1:E:40:PHE:HD2	1:E:127:ILE:HG22	1.34	0.92
1:B:40:PHE:HB2	1:B:127:ILE:HD12	1.52	0.91
1:I:171:VAL:HA	1:I:174:MET:HB3	1.52	0.91
1:G:185:GLU:HA	1:G:188:GLU:HB3	1.53	0.91
1:A:214:ARG:HD3	1:A:214:ARG:H	1.32	0.90
1:B:116:ILE:HD11	1:B:126:LEU:HB2	1.52	0.89
1:E:145:TYR:CE2	1:F:145:TYR:HA	2.07	0.89
1:D:38:ASN:HD22	1:D:53:ILE:HG22	1.36	0.89
1:D:160:GLU:HA	1:D:163:GLU:HB2	1.54	0.89
1:A:145:TYR:HE1	1:B:145:TYR:HA	1.36	0.88
1:B:43:SER:HB3	1:B:49:LEU:HD11	1.54	0.88
1:D:155:LEU:O	1:D:159:ALA:HB3	1.72	0.88
1:I:22:VAL:HG11	1:I:157:GLU:HB2	1.54	0.88
1:J:63:LYS:HA	1:J:66:LEU:HB3	1.56	0.88
1:A:65:MET:O	1:A:69:ARG:HA	1.73	0.87
1:B:173:GLN:HE21	1:C:166:ALA:HA	1.39	0.87
1:G:145:TYR:HA	1:H:145:TYR:CE1	2.09	0.86
1:D:145:TYR:O	1:D:149:VAL:HG13	1.75	0.86
1:G:145:TYR:CD2	1:H:145:TYR:CD1	2.56	0.86
1:K:179:LEU:HB2	1:K:183:GLU:HB2	1.58	0.85
1:A:170:ALA:HB2	1:D:173:GLN:HB3	1.58	0.85
1:H:40:PHE:HB2	1:H:127:ILE:HB	1.59	0.85
1:D:187:ILE:HD13	1:D:220:ALA:HB1	1.58	0.85
1:C:224:LEU:HB3	1:C:230:ILE:HG12	1.58	0.85
1:E:148:THR:HG21	1:F:14:LEU:HG	1.57	0.84
1:L:115:PRO:CB	1:L:122:ARG:HD2	2.07	0.84
1:C:61:ARG:HG3	1:C:105:LEU:HD13	1.59	0.84
1:A:116:ILE:HG12	1:A:147:ALA:HB1	1.60	0.83
1:D:190:ILE:HD13	1:D:221:LEU:HD11	1.60	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:219:ASN:HB2	1:H:19:GLY:HA2	1.60	0.83
1:F:228:GLY:HA3	1:H:228:GLY:HA3	1.61	0.83
1:A:183:GLU:O	1:A:187:ILE:HG12	1.79	0.82
1:A:145:TYR:CA	1:B:145:TYR:CE1	2.59	0.82
1:G:145:TYR:CA	1:H:145:TYR:CZ	2.56	0.82
1:A:145:TYR:HA	1:B:145:TYR:CE1	2.14	0.82
1:F:86:SER:HB3	1:F:113:ILE:H	1.44	0.82
1:L:180:SER:H	1:L:183:GLU:HG3	1.45	0.82
1:C:6:LYS:HD2	1:C:142:LEU:HD13	1.60	0.81
1:I:167:ARG:HE	1:K:227:ALA:HA	1.45	0.81
1:J:115:PRO:HA	1:J:125:THR:HA	1.62	0.81
1:C:205:LYS:O	1:C:209:ARG:HG2	1.79	0.81
1:B:144:GLU:C	1:B:146:GLY:H	1.83	0.81
1:G:32:ARG:HD3	1:G:54:ASN:HB3	1.62	0.81
1:H:179:LEU:HA	1:H:183:GLU:HB2	1.59	0.81
1:A:145:TYR:HE1	1:B:145:TYR:CA	1.92	0.81
1:F:83:PRO:HA	1:F:122:ARG:HH12	1.45	0.81
1:L:179:LEU:HD12	1:L:183:GLU:HB2	1.63	0.81
1:F:219:ASN:CB	1:H:19:GLY:HA2	2.11	0.81
1:B:194:LEU:O	1:B:195:ASP:HB2	1.79	0.80
1:A:157:GLU:HG3	1:A:158:LYS:HG2	1.63	0.80
1:C:138:ASP:C	1:C:140:LEU:H	1.84	0.80
1:C:186:ALA:O	1:C:190:ILE:HG13	1.81	0.80
1:I:19:GLY:HA2	1:K:219:ASN:HB3	1.64	0.80
1:J:117:ILE:HG22	1:J:118:GLY:N	1.97	0.80
1:K:130:ARG:HG3	1:K:130:ARG:NH1	1.92	0.80
1:D:170:ALA:O	1:D:174:MET:HB3	1.82	0.79
1:A:81:ASN:O	1:A:83:PRO:HD3	1.81	0.79
1:C:237:MET:HG3	1:C:238:LYS:N	1.95	0.79
1:G:158:LYS:HA	1:G:161:GLU:HB3	1.62	0.79
1:K:48:LEU:HD11	1:K:51:TYR:HB3	1.63	0.79
1:B:103:ARG:HH11	1:B:103:ARG:HB3	1.48	0.79
1:G:200:LEU:HA	1:G:240:THR:O	1.82	0.79
1:H:14:LEU:HD13	1:H:16:ALA:H	1.47	0.79
1:D:55:GLN:HG2	1:D:56:GLN:H	1.46	0.79
1:B:60:ASP:HB3	1:B:104:ASP:CB	2.09	0.79
1:D:90:ASP:HA	1:D:106:PHE:HB2	1.62	0.79
1:C:172:VAL:O	1:C:172:VAL:HG12	1.83	0.78
1:A:40:PHE:HB2	1:A:127:ILE:HB	1.64	0.78
1:A:237:MET:HG3	1:A:238:LYS:H	1.48	0.78
1:F:183:GLU:O	1:F:187:ILE:HG12	1.84	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:TYR:CE1	1:B:145:TYR:HA	2.19	0.78
1:B:91:ILE:HA	1:B:103:ARG:HG2	1.66	0.78
1:E:161:GLU:HG3	1:E:162:ILE:N	1.98	0.78
1:K:145:TYR:CE2	1:L:145:TYR:CA	2.53	0.78
1:L:115:PRO:HB2	1:L:122:ARG:HD2	1.65	0.78
1:B:40:PHE:HB2	1:B:127:ILE:CD1	2.15	0.77
1:J:61:ARG:C	1:J:63:LYS:H	1.86	0.77
1:E:169:LYS:HB2	1:H:173:GLN:HG2	1.66	0.77
1:M:106:PHE:HD1	1:M:111:THR:HG21	1.48	0.77
1:A:214:ARG:CD	1:A:214:ARG:H	1.96	0.77
1:K:145:TYR:CE1	1:L:145:TYR:C	2.44	0.77
1:D:183:GLU:O	1:D:185:GLU:N	2.18	0.77
1:D:88:ASN:OD1	1:D:135:PHE:HB2	1.83	0.77
1:I:40:PHE:HB2	1:I:127:ILE:O	1.85	0.77
1:G:254:GLU:HG2	1:G:257:LYS:HE2	1.67	0.76
1:A:100:VAL:HA	1:A:103:ARG:HD3	1.66	0.76
1:D:91:ILE:HG12	1:D:107:GLN:HA	1.66	0.76
1:L:103:ARG:C	1:L:105:LEU:H	1.88	0.76
1:A:145:TYR:HE1	1:B:145:TYR:CB	1.99	0.76
1:I:184:LEU:O	1:I:188:GLU:N	2.18	0.76
1:I:187:ILE:C	1:I:189:HIS:H	1.86	0.76
1:A:210:VAL:HG11	1:A:212:ILE:HD12	1.66	0.76
1:E:173:GLN:HG2	1:H:169:LYS:CB	2.15	0.76
1:K:244:VAL:HG21	1:K:250:LEU:HD21	1.65	0.76
1:D:117:ILE:HG23	1:D:118:GLY:H	1.50	0.76
1:D:33:ASP:O	1:D:35:ILE:N	2.17	0.75
1:I:224:LEU:O	1:I:229:VAL:HB	1.85	0.75
1:K:145:TYR:CE2	1:L:145:TYR:CB	2.69	0.75
1:J:14:LEU:HG	1:J:149:VAL:HB	1.66	0.75
1:A:223:LYS:CA	1:A:226:SER:HB3	2.16	0.75
1:B:24:PHE:CE1	1:B:154:ILE:HG12	2.21	0.75
1:D:117:ILE:HG23	1:D:118:GLY:N	2.01	0.75
1:H:47:LYS:HA	1:H:70:GLN:HA	1.67	0.75
1:L:234:SER:HA	1:L:240:THR:OG1	1.86	0.75
1:K:234:SER:HB2	1:K:240:THR:HB	1.69	0.75
1:F:90:ASP:HA	1:F:110:LEU:HA	1.69	0.75
1:F:146:GLY:HA2	1:F:149:VAL:HG22	1.69	0.74
1:E:22:VAL:HG22	1:E:153:GLU:HG3	1.68	0.74
1:A:14:LEU:HD11	1:B:117:ILE:O	1.88	0.74
1:D:203:ALA:HB3	1:D:238:LYS:HE2	1.68	0.74
1:K:43:SER:HB2	1:K:49:LEU:HD11	1.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:40:PHE:CD2	1:E:127:ILE:HG22	2.21	0.74
1:E:251:ILE:O	1:E:255:ASN:ND2	2.20	0.74
1:I:110:LEU:HD23	1:I:132:GLN:HA	1.70	0.74
1:J:117:ILE:CG2	1:J:118:GLY:H	2.01	0.74
1:L:65:MET:HG3	1:L:71:PHE:HD1	1.53	0.74
1:H:217:ILE:O	1:H:221:LEU:HD23	1.88	0.74
1:B:158:LYS:HD3	1:C:181:TYR:CE2	2.16	0.74
1:D:147:ALA:C	1:D:149:VAL:H	1.88	0.74
1:G:173:GLN:HA	1:G:176:ILE:HG22	1.69	0.74
1:A:17:ALA:HA	1:A:20:LYS:O	1.87	0.73
1:D:25:LYS:O	1:D:29:GLU:N	2.19	0.73
1:E:76:THR:HA	1:E:79:LEU:HB2	1.68	0.73
1:I:183:GLU:HG2	1:I:219:ASN:OD1	1.87	0.73
1:G:145:TYR:CA	1:H:145:TYR:CE1	2.70	0.73
1:C:87:SER:HA	1:C:112:THR:HG23	1.71	0.73
1:J:13:MET:HG3	1:J:14:LEU:N	2.03	0.73
1:C:22:VAL:HG11	1:C:157:GLU:HB2	1.70	0.73
1:I:14:LEU:HD12	1:I:149:VAL:HB	1.68	0.73
1:M:247:ASN:H	1:M:247:ASN:HD22	1.34	0.73
1:A:2:ALA:HB1	1:A:6:LYS:CG	2.17	0.73
1:F:210:VAL:HB	1:F:212:ILE:HD11	1.70	0.73
1:B:157:GLU:HG3	1:B:158:LYS:HG3	1.69	0.72
1:D:232:SER:HB3	1:D:242:ILE:HD12	1.71	0.72
1:C:145:TYR:CE2	1:D:145:TYR:HB2	2.24	0.72
1:H:231:GLU:HG2	1:H:243:LYS:HB3	1.70	0.72
1:E:145:TYR:CE2	1:F:145:TYR:CA	2.72	0.72
1:K:32:ARG:HE	1:K:54:ASN:HB3	1.51	0.72
1:C:247:ASN:HD22	1:C:247:ASN:H	1.36	0.72
1:D:235:LEU:HG	1:D:236:GLY:H	1.55	0.72
1:D:201:LEU:HB3	1:D:240:THR:O	1.88	0.72
1:I:6:LYS:HB3	1:I:142:LEU:HD11	1.71	0.72
1:L:32:ARG:HH21	1:L:33:ASP:HB2	1.54	0.72
1:J:158:LYS:O	1:J:162:ILE:HG12	1.89	0.72
1:B:2:ALA:O	1:B:6:LYS:HG3	1.88	0.72
1:E:34:VAL:HG13	1:E:142:LEU:HD22	1.72	0.71
1:H:194:LEU:HG	1:H:199:GLY:HA2	1.73	0.71
1:L:178:SER:HB2	1:L:223:LYS:HD3	1.71	0.71
1:A:178:SER:HB3	1:C:167:ARG:HD2	1.72	0.71
1:A:32:ARG:HD3	1:A:33:ASP:OD1	1.90	0.71
1:C:150:VAL:O	1:C:154:ILE:HG13	1.89	0.71
1:D:190:ILE:HD13	1:D:221:LEU:CD1	2.20	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:171:VAL:HA	1:G:174:MET:HB2	1.70	0.71
1:M:48:LEU:HD23	1:M:69:ARG:HD3	1.72	0.71
1:B:37:SER:HB2	1:B:130:ARG:HE	1.56	0.71
1:A:122:ARG:NH2	1:A:125:THR:HB	2.05	0.71
1:L:32:ARG:HD3	1:L:52:SER:HB3	1.72	0.71
1:M:106:PHE:CD1	1:M:111:THR:HG21	2.25	0.71
1:L:91:ILE:HA	1:L:106:PHE:HD1	1.56	0.71
1:A:27:MET:HA	1:A:27:MET:HE2	1.73	0.71
1:J:90:ASP:HA	1:J:106:PHE:HB3	1.73	0.71
1:L:39:ILE:HG23	1:L:126:LEU:HD11	1.72	0.71
1:F:146:GLY:C	1:F:148:THR:H	1.93	0.70
1:G:239:GLY:O	1:G:240:THR:HB	1.91	0.70
1:C:234:SER:HB3	1:C:240:THR:HA	1.73	0.70
1:F:178:SER:OG	1:H:167:ARG:HD2	1.91	0.70
1:K:179:LEU:CB	1:K:183:GLU:HB2	2.21	0.70
1:G:158:LYS:O	1:G:162:ILE:HG13	1.91	0.70
1:I:212:ILE:HB	1:I:216:VAL:HG21	1.74	0.70
1:A:88:ASN:HA	1:A:110:LEU:HG	1.74	0.70
1:B:103:ARG:CB	1:B:103:ARG:HH11	2.04	0.70
1:B:136:ASN:O	1:B:140:LEU:HG	1.91	0.70
1:G:172:VAL:HG13	1:G:249:PHE:HD1	1.56	0.70
1:H:78:ASN:O	1:H:81:ASN:HB2	1.91	0.70
1:C:203:ALA:O	1:C:207:ALA:HB2	1.92	0.70
1:F:43:SER:HB3	1:F:49:LEU:HD21	1.72	0.70
1:A:59:ASN:HD22	1:A:62:MET:HG2	1.57	0.70
1:A:73:GLU:O	1:A:77:LYS:HB2	1.90	0.70
1:F:153:GLU:OE2	1:F:153:GLU:HA	1.92	0.70
1:J:40:PHE:HA	1:J:51:TYR:HB2	1.72	0.70
1:A:250:LEU:CD2	1:A:250:LEU:H	2.04	0.70
1:B:203:ALA:N	1:B:239:GLY:HA3	2.07	0.70
1:J:130:ARG:HD2	1:J:133:ASP:HB3	1.73	0.70
1:B:158:LYS:CD	1:C:181:TYR:HE2	2.03	0.69
1:C:45:ARG:HH11	1:C:47:LYS:NZ	1.90	0.69
1:G:185:GLU:HA	1:G:188:GLU:CB	2.21	0.69
1:K:225:GLU:OE1	1:K:232:SER:HB3	1.92	0.69
1:B:212:ILE:HA	1:C:121:GLU:HB3	1.73	0.69
1:I:183:GLU:HA	1:I:186:ALA:HB3	1.74	0.69
1:B:103:ARG:HH11	1:B:103:ARG:CG	2.05	0.69
1:D:131:LEU:HG	1:D:132:GLN:H	1.56	0.69
1:E:114:VAL:HG11	1:E:147:ALA:HB2	1.74	0.69
1:G:201:LEU:O	1:G:239:GLY:HA2	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:40:PHE:HB2	1:N:127:ILE:HB	1.74	0.69
1:D:55:GLN:CG	1:D:56:GLN:H	2.06	0.69
1:K:113:ILE:HG12	1:K:127:ILE:HG13	1.74	0.69
1:G:145:TYR:C	1:H:145:TYR:CE1	2.64	0.69
1:J:35:ILE:HG21	1:J:39:ILE:HD11	1.74	0.69
1:D:26:GLU:HA	1:D:29:GLU:HB2	1.75	0.69
1:F:32:ARG:HD3	1:F:52:SER:HB3	1.73	0.69
1:D:169:LYS:HG2	1:D:248:LYS:HG2	1.75	0.69
1:F:242:ILE:HG22	1:F:243:LYS:H	1.58	0.69
1:I:145:TYR:HA	1:J:145:TYR:OH	1.93	0.69
1:A:172:VAL:O	1:A:172:VAL:CG1	2.41	0.69
1:D:187:ILE:O	1:D:190:ILE:HB	1.92	0.69
1:C:147:ALA:O	1:C:150:VAL:HB	1.93	0.69
1:A:190:ILE:O	1:A:194:LEU:HB2	1.91	0.68
1:B:159:ALA:O	1:B:163:GLU:HB2	1.93	0.68
1:G:145:TYR:CE2	1:H:145:TYR:CD1	2.72	0.68
1:A:2:ALA:HA	1:A:5:GLN:CD	2.14	0.68
1:H:159:ALA:HA	1:H:162:ILE:HG12	1.76	0.68
1:G:145:TYR:HA	1:H:145:TYR:CE2	2.25	0.68
1:B:57:ILE:HB	1:B:63:LYS:HD2	1.74	0.68
1:A:87:SER:HA	1:A:112:THR:HG23	1.74	0.68
1:C:115:PRO:HA	1:C:125:THR:HA	1.76	0.68
1:F:22:VAL:HG11	1:F:153:GLU:HB3	1.74	0.68
1:L:240:THR:OG1	1:L:241:TYR:N	2.26	0.68
1:B:15:GLN:NE2	1:B:20:LYS:HZ3	1.92	0.67
1:J:16:ALA:HA	1:J:153:GLU:HG2	1.76	0.67
1:B:10:ILE:HG21	1:B:145:TYR:O	1.94	0.67
1:D:149:VAL:HA	1:D:152:MET:SD	2.34	0.67
1:H:88:ASN:HB2	1:H:135:PHE:HB2	1.76	0.67
1:J:29:GLU:HG2	1:J:52:SER:HB3	1.76	0.67
1:A:184:LEU:HG	1:A:185:GLU:N	2.09	0.67
1:A:224:LEU:HB2	1:A:230:ILE:HG12	1.76	0.67
1:D:180:SER:H	1:D:183:GLU:HG3	1.58	0.67
1:D:205:LYS:O	1:D:209:ARG:HB2	1.94	0.67
1:A:136:ASN:O	1:A:138:ASP:N	2.23	0.67
1:E:44:ARG:HH11	1:E:122:ARG:HB3	1.59	0.67
1:B:111:THR:OG1	1:B:129:SER:HB3	1.94	0.67
1:D:242:ILE:HG13	1:D:243:LYS:H	1.60	0.67
1:C:61:ARG:HB3	1:C:105:LEU:HA	1.76	0.67
1:F:3:LEU:HD21	1:F:141:ILE:HD13	1.77	0.67
1:G:252:GLU:HA	1:G:255:ASN:HB2	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:ILE:HD12	1:A:224:LEU:HD11	1.75	0.67
1:F:10:ILE:HD13	1:F:146:GLY:HA3	1.76	0.67
1:F:176:ILE:HA	1:F:179:LEU:HD12	1.77	0.66
1:H:207:ALA:HA	1:H:212:ILE:O	1.94	0.66
1:K:130:ARG:HH11	1:K:130:ARG:CG	2.04	0.66
1:M:228:GLY:HA3	1:N:228:GLY:HA3	1.77	0.66
1:E:32:ARG:HE	1:E:52:SER:HB3	1.61	0.66
1:F:114:VAL:HG22	1:F:115:PRO:HD2	1.76	0.66
1:G:202:VAL:HG23	1:G:206:ILE:HG12	1.78	0.66
1:J:117:ILE:HG13	1:J:122:ARG:HB2	1.76	0.66
1:L:190:ILE:O	1:L:194:LEU:HB2	1.95	0.66
1:A:106:PHE:O	1:A:108:ALA:N	2.29	0.66
1:A:197:ASN:HD21	1:A:243:LYS:HE3	1.59	0.66
1:D:118:GLY:C	1:D:120:GLY:H	1.99	0.66
1:J:40:PHE:HB2	1:J:127:ILE:HB	1.78	0.66
1:E:3:LEU:HD22	1:E:138:ASP:HB3	1.78	0.66
1:G:130:ARG:HH21	1:G:133:ASP:HB3	1.61	0.66
1:F:228:GLY:CA	1:H:228:GLY:HA3	2.25	0.66
1:I:88:ASN:HA	1:I:110:LEU:HD12	1.76	0.66
1:A:145:TYR:HA	1:B:145:TYR:CZ	2.31	0.66
1:E:103:ARG:C	1:E:105:LEU:H	1.98	0.66
1:E:174:MET:HG3	1:F:174:MET:SD	2.34	0.66
1:B:20:LYS:HB2	1:B:21:PRO:HD2	1.77	0.66
1:D:233:ARG:O	1:D:240:THR:OG1	2.11	0.66
1:J:183:GLU:O	1:J:187:ILE:HG12	1.95	0.66
1:K:122:ARG:HD2	1:K:124:GLY:O	1.94	0.66
1:B:98:PHE:CD2	1:B:106:PHE:HZ	2.14	0.66
1:A:98:PHE:CB	1:A:106:PHE:CZ	2.71	0.66
1:C:179:LEU:HD23	1:C:183:GLU:HB3	1.77	0.66
1:E:78:ASN:O	1:E:81:ASN:HB2	1.96	0.66
1:E:83:PRO:O	1:E:115:PRO:HG2	1.96	0.65
1:E:20:LYS:CD	1:E:20:LYS:NZ	2.58	0.65
1:A:98:PHE:O	1:A:103:ARG:NH1	2.29	0.65
1:C:6:LYS:HB2	1:C:142:LEU:HD22	1.78	0.65
1:E:171:VAL:HG23	1:E:172:VAL:H	1.62	0.65
1:G:200:LEU:HD23	1:G:240:THR:H	1.61	0.65
1:A:172:VAL:HA	1:A:175:ALA:HB3	1.79	0.65
1:L:123:LEU:HD13	1:L:154:ILE:HB	1.78	0.65
1:A:172:VAL:HG12	1:A:172:VAL:O	1.97	0.65
1:A:79:LEU:HG	1:A:98:PHE:CE1	2.32	0.65
1:F:118:GLY:HA3	1:F:123:LEU:HD12	1.76	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:111:THR:HA	1:L:128:LEU:O	1.96	0.65
1:D:215:SER:O	1:D:218:VAL:HB	1.97	0.65
1:K:160:GLU:HA	1:K:163:GLU:HB2	1.78	0.65
1:K:55:GLN:HE22	1:K:130:ARG:HG2	1.61	0.65
1:A:109:GLY:HA2	1:A:131:LEU:O	1.96	0.65
1:A:42:VAL:HA	1:A:48:LEU:HA	1.79	0.65
1:B:144:GLU:C	1:B:146:GLY:N	2.50	0.65
1:B:183:GLU:HB2	1:B:220:ALA:HB2	1.79	0.65
1:L:206:ILE:O	1:L:214:ARG:N	2.30	0.65
1:B:106:PHE:HD2	1:B:111:THR:CB	2.07	0.65
1:K:74:GLU:O	1:K:78:ASN:HB2	1.96	0.65
1:M:174:MET:HE3	1:N:171:VAL:HG12	1.77	0.65
1:B:60:ASP:CB	1:B:104:ASP:HB2	2.11	0.64
1:C:16:ALA:HA	1:C:156:ARG:CB	2.27	0.64
1:I:153:GLU:HA	1:I:156:ARG:CB	2.27	0.64
1:K:229:VAL:HG12	1:K:230:ILE:HG23	1.79	0.64
1:B:158:LYS:HB2	1:C:181:TYR:CD2	2.33	0.64
1:I:44:ARG:HH11	1:I:121:GLU:HB2	1.62	0.64
1:K:41:VAL:H	1:K:48:LEU:HD12	1.62	0.64
1:L:231:GLU:HG2	1:L:245:LEU:HG	1.78	0.64
1:G:214:ARG:HG2	1:G:215:SER:N	2.11	0.64
1:C:40:PHE:CZ	1:C:62:MET:HE1	2.32	0.64
1:D:136:ASN:C	1:D:138:ASP:H	2.01	0.64
1:L:221:LEU:O	1:L:230:ILE:HD11	1.97	0.64
1:D:38:ASN:O	1:D:128:LEU:HA	1.98	0.64
1:B:72:PRO:O	1:B:75:TYR:HB2	1.97	0.64
1:D:169:LYS:HE2	1:D:248:LYS:HE2	1.80	0.64
1:G:32:ARG:HD3	1:G:54:ASN:CB	2.27	0.64
1:M:59:ASN:HB2	1:M:108:ALA:HB3	1.79	0.64
1:A:141:ILE:HD11	1:B:4:LEU:HA	1.78	0.64
1:B:186:ALA:O	1:B:190:ILE:HG12	1.97	0.64
1:D:137:ASP:HA	1:D:140:LEU:HD22	1.80	0.64
1:E:166:ALA:O	1:H:173:GLN:HB3	1.98	0.64
1:L:122:ARG:HE	1:L:125:THR:HG23	1.62	0.64
1:B:24:PHE:CZ	1:B:154:ILE:HG12	2.32	0.63
1:F:221:LEU:O	1:F:225:GLU:HB2	1.99	0.63
1:A:78:ASN:HD22	1:A:99:PRO:HG2	1.62	0.63
1:J:38:ASN:HB3	1:J:53:ILE:HG22	1.80	0.63
1:G:136:ASN:HD22	1:G:137:ASP:H	1.45	0.63
1:I:3:LEU:HA	1:I:6:LYS:HG3	1.79	0.63
1:A:250:LEU:N	1:A:250:LEU:HD23	2.06	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:145:TYR:HE2	1:F:145:TYR:CA	2.10	0.63
1:F:180:SER:H	1:F:183:GLU:CG	2.11	0.63
1:I:187:ILE:C	1:I:189:HIS:N	2.51	0.63
1:A:103:ARG:HA	1:A:106:PHE:CE2	2.33	0.63
1:E:130:ARG:HG2	1:E:131:LEU:H	1.64	0.63
1:L:99:PRO:HB2	1:L:102:ASN:HB3	1.81	0.63
1:F:10:ILE:CD1	1:F:146:GLY:HA3	2.29	0.63
1:F:187:ILE:HD12	1:F:224:LEU:HD12	1.80	0.63
1:I:19:GLY:HA3	1:K:215:SER:O	1.98	0.63
1:L:194:LEU:HD23	1:L:195:ASP:H	1.63	0.63
1:E:74:GLU:HA	1:E:77:LYS:HB2	1.80	0.63
1:K:48:LEU:HB3	1:K:69:ARG:HD2	1.81	0.63
1:C:200:LEU:HD12	1:C:241:TYR:HB2	1.79	0.63
1:C:247:ASN:HA	1:C:250:LEU:HD21	1.80	0.63
1:K:17:ALA:HB2	1:L:155:LEU:HD21	1.81	0.63
1:L:115:PRO:HA	1:L:125:THR:CG2	2.29	0.63
1:J:181:TYR:CE1	1:J:185:GLU:HG3	2.33	0.62
1:L:31:LEU:O	1:L:35:ILE:HG22	1.98	0.62
1:L:133:ASP:CG	1:L:134:GLN:H	2.02	0.62
1:A:162:ILE:HD13	1:D:184:LEU:HD12	1.79	0.62
1:C:126:LEU:HD23	1:C:147:ALA:HB2	1.81	0.62
1:D:3:LEU:HD12	1:D:3:LEU:O	1.99	0.62
1:A:103:ARG:HA	1:A:106:PHE:CD2	2.35	0.62
1:E:201:LEU:HD23	1:E:206:ILE:HD11	1.81	0.62
1:J:190:ILE:HD11	1:J:217:ILE:HG23	1.82	0.62
1:L:213:THR:HB	1:L:216:VAL:HB	1.82	0.62
1:C:172:VAL:O	1:C:173:GLN:NE2	2.32	0.62
1:D:180:SER:H	1:D:183:GLU:CG	2.12	0.62
1:F:230:ILE:HB	1:F:242:ILE:CG2	2.29	0.62
1:G:184:LEU:O	1:G:188:GLU:HB2	2.00	0.62
1:J:159:ALA:O	1:J:163:GLU:HB2	2.00	0.62
1:E:177:SER:HB2	1:H:163:GLU:HA	1.81	0.62
1:F:167:ARG:HH21	1:H:227:ALA:HB2	1.64	0.62
1:K:155:LEU:O	1:K:159:ALA:HB2	2.00	0.62
1:L:103:ARG:O	1:L:105:LEU:N	2.33	0.62
1:L:79:LEU:O	1:L:82:VAL:HG23	1.99	0.62
1:A:91:ILE:HD13	1:A:107:GLN:HA	1.82	0.62
1:A:222:ARG:O	1:A:224:LEU:N	2.33	0.62
1:F:199:GLY:H	1:F:241:TYR:HE1	1.48	0.62
1:G:32:ARG:CD	1:G:54:ASN:HB3	2.29	0.62
1:I:19:GLY:HA3	1:K:216:VAL:HA	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:25:LYS:O	1:F:29:GLU:N	2.25	0.62
1:J:117:ILE:CG1	1:J:122:ARG:HB2	2.30	0.62
1:J:184:LEU:HD13	1:K:162:ILE:HD12	1.82	0.62
1:K:35:ILE:O	1:K:36:ASP:HB3	2.00	0.62
1:L:13:MET:HG3	1:L:14:LEU:N	2.15	0.62
1:A:145:TYR:CE1	1:B:145:TYR:CB	2.78	0.62
1:K:123:LEU:HB2	1:K:154:ILE:HD13	1.82	0.62
1:A:237:MET:HG3	1:A:238:LYS:N	2.14	0.61
1:D:32:ARG:HB2	1:D:52:SER:HB3	1.80	0.61
1:D:3:LEU:HD13	1:D:138:ASP:OD2	2.00	0.61
1:G:61:ARG:HH21	1:G:75:TYR:HE1	1.48	0.61
1:A:197:ASN:C	1:A:197:ASN:HD22	2.04	0.61
1:D:121:GLU:HB3	1:D:123:LEU:HG	1.83	0.61
1:F:185:GLU:O	1:F:189:HIS:HD2	1.81	0.61
1:D:160:GLU:C	1:D:162:ILE:H	2.02	0.61
1:M:219:ASN:HA	1:M:222:ARG:HB2	1.82	0.61
1:A:203:ALA:H	1:A:239:GLY:HA3	1.63	0.61
1:C:41:VAL:HG22	1:C:126:LEU:HD13	1.82	0.61
1:I:216:VAL:HA	1:I:219:ASN:HD21	1.66	0.61
1:J:35:ILE:O	1:J:36:ASP:HB2	2.01	0.61
1:H:214:ARG:O	1:H:217:ILE:HG22	2.01	0.61
1:I:161:GLU:OE2	1:I:162:ILE:HG23	2.01	0.61
1:C:7:THR:C	1:C:9:ILE:H	2.02	0.60
1:F:181:TYR:HD2	1:G:158:LYS:HG3	1.64	0.60
1:A:153:GLU:O	1:A:153:GLU:HG3	2.00	0.60
1:B:158:LYS:HB2	1:C:181:TYR:HD2	1.63	0.60
1:L:115:PRO:HA	1:L:125:THR:HG22	1.83	0.60
1:A:90:ASP:HA	1:A:109:GLY:O	2.02	0.60
1:C:247:ASN:ND2	1:C:247:ASN:H	1.99	0.60
1:A:220:ALA:C	1:A:222:ARG:H	2.03	0.60
1:C:203:ALA:O	1:C:207:ALA:CB	2.49	0.60
1:D:31:LEU:HB2	1:D:39:ILE:CD1	2.31	0.60
1:G:202:VAL:HB	1:G:205:LYS:HB2	1.82	0.60
1:I:38:ASN:HB2	1:I:129:SER:H	1.67	0.60
1:I:91:ILE:HB	1:I:108:ALA:H	1.65	0.60
1:E:250:LEU:HD23	1:E:250:LEU:H	1.67	0.60
1:G:39:ILE:HA	1:G:128:LEU:HD22	1.82	0.60
1:J:32:ARG:HA	1:J:39:ILE:HG12	1.84	0.60
1:J:250:LEU:HD23	1:J:253:LEU:HD12	1.83	0.60
1:A:149:VAL:O	1:A:152:MET:HB3	2.02	0.60
1:C:138:ASP:C	1:C:140:LEU:N	2.55	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:114:VAL:CG1	1:E:147:ALA:HB2	2.32	0.60
1:E:158:LYS:O	1:E:162:ILE:HG12	2.01	0.60
1:F:27:MET:HE3	1:F:150:VAL:HG13	1.84	0.60
1:G:248:LYS:HA	1:G:251:ILE:HG12	1.83	0.60
1:I:43:SER:OG	1:I:44:ARG:N	2.35	0.60
1:J:212:ILE:HG12	1:K:121:GLU:CB	2.23	0.60
1:A:224:LEU:O	1:A:228:GLY:N	2.31	0.60
1:B:37:SER:HB2	1:B:130:ARG:NE	2.17	0.60
1:C:172:VAL:HG11	1:C:249:PHE:CD1	2.37	0.60
1:D:180:SER:HB3	1:D:183:GLU:HG2	1.82	0.60
1:H:212:ILE:HG22	1:H:212:ILE:O	2.02	0.60
1:N:79:LEU:HD21	1:N:113:ILE:HD13	1.82	0.60
1:A:113:ILE:HA	1:A:126:LEU:O	2.02	0.59
1:G:190:ILE:HG23	1:G:201:LEU:HD13	1.84	0.59
1:A:171:VAL:HG12	1:C:174:MET:HE3	1.83	0.59
1:B:254:GLU:H	1:B:254:GLU:CD	2.05	0.59
1:H:91:ILE:HG23	1:H:107:GLN:HA	1.85	0.59
1:K:98:PHE:HB3	1:K:103:ARG:HH22	1.66	0.59
1:J:168:SER:O	1:J:172:VAL:HG23	2.02	0.59
1:D:6:LYS:HB3	1:D:142:LEU:HD11	1.83	0.59
1:F:213:THR:C	1:F:215:SER:H	2.05	0.59
1:F:212:ILE:HA	1:G:121:GLU:HB3	1.84	0.59
1:I:169:LYS:HB2	1:L:173:GLN:CD	2.23	0.59
1:D:24:PHE:O	1:D:50:GLY:HA3	2.03	0.59
1:E:17:ALA:HA	1:E:156:ARG:CB	2.32	0.59
1:I:41:VAL:O	1:I:48:LEU:HA	2.02	0.59
1:D:33:ASP:HA	1:D:36:ASP:HA	1.84	0.59
1:L:256:LEU:C	1:L:258:SER:H	2.05	0.59
1:L:65:MET:HA	1:L:72:PRO:HD3	1.84	0.59
1:J:61:ARG:C	1:J:63:LYS:N	2.54	0.59
1:B:46:GLY:O	1:B:47:LYS:HB2	2.02	0.59
1:D:13:MET:HG2	1:D:30:THR:HG21	1.85	0.59
1:F:111:THR:HG23	1:F:127:ILE:HG23	1.85	0.59
1:F:230:ILE:HB	1:F:242:ILE:HG21	1.83	0.59
1:E:155:LEU:HG	1:H:181:TYR:HB3	1.85	0.59
1:K:25:LYS:HG3	1:K:51:TYR:O	2.02	0.59
1:B:114:VAL:HB	1:B:126:LEU:HB3	1.84	0.59
1:A:137:ASP:HA	1:B:4:LEU:HD22	1.85	0.59
1:C:252:GLU:O	1:C:256:LEU:HB2	2.02	0.59
1:C:48:LEU:HD23	1:C:69:ARG:HG2	1.84	0.59
1:E:24:PHE:HB2	1:E:49:LEU:HB3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:201:LEU:HD22	1:F:242:ILE:HD11	1.83	0.59
1:A:2:ALA:O	1:A:4:LEU:N	2.36	0.59
1:B:3:LEU:HA	1:B:6:LYS:HD2	1.85	0.59
1:G:110:LEU:HB2	1:G:130:ARG:HB2	1.84	0.59
1:I:186:ALA:HB2	1:I:212:ILE:HD13	1.84	0.59
1:B:103:ARG:HH11	1:B:103:ARG:HG2	1.68	0.58
1:C:85:THR:HG23	1:C:114:VAL:HG22	1.85	0.58
1:I:187:ILE:HD13	1:I:190:ILE:HD12	1.84	0.58
1:I:7:THR:C	1:I:9:ILE:H	2.07	0.58
1:I:170:ALA:HB1	1:K:174:MET:HE3	1.84	0.58
1:C:31:LEU:C	1:C:39:ILE:HG13	2.24	0.58
1:F:2:ALA:O	1:F:6:LYS:HG3	2.04	0.58
1:I:35:ILE:HG23	1:I:139:ASP:HB3	1.84	0.58
1:C:138:ASP:HA	1:C:141:ILE:HG22	1.85	0.58
1:H:198:GLU:OE2	1:H:243:LYS:HG3	2.04	0.58
1:L:65:MET:HG3	1:L:71:PHE:CD1	2.37	0.58
1:E:75:TYR:O	1:E:79:LEU:HD12	2.02	0.58
1:H:10:ILE:HD11	1:H:34:VAL:HG11	1.84	0.58
1:D:169:LYS:HB3	1:D:252:GLU:OE2	2.03	0.58
1:K:113:ILE:CG1	1:K:127:ILE:HG13	2.32	0.58
1:L:185:GLU:HA	1:L:188:GLU:HB2	1.85	0.58
1:L:98:PHE:CG	1:L:99:PRO:HD2	2.38	0.58
1:D:162:ILE:HG13	1:D:163:GLU:N	2.19	0.58
1:E:28:ALA:O	1:E:32:ARG:HB3	2.03	0.58
1:F:168:SER:HB3	1:F:246:ASN:HD21	1.68	0.58
1:F:217:ILE:O	1:F:221:LEU:CD1	2.52	0.58
1:L:224:LEU:HB3	1:L:230:ILE:CG1	2.33	0.58
1:A:145:TYR:HA	1:B:145:TYR:OH	2.03	0.58
1:C:163:GLU:O	1:C:164:GLU:HG2	2.04	0.58
1:C:31:LEU:O	1:C:39:ILE:HG13	2.03	0.58
1:L:252:GLU:O	1:L:255:ASN:HB3	2.04	0.58
1:D:141:ILE:HD12	1:D:142:LEU:HG	1.85	0.58
1:I:135:PHE:O	1:I:140:LEU:HB2	2.03	0.58
1:K:66:LEU:HA	1:K:69:ARG:HD3	1.86	0.58
1:C:249:PHE:O	1:C:252:GLU:N	2.37	0.58
1:F:224:LEU:HD22	1:F:230:ILE:HG12	1.86	0.58
1:K:252:GLU:O	1:K:256:LEU:HB2	2.03	0.58
1:L:115:PRO:HB3	1:L:122:ARG:HD2	1.86	0.58
1:L:181:TYR:HA	1:L:184:LEU:HB3	1.85	0.58
1:A:57:ILE:HG23	1:A:131:LEU:CD1	2.34	0.58
1:C:43:SER:HB3	1:C:47:LYS:CG	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:202:VAL:HG23	1:G:206:ILE:CG1	2.34	0.58
1:K:65:MET:O	1:K:69:ARG:N	2.33	0.58
1:B:99:PRO:O	1:B:103:ARG:HB2	2.04	0.57
1:F:136:ASN:H	1:F:139:ASP:HB2	1.68	0.57
1:I:157:GLU:C	1:I:159:ALA:H	2.05	0.57
1:L:162:ILE:HG13	1:L:163:GLU:N	2.17	0.57
1:A:6:LYS:HA	1:A:9:ILE:CD1	2.34	0.57
1:B:38:ASN:O	1:B:128:LEU:HB3	2.03	0.57
1:E:10:ILE:HG21	1:E:145:TYR:O	2.03	0.57
1:A:25:LYS:O	1:A:29:GLU:HG3	2.04	0.57
1:A:215:SER:HB3	1:C:19:GLY:HA3	1.87	0.57
1:D:114:VAL:HG11	1:D:143:ALA:O	2.03	0.57
1:E:116:ILE:HD13	1:E:150:VAL:HG11	1.86	0.57
1:G:172:VAL:HG13	1:G:249:PHE:CD1	2.39	0.57
1:I:212:ILE:CG2	1:I:216:VAL:HG11	2.34	0.57
1:B:126:LEU:C	1:B:127:ILE:HG13	2.24	0.57
1:J:151:GLY:HA2	1:J:154:ILE:HD12	1.85	0.57
1:L:207:ALA:HA	1:L:212:ILE:O	2.04	0.57
1:C:103:ARG:HA	1:C:106:PHE:HE1	1.70	0.57
1:C:86:SER:O	1:C:112:THR:HG23	2.05	0.57
1:K:41:VAL:H	1:K:48:LEU:CD1	2.18	0.57
1:D:106:PHE:HB3	1:D:111:THR:HB	1.85	0.57
1:D:31:LEU:HB2	1:D:39:ILE:HG13	1.87	0.57
1:F:113:ILE:HG23	1:F:125:THR:HG21	1.85	0.57
1:H:172:VAL:O	1:H:176:ILE:N	2.37	0.57
1:N:74:GLU:HB3	1:N:102:ASN:HD21	1.70	0.57
1:B:111:THR:HG1	1:B:129:SER:HB3	1.68	0.57
1:F:157:GLU:HG3	1:F:158:LYS:N	2.20	0.57
1:G:139:ASP:O	1:G:143:ALA:HB2	2.04	0.57
1:F:204:SER:HB3	1:F:214:ARG:HB3	1.86	0.56
1:M:167:ARG:HG3	1:N:174:MET:CE	2.34	0.56
1:A:100:VAL:HA	1:A:103:ARG:CD	2.33	0.56
1:K:4:LEU:HB2	1:L:137:ASP:OD2	2.05	0.56
1:B:105:LEU:H	1:B:105:LEU:HD12	1.70	0.56
1:B:182:SER:HA	1:C:121:GLU:OE1	2.05	0.56
1:C:138:ASP:O	1:C:140:LEU:N	2.38	0.56
1:F:187:ILE:HD13	1:F:190:ILE:HD12	1.86	0.56
1:A:138:ASP:C	1:A:140:LEU:H	2.09	0.56
1:C:173:GLN:C	1:C:175:ALA:N	2.59	0.56
1:D:38:ASN:ND2	1:D:53:ILE:HG22	2.15	0.56
1:G:157:GLU:HG3	1:G:158:LYS:H	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:15:GLN:HG3	1:J:20:LYS:HE3	1.87	0.56
1:L:103:ARG:C	1:L:105:LEU:N	2.58	0.56
1:A:203:ALA:H	1:A:239:GLY:CA	2.18	0.56
1:F:215:SER:O	1:F:218:VAL:HB	2.05	0.56
1:H:179:LEU:CA	1:H:183:GLU:HB2	2.34	0.56
1:F:219:ASN:HB2	1:H:19:GLY:CA	2.33	0.56
1:L:91:ILE:HG23	1:L:106:PHE:C	2.25	0.56
1:M:233:ARG:H	1:M:241:TYR:HD2	1.53	0.56
1:N:175:ALA:HB1	1:N:224:LEU:HD12	1.87	0.56
1:I:72:PRO:HG2	1:I:75:TYR:HB2	1.87	0.56
1:I:80:PHE:HE2	1:I:122:ARG:HB3	1.71	0.56
1:J:202:VAL:O	1:J:206:ILE:HB	2.05	0.56
1:L:171:VAL:O	1:L:175:ALA:N	2.37	0.56
1:L:65:MET:CG	1:L:71:PHE:HD1	2.17	0.56
1:L:191:PHE:HA	1:L:194:LEU:HB2	1.87	0.56
1:B:122:ARG:C	1:B:124:GLY:H	2.08	0.56
1:F:39:ILE:HB	1:F:52:SER:HB2	1.88	0.56
1:E:216:VAL:HB	1:G:19:GLY:HA2	1.87	0.56
1:G:248:LYS:HA	1:G:251:ILE:CG1	2.36	0.56
1:G:116:ILE:HD13	1:G:150:VAL:HB	1.87	0.56
1:L:40:PHE:HB2	1:L:127:ILE:HG13	1.87	0.56
1:M:202:VAL:HG11	1:M:205:LYS:HB2	1.86	0.56
1:D:130:ARG:HB2	1:D:135:PHE:HZ	1.71	0.56
1:D:242:ILE:HG13	1:D:243:LYS:N	2.20	0.56
1:F:150:VAL:O	1:F:153:GLU:HB2	2.06	0.56
1:G:24:PHE:CE1	1:G:49:LEU:HD23	2.41	0.56
1:A:24:PHE:O	1:A:27:MET:HB3	2.06	0.55
1:K:3:LEU:HA	1:K:6:LYS:HB2	1.88	0.55
1:D:224:LEU:CB	1:D:230:ILE:HG12	2.35	0.55
1:E:44:ARG:NE	1:E:122:ARG:O	2.39	0.55
1:F:181:TYR:CE2	1:G:158:LYS:HE2	2.41	0.55
1:L:191:PHE:HA	1:L:194:LEU:CB	2.35	0.55
1:L:221:LEU:O	1:L:225:GLU:N	2.37	0.55
1:A:217:ILE:O	1:A:221:LEU:HB2	2.07	0.55
1:B:250:LEU:HA	1:B:253:LEU:HB2	1.88	0.55
1:D:224:LEU:HB2	1:D:230:ILE:HG12	1.89	0.55
1:E:158:LYS:O	1:E:161:GLU:HG2	2.06	0.55
1:K:83:PRO:O	1:K:115:PRO:HG2	2.07	0.55
1:A:187:ILE:HD13	1:A:221:LEU:HD22	1.89	0.55
1:F:81:ASN:O	1:F:83:PRO:HD3	2.05	0.55
1:H:180:SER:O	1:H:182:SER:N	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:9:ILE:HG21	1:I:34:VAL:HG21	1.87	0.55
1:E:45:ARG:HD2	1:E:47:LYS:HZ2	1.71	0.55
1:I:9:ILE:O	1:I:13:MET:HB3	2.06	0.55
1:A:223:LYS:HA	1:A:226:SER:CB	2.27	0.55
1:G:194:LEU:HD11	1:G:199:GLY:HA2	1.87	0.55
1:H:3:LEU:HD22	1:H:138:ASP:HB3	1.89	0.55
1:K:123:LEU:HB3	1:K:154:ILE:HG21	1.88	0.55
1:A:4:LEU:HA	1:B:141:ILE:HG13	1.89	0.55
1:I:222:ARG:C	1:I:224:LEU:H	2.11	0.55
1:K:230:ILE:HB	1:K:243:LYS:O	2.07	0.55
1:L:180:SER:N	1:L:183:GLU:HG3	2.20	0.55
1:L:71:PHE:CD1	1:L:72:PRO:HD2	2.42	0.55
1:C:172:VAL:O	1:C:172:VAL:CG1	2.54	0.55
1:C:202:VAL:HG12	1:C:203:ALA:H	1.71	0.55
1:C:45:ARG:HH11	1:C:47:LYS:HZ3	1.52	0.55
1:D:213:THR:O	1:D:217:ILE:HD12	2.07	0.55
1:E:198:GLU:HG2	1:E:243:LYS:HD2	1.88	0.55
1:L:213:THR:O	1:L:216:VAL:HG12	2.07	0.55
1:N:172:VAL:HG11	1:N:252:GLU:HG3	1.88	0.55
1:A:181:TYR:HE1	1:A:185:GLU:HG3	1.72	0.55
1:B:37:SER:OG	1:B:38:ASN:N	2.40	0.55
1:D:185:GLU:O	1:D:189:HIS:CD2	2.59	0.55
1:E:145:TYR:HE2	1:F:145:TYR:O	1.90	0.55
1:H:221:LEU:O	1:H:225:GLU:HB2	2.06	0.55
1:J:220:ALA:O	1:J:223:LYS:HB2	2.07	0.55
1:J:88:ASN:CG	1:J:110:LEU:HG	2.26	0.55
1:J:181:TYR:HE2	1:K:123:LEU:HD22	1.71	0.55
1:K:55:GLN:OE1	1:K:130:ARG:HD3	2.07	0.55
1:B:12:SER:C	1:B:14:LEU:H	2.10	0.54
1:C:176:ILE:C	1:C:178:SER:H	2.10	0.54
1:E:103:ARG:HG3	1:E:106:PHE:CZ	2.43	0.54
1:E:111:THR:HA	1:E:129:SER:HA	1.89	0.54
1:L:5:GLN:O	1:L:9:ILE:HG13	2.07	0.54
1:N:224:LEU:HB3	1:N:229:VAL:HB	1.89	0.54
1:B:233:ARG:HD3	1:G:233:ARG:HH11	1.71	0.54
1:C:29:GLU:HA	1:C:52:SER:OG	2.06	0.54
1:D:131:LEU:HG	1:D:132:GLN:N	2.22	0.54
1:H:149:VAL:HA	1:H:152:MET:HB2	1.88	0.54
1:H:163:GLU:O	1:H:167:ARG:N	2.36	0.54
1:A:40:PHE:HD2	1:A:127:ILE:HG22	1.71	0.54
1:A:150:VAL:C	1:A:152:MET:H	2.10	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:151:GLY:HA2	1:C:154:ILE:HD12	1.88	0.54
1:F:71:PHE:HE2	1:F:105:LEU:HD21	1.72	0.54
1:H:88:ASN:OD1	1:H:110:LEU:HB3	2.07	0.54
1:J:35:ILE:HG23	1:J:37:SER:H	1.72	0.54
1:N:197:ASN:HD21	1:N:244:VAL:HG22	1.73	0.54
1:D:147:ALA:C	1:D:149:VAL:N	2.57	0.54
1:J:115:PRO:CA	1:J:125:THR:HA	2.33	0.54
1:J:228:GLY:HA3	1:L:228:GLY:HA3	1.90	0.54
1:L:231:GLU:HG3	1:L:243:LYS:O	2.07	0.54
1:A:188:GLU:OE2	1:A:189:HIS:HD2	1.90	0.54
1:B:187:ILE:HA	1:B:190:ILE:HG12	1.89	0.54
1:C:43:SER:HB3	1:C:47:LYS:HG2	1.88	0.54
1:H:249:PHE:O	1:H:253:LEU:N	2.40	0.54
1:L:146:GLY:O	1:L:149:VAL:HG22	2.08	0.54
1:H:247:ASN:OD1	1:H:248:LYS:HD2	2.08	0.54
1:J:106:PHE:HD1	1:J:111:THR:HB	1.71	0.54
1:L:114:VAL:HG11	1:L:147:ALA:HB3	1.89	0.54
1:L:203:ALA:O	1:L:214:ARG:HB3	2.07	0.54
1:D:235:LEU:CG	1:D:236:GLY:H	2.21	0.54
1:H:191:PHE:HA	1:H:194:LEU:HB3	1.90	0.54
1:J:250:LEU:HA	1:J:253:LEU:HB3	1.90	0.54
1:L:205:LYS:HG2	1:L:206:ILE:HD12	1.90	0.54
1:G:115:PRO:HA	1:G:126:LEU:HD13	1.89	0.54
1:C:111:THR:HG22	1:C:129:SER:OG	2.08	0.54
1:D:106:PHE:HD2	1:D:111:THR:HB	1.73	0.54
1:E:3:LEU:HD11	1:E:141:ILE:HD12	1.89	0.54
1:H:237:MET:HG3	1:H:239:GLY:H	1.73	0.54
1:L:91:ILE:HA	1:L:106:PHE:CD1	2.41	0.54
1:B:48:LEU:HD11	1:B:51:TYR:HB3	1.90	0.54
1:C:171:VAL:O	1:C:173:GLN:N	2.38	0.54
1:D:250:LEU:HD13	1:D:253:LEU:HD22	1.89	0.54
1:D:5:GLN:HB3	1:D:9:ILE:HD12	1.89	0.54
1:G:91:ILE:HG22	1:G:103:ARG:HG2	1.89	0.54
1:I:63:LYS:HA	1:I:66:LEU:HB2	1.89	0.54
1:I:145:TYR:CA	1:J:145:TYR:OH	2.56	0.54
1:J:72:PRO:HD2	1:J:75:TYR:HB2	1.89	0.54
1:L:114:VAL:HG11	1:L:147:ALA:CB	2.37	0.54
1:G:180:SER:O	1:G:183:GLU:N	2.41	0.53
1:L:112:THR:HB	1:L:128:LEU:HB2	1.89	0.53
1:M:57:ILE:HG22	1:M:108:ALA:HB1	1.90	0.53
1:B:233:ARG:H	1:B:242:ILE:CG1	2.20	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:173:GLN:HA	1:I:176:ILE:CD1	2.38	0.53
1:I:42:VAL:HG11	1:I:71:PHE:HE2	1.72	0.53
1:M:32:ARG:O	1:M:36:ASP:HA	2.08	0.53
1:A:54:ASN:CG	1:A:55:GLN:H	2.12	0.53
1:B:116:ILE:HG21	1:B:150:VAL:HG12	1.89	0.53
1:E:51:TYR:HB3	1:E:66:LEU:HD21	1.90	0.53
1:H:34:VAL:HG12	1:H:142:LEU:HD13	1.90	0.53
1:B:24:PHE:HE1	1:B:154:ILE:HG12	1.71	0.53
1:C:161:GLU:HG3	1:C:162:ILE:N	2.24	0.53
1:E:6:LYS:HD3	1:E:142:LEU:HD11	1.90	0.53
1:G:17:ALA:HB3	1:H:119:GLY:HA3	1.91	0.53
1:K:176:ILE:C	1:K:178:SER:H	2.11	0.53
1:E:130:ARG:HB2	1:E:135:PHE:HZ	1.74	0.53
1:J:40:PHE:CB	1:J:127:ILE:HB	2.39	0.53
1:J:229:VAL:HB	1:J:249:PHE:CE2	2.42	0.53
1:A:202:VAL:HB	1:A:206:ILE:H	1.74	0.53
1:E:141:ILE:HG23	1:F:7:THR:HG21	1.90	0.53
1:F:169:LYS:NZ	1:G:252:GLU:OE1	2.42	0.53
1:K:65:MET:O	1:K:67:GLU:N	2.42	0.53
1:K:145:TYR:CD2	1:L:145:TYR:CB	2.87	0.53
1:A:217:ILE:HG23	1:A:221:LEU:HD23	1.91	0.53
1:F:24:PHE:HE1	1:F:41:VAL:HG21	1.74	0.53
1:F:78:ASN:O	1:F:82:VAL:HG23	2.09	0.53
1:H:170:ALA:O	1:H:174:MET:HG2	2.08	0.53
1:K:187:ILE:HA	1:K:190:ILE:HD12	1.91	0.53
1:K:79:LEU:C	1:K:81:ASN:H	2.11	0.53
1:A:145:TYR:O	1:A:149:VAL:HG23	2.09	0.53
1:E:68:ASP:N	1:E:68:ASP:OD1	2.42	0.53
1:F:30:THR:HA	1:F:33:ASP:HB2	1.90	0.53
1:G:150:VAL:O	1:G:154:ILE:N	2.42	0.53
1:L:214:ARG:O	1:L:217:ILE:HB	2.09	0.53
1:C:114:VAL:O	1:C:126:LEU:N	2.39	0.53
1:C:117:ILE:HG23	1:C:122:ARG:HA	1.92	0.53
1:D:194:LEU:H	1:D:194:LEU:HD22	1.74	0.53
1:H:117:ILE:O	1:H:121:GLU:O	2.27	0.53
1:K:98:PHE:HB3	1:K:103:ARG:NH2	2.24	0.53
1:A:253:LEU:O	1:A:256:LEU:HB2	2.10	0.52
1:C:10:ILE:HG21	1:C:31:LEU:HD21	1.91	0.52
1:K:210:VAL:HB	1:K:212:ILE:HG12	1.89	0.52
1:M:228:GLY:HA3	1:N:228:GLY:CA	2.39	0.52
1:F:153:GLU:CA	1:F:153:GLU:OE2	2.57	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:116:ILE:HG21	1:H:150:VAL:HG13	1.90	0.52
1:H:117:ILE:HA	1:H:122:ARG:HA	1.91	0.52
1:J:90:ASP:HA	1:J:106:PHE:CB	2.40	0.52
1:D:39:ILE:O	1:D:51:TYR:HB2	2.09	0.52
1:J:181:TYR:HE1	1:J:185:GLU:HG3	1.74	0.52
1:A:181:TYR:CE1	1:A:185:GLU:HG3	2.44	0.52
1:B:121:GLU:OE2	1:C:181:TYR:HE1	1.91	0.52
1:I:15:GLN:HB2	1:J:119:GLY:HA2	1.90	0.52
1:L:35:ILE:HD13	1:L:128:LEU:HD21	1.92	0.52
1:E:201:LEU:HB2	1:E:242:ILE:HD12	1.92	0.52
1:F:32:ARG:C	1:F:34:VAL:H	2.12	0.52
1:G:114:VAL:HG21	1:G:140:LEU:HD13	1.91	0.52
1:K:118:GLY:C	1:K:120:GLY:H	2.13	0.52
1:K:170:ALA:O	1:K:174:MET:HB2	2.09	0.52
1:K:145:TYR:CD2	1:L:145:TYR:HB2	2.44	0.52
1:D:136:ASN:O	1:D:138:ASP:N	2.41	0.52
1:D:244:VAL:HG12	1:D:245:LEU:N	2.25	0.52
1:G:111:THR:HG21	1:G:127:ILE:HG23	1.91	0.52
1:A:214:ARG:O	1:A:218:VAL:HG22	2.09	0.52
1:C:226:SER:C	1:C:228:GLY:H	2.13	0.52
1:D:149:VAL:O	1:D:152:MET:HB2	2.10	0.52
1:H:171:VAL:O	1:H:175:ALA:N	2.43	0.52
1:I:173:GLN:HA	1:I:176:ILE:HD13	1.92	0.52
1:J:25:LYS:O	1:J:29:GLU:HB2	2.10	0.52
1:K:231:GLU:HB3	1:K:243:LYS:HB3	1.91	0.52
1:K:60:ASP:O	1:K:63:LYS:HB2	2.10	0.52
1:D:74:GLU:C	1:D:76:THR:H	2.12	0.52
1:E:40:PHE:CD2	1:E:127:ILE:CG2	2.92	0.52
1:H:187:ILE:HG12	1:H:220:ALA:HB1	1.92	0.52
1:K:172:VAL:HG22	1:K:246:ASN:OD1	2.09	0.52
1:K:25:LYS:O	1:K:29:GLU:HG3	2.09	0.52
1:A:180:SER:O	1:A:181:TYR:C	2.47	0.52
1:D:10:ILE:O	1:D:13:MET:HG3	2.10	0.52
1:C:144:GLU:HG3	1:D:8:ARG:HE	1.73	0.52
1:F:114:VAL:CG2	1:F:115:PRO:HD2	2.40	0.52
1:F:219:ASN:HD21	1:F:223:LYS:HE3	1.75	0.52
1:A:191:PHE:CE2	1:A:249:PHE:HE2	2.28	0.52
1:F:165:GLU:HG2	1:F:248:LYS:HE2	1.91	0.52
1:G:139:ASP:O	1:G:143:ALA:CB	2.58	0.52
1:J:162:ILE:HG13	1:J:163:GLU:N	2.25	0.52
1:B:23:ASN:O	1:B:27:MET:HG3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:32:ARG:HB2	1:C:52:SER:HB3	1.90	0.51
1:D:32:ARG:HB2	1:D:52:SER:CB	2.40	0.51
1:L:3:LEU:HD21	1:L:138:ASP:HB3	1.92	0.51
1:M:15:GLN:HB3	1:M:18:ALA:HB2	1.91	0.51
1:N:250:LEU:HA	1:N:253:LEU:HD13	1.92	0.51
1:A:216:VAL:O	1:A:217:ILE:C	2.47	0.51
1:B:109:GLY:O	1:B:110:LEU:HD12	2.11	0.51
1:C:110:LEU:HD23	1:C:132:GLN:HA	1.92	0.51
1:H:126:LEU:HD23	1:H:128:LEU:HD11	1.90	0.51
1:J:115:PRO:HD3	1:J:125:THR:HG23	1.91	0.51
1:J:191:PHE:HB3	1:J:250:LEU:HD21	1.90	0.51
1:K:103:ARG:HG3	1:K:106:PHE:CD1	2.45	0.51
1:A:179:LEU:HD22	1:A:183:GLU:HB3	1.92	0.51
1:A:22:VAL:HG13	1:A:153:GLU:HG3	1.93	0.51
1:D:116:ILE:HG23	1:D:148:THR:HA	1.92	0.51
1:D:55:GLN:HG2	1:D:56:GLN:N	2.21	0.51
1:E:172:VAL:O	1:E:176:ILE:HB	2.10	0.51
1:K:55:GLN:HE22	1:K:130:ARG:HA	1.76	0.51
1:K:91:ILE:HG22	1:K:106:PHE:O	2.10	0.51
1:D:240:THR:OG1	1:D:241:TYR:N	2.42	0.51
1:I:38:ASN:HD22	1:I:40:PHE:HE1	1.57	0.51
1:M:27:MET:SD	1:M:150:VAL:HA	2.49	0.51
1:A:79:LEU:HG	1:A:98:PHE:HE1	1.74	0.51
1:C:128:LEU:HD21	1:C:143:ALA:HB1	1.93	0.51
1:C:40:PHE:HB3	1:C:51:TYR:HB2	1.93	0.51
1:F:151:GLY:C	1:F:153:GLU:N	2.64	0.51
1:J:53:ILE:HD13	1:J:56:GLN:HA	1.93	0.51
1:B:185:GLU:HA	1:B:188:GLU:HB3	1.91	0.51
1:F:181:TYR:HE1	1:F:185:GLU:OE1	1.94	0.51
1:J:117:ILE:CG2	1:J:118:GLY:N	2.66	0.51
1:L:56:GLN:H	1:L:57:ILE:HD12	1.75	0.51
1:M:37:SER:HB2	1:M:130:ARG:HH11	1.75	0.51
1:M:30:THR:HG22	1:M:34:VAL:HG21	1.93	0.51
1:C:53:ILE:HG12	1:C:56:GLN:HA	1.93	0.51
1:G:112:THR:H	1:G:128:LEU:H	1.58	0.51
1:H:201:LEU:HD12	1:H:201:LEU:H	1.76	0.51
1:H:6:LYS:HB3	1:H:34:VAL:HG13	1.93	0.51
1:L:37:SER:HB2	1:L:130:ARG:HE	1.75	0.51
1:B:47:LYS:HE3	1:B:70:GLN:HB2	1.92	0.51
1:E:4:LEU:HD21	1:F:141:ILE:HB	1.93	0.51
1:G:213:THR:O	1:G:217:ILE:HG13	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:19:GLY:HA3	1:K:215:SER:C	2.30	0.51
1:K:224:LEU:HD12	1:K:229:VAL:HG11	1.91	0.51
1:N:239:GLY:O	1:N:240:THR:HB	2.11	0.51
1:A:90:ASP:CG	1:A:91:ILE:H	2.14	0.51
1:B:103:ARG:NH1	1:B:103:ARG:HB3	2.22	0.51
1:B:122:ARG:O	1:B:124:GLY:N	2.42	0.51
1:B:6:LYS:O	1:B:9:ILE:HG22	2.11	0.51
1:I:185:GLU:HB3	1:I:189:HIS:HD2	1.76	0.51
1:L:15:GLN:HG2	1:L:16:ALA:H	1.76	0.51
1:A:126:LEU:HD12	1:A:127:ILE:H	1.76	0.51
1:B:121:GLU:HB3	1:B:123:LEU:HD23	1.93	0.51
1:E:171:VAL:HG23	1:E:172:VAL:N	2.26	0.51
1:J:113:ILE:HA	1:J:126:LEU:O	2.10	0.51
1:K:218:VAL:C	1:K:220:ALA:H	2.14	0.51
1:N:65:MET:HG3	1:N:71:PHE:CZ	2.46	0.51
1:C:40:PHE:CE2	1:C:127:ILE:HB	2.46	0.50
1:F:87:SER:O	1:F:88:ASN:HB2	2.11	0.50
1:K:150:VAL:HG12	1:K:154:ILE:HG13	1.94	0.50
1:K:203:ALA:HB2	1:K:240:THR:HG22	1.93	0.50
1:N:217:ILE:HA	1:N:220:ALA:HB3	1.92	0.50
1:C:136:ASN:O	1:C:139:ASP:N	2.44	0.50
1:D:126:LEU:HD13	1:D:150:VAL:HG21	1.92	0.50
1:M:85:THR:HG22	1:M:86:SER:H	1.76	0.50
1:A:179:LEU:HA	1:A:183:GLU:HB2	1.92	0.50
1:F:165:GLU:O	1:F:168:SER:HB2	2.11	0.50
1:F:168:SER:HB3	1:F:246:ASN:ND2	2.26	0.50
1:K:59:ASN:HD21	1:K:105:LEU:HD12	1.76	0.50
1:N:235:LEU:HG	1:N:237:MET:SD	2.51	0.50
1:D:37:SER:HB2	1:D:130:ARG:NH2	2.25	0.50
1:E:162:ILE:C	1:E:164:GLU:H	2.12	0.50
1:F:200:LEU:O	1:F:200:LEU:HD23	2.12	0.50
1:G:38:ASN:HB2	1:G:129:SER:OG	2.10	0.50
1:K:37:SER:HB3	1:K:130:ARG:NH1	2.26	0.50
1:A:22:VAL:HG21	1:A:156:ARG:O	2.11	0.50
1:A:4:LEU:HD22	1:B:137:ASP:HA	1.94	0.50
1:B:184:LEU:HD13	1:C:162:ILE:HD13	1.93	0.50
1:H:206:ILE:HA	1:H:209:ARG:HG2	1.94	0.50
1:I:3:LEU:HA	1:I:6:LYS:CG	2.41	0.50
1:L:48:LEU:HD22	1:L:65:MET:SD	2.52	0.50
1:M:167:ARG:HA	1:N:174:MET:HE1	1.94	0.50
1:M:229:VAL:O	1:M:245:LEU:HB3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:237:MET:HG3	1:C:238:LYS:H	1.72	0.50
1:A:173:GLN:NE2	1:D:169:LYS:HD2	2.27	0.50
1:G:145:TYR:O	1:H:145:TYR:CD1	2.63	0.50
1:H:32:ARG:HG2	1:H:54:ASN:HD22	1.77	0.50
1:J:37:SER:HB2	1:J:130:ARG:NE	2.27	0.50
1:K:86:SER:HB3	1:K:89:LEU:HD22	1.92	0.50
1:B:222:ARG:HB2	1:B:222:ARG:CZ	2.41	0.50
1:B:42:VAL:HG23	1:B:125:THR:HB	1.92	0.50
1:E:40:PHE:HE1	1:E:66:LEU:HD12	1.77	0.50
1:F:160:GLU:OE2	1:H:223:LYS:NZ	2.44	0.50
1:H:106:PHE:CD2	1:H:111:THR:HB	2.46	0.50
1:I:6:LYS:HB3	1:I:142:LEU:CD1	2.38	0.50
1:A:174:MET:O	1:A:177:SER:N	2.43	0.50
1:A:190:ILE:HG13	1:A:201:LEU:HD23	1.94	0.50
1:D:213:THR:HB	1:D:216:VAL:H	1.75	0.50
1:F:151:GLY:O	1:F:153:GLU:N	2.45	0.50
1:E:223:LYS:HE2	1:G:164:GLU:OE2	2.12	0.50
1:J:149:VAL:HA	1:J:152:MET:SD	2.52	0.50
1:K:88:ASN:HD21	1:K:135:PHE:HB2	1.77	0.50
1:L:224:LEU:HB3	1:L:230:ILE:HG13	1.94	0.50
1:M:116:ILE:HG12	1:M:147:ALA:HB1	1.94	0.50
1:F:181:TYR:C	1:F:181:TYR:CD1	2.85	0.50
1:F:169:LYS:HB3	1:G:173:GLN:HE21	1.77	0.50
1:C:81:ASN:O	1:C:82:VAL:C	2.49	0.49
1:G:190:ILE:O	1:G:194:LEU:HB2	2.12	0.49
1:H:186:ALA:HB3	1:H:220:ALA:HB2	1.93	0.49
1:K:114:VAL:O	1:K:126:LEU:N	2.45	0.49
1:K:115:PRO:HB3	1:K:122:ARG:CZ	2.41	0.49
1:K:197:ASN:HD21	1:K:244:VAL:HG22	1.77	0.49
1:L:64:LYS:HG2	1:L:67:GLU:OE1	2.12	0.49
1:E:183:GLU:O	1:E:187:ILE:HG13	2.12	0.49
1:I:55:GLN:HE22	1:I:130:ARG:HG2	1.77	0.49
1:J:35:ILE:CG2	1:J:39:ILE:HD11	2.40	0.49
1:M:178:SER:HB2	1:N:163:GLU:HB3	1.94	0.49
1:A:30:THR:HA	1:A:33:ASP:HB2	1.93	0.49
1:B:230:ILE:O	1:B:245:LEU:HD22	2.11	0.49
1:C:30:THR:O	1:C:30:THR:HG22	2.12	0.49
1:I:84:GLU:HA	1:I:115:PRO:HG3	1.95	0.49
1:I:187:ILE:HD13	1:I:190:ILE:HB	1.93	0.49
1:L:114:VAL:HB	1:L:126:LEU:HB3	1.94	0.49
1:E:44:ARG:NH1	1:H:210:VAL:O	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:204:SER:HA	1:F:207:ALA:HB3	1.94	0.49
1:J:29:GLU:HG2	1:J:52:SER:CB	2.42	0.49
1:B:218:VAL:O	1:B:222:ARG:NH1	2.46	0.49
1:F:5:GLN:HE21	1:F:5:GLN:N	2.10	0.49
1:J:229:VAL:HB	1:J:249:PHE:HE2	1.77	0.49
1:M:195:ASP:O	1:M:197:ASN:N	2.46	0.49
1:B:222:ARG:HB2	1:B:222:ARG:NH1	2.27	0.49
1:D:115:PRO:HB3	1:D:122:ARG:NH1	2.27	0.49
1:A:170:ALA:HB2	1:D:173:GLN:CB	2.39	0.49
1:B:37:SER:HA	1:B:130:ARG:HG3	1.94	0.49
1:C:51:TYR:HD1	1:C:51:TYR:C	2.16	0.49
1:D:174:MET:O	1:D:177:SER:OG	2.22	0.49
1:F:228:GLY:HA3	1:H:228:GLY:CA	2.37	0.49
1:L:68:ASP:O	1:L:70:GLN:N	2.44	0.49
1:M:113:ILE:HG23	1:M:125:THR:CG2	2.43	0.49
1:N:200:LEU:HB2	1:N:241:TYR:HA	1.95	0.49
1:B:72:PRO:HB2	1:B:75:TYR:CD1	2.48	0.49
1:C:98:PHE:O	1:C:103:ARG:HD2	2.12	0.49
1:D:60:ASP:O	1:D:64:LYS:HB2	2.13	0.49
1:H:231:GLU:HG3	1:H:231:GLU:O	2.13	0.49
1:H:246:ASN:O	1:H:247:ASN:C	2.51	0.49
1:M:114:VAL:HB	1:M:126:LEU:HB3	1.94	0.49
1:A:22:VAL:HG22	1:A:153:GLU:OE2	2.12	0.49
1:D:17:ALA:O	1:D:18:ALA:CB	2.60	0.49
1:J:178:SER:OG	1:L:167:ARG:HD2	2.12	0.49
1:I:173:GLN:HB3	1:L:166:ALA:HB1	1.95	0.49
1:L:61:ARG:HG2	1:L:105:LEU:HD12	1.94	0.49
1:A:42:VAL:HG13	1:A:48:LEU:HB2	1.94	0.49
1:F:216:VAL:HB	1:H:18:ALA:HB1	1.95	0.49
1:J:115:PRO:HA	1:J:126:LEU:N	2.28	0.49
1:L:17:ALA:O	1:L:20:LYS:NZ	2.39	0.49
1:A:27:MET:HA	1:A:27:MET:CE	2.42	0.48
1:A:6:LYS:HA	1:A:9:ILE:HD11	1.95	0.48
1:D:160:GLU:C	1:D:162:ILE:N	2.66	0.48
1:A:159:ALA:HB2	1:D:181:TYR:HB2	1.94	0.48
1:I:29:GLU:HG3	1:I:51:TYR:O	2.13	0.48
1:J:85:THR:HA	1:J:114:VAL:HG13	1.95	0.48
1:L:190:ILE:HD11	1:L:217:ILE:HG23	1.95	0.48
1:L:187:ILE:HD11	1:L:224:LEU:HD12	1.95	0.48
1:C:188:GLU:O	1:C:192:GLU:HB3	2.13	0.48
1:F:217:ILE:O	1:F:221:LEU:HD11	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:123:LEU:HD13	1:G:154:ILE:CG2	2.43	0.48
1:H:214:ARG:H	1:H:214:ARG:HG2	1.44	0.48
1:H:61:ARG:HB3	1:H:105:LEU:HA	1.96	0.48
1:C:31:LEU:HB2	1:C:39:ILE:HG21	1.94	0.48
1:J:115:PRO:HB3	1:J:122:ARG:HH21	1.78	0.48
1:J:63:LYS:CA	1:J:66:LEU:HB3	2.37	0.48
1:A:116:ILE:HG22	1:A:151:GLY:HA3	1.95	0.48
1:D:187:ILE:HA	1:D:190:ILE:HD12	1.96	0.48
1:F:231:GLU:HB2	1:F:233:ARG:CZ	2.43	0.48
1:H:217:ILE:O	1:H:221:LEU:CD2	2.59	0.48
1:L:224:LEU:HB3	1:L:230:ILE:HG12	1.95	0.48
1:A:181:TYR:CD1	1:A:181:TYR:C	2.87	0.48
1:A:96:THR:O	1:A:98:PHE:N	2.47	0.48
1:C:22:VAL:HG21	1:C:157:GLU:HA	1.95	0.48
1:G:247:ASN:H	1:G:247:ASN:HD22	1.62	0.48
1:H:176:ILE:HG13	1:H:179:LEU:HD12	1.94	0.48
1:I:157:GLU:C	1:I:159:ALA:N	2.66	0.48
1:L:136:ASN:O	1:L:139:ASP:HB2	2.14	0.48
1:B:17:ALA:O	1:B:20:LYS:NZ	2.44	0.48
1:C:141:ILE:HG23	1:C:142:LEU:HG	1.96	0.48
1:E:116:ILE:HA	1:E:147:ALA:O	2.14	0.48
1:G:24:PHE:CG	1:G:49:LEU:HB3	2.48	0.48
1:K:9:ILE:O	1:K:9:ILE:HG22	2.14	0.48
1:L:6:LYS:HA	1:L:9:ILE:HD12	1.96	0.48
1:N:141:ILE:HG12	1:N:144:GLU:OE1	2.13	0.48
1:C:122:ARG:HD2	1:C:124:GLY:H	1.77	0.48
1:C:184:LEU:CD2	1:C:185:GLU:HG2	2.44	0.48
1:D:154:ILE:HA	1:D:157:GLU:HB3	1.96	0.48
1:E:145:TYR:HA	1:F:145:TYR:HE2	1.78	0.48
1:F:217:ILE:O	1:F:221:LEU:HD13	2.14	0.48
1:F:219:ASN:HD21	1:F:223:LYS:CE	2.26	0.48
1:L:240:THR:HG1	1:L:241:TYR:H	1.59	0.48
1:M:24:PHE:HA	1:M:27:MET:HB2	1.95	0.48
1:A:202:VAL:HA	1:A:239:GLY:HA3	1.95	0.48
1:C:112:THR:O	1:C:128:LEU:HD12	2.14	0.48
1:C:88:ASN:OD1	1:C:135:PHE:HB2	2.13	0.48
1:E:31:LEU:HA	1:E:34:VAL:HG12	1.95	0.48
1:J:230:ILE:HG23	1:J:249:PHE:CE2	2.49	0.48
1:I:216:VAL:HG12	1:K:18:ALA:HA	1.95	0.48
1:L:202:VAL:HA	1:L:239:GLY:HA3	1.95	0.48
1:A:188:GLU:OE2	1:A:189:HIS:CD2	2.66	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:ARG:C	1:A:224:LEU:H	2.17	0.48
1:A:57:ILE:HG23	1:A:131:LEU:HD11	1.95	0.48
1:C:207:ALA:HA	1:C:217:ILE:HD11	1.94	0.48
1:C:249:PHE:O	1:C:252:GLU:HB2	2.14	0.48
1:E:114:VAL:HB	1:E:126:LEU:HB3	1.95	0.48
1:E:172:VAL:HG22	1:E:249:PHE:HD1	1.78	0.48
1:F:155:LEU:C	1:F:157:GLU:H	2.17	0.48
1:G:123:LEU:HD13	1:G:154:ILE:HG21	1.96	0.48
1:I:44:ARG:HB2	1:I:45:ARG:HD2	1.96	0.48
1:M:19:GLY:H	1:N:215:SER:HB3	1.78	0.48
1:M:40:PHE:HE1	1:M:66:LEU:HD21	1.79	0.48
1:N:28:ALA:O	1:N:39:ILE:HG13	2.13	0.48
1:A:138:ASP:C	1:A:140:LEU:N	2.66	0.48
1:A:42:VAL:HG22	1:A:48:LEU:HD13	1.95	0.48
1:B:88:ASN:N	1:B:88:ASN:OD1	2.47	0.48
1:D:22:VAL:HG21	1:D:157:GLU:HB2	1.96	0.48
1:F:10:ILE:HA	1:F:13:MET:HB2	1.96	0.48
1:H:38:ASN:HD21	1:H:53:ILE:HG13	1.79	0.48
1:J:219:ASN:O	1:J:223:LYS:HG2	2.14	0.48
1:C:103:ARG:HG3	1:C:106:PHE:CE1	2.49	0.47
1:C:124:GLY:O	1:C:125:THR:HG23	2.14	0.47
1:E:137:ASP:OD2	1:F:5:GLN:NE2	2.41	0.47
1:F:98:PHE:HB3	1:F:103:ARG:NH2	2.29	0.47
1:F:187:ILE:HD11	1:F:220:ALA:HB1	1.96	0.47
1:E:21:PRO:HG3	1:G:222:ARG:HH12	1.79	0.47
1:I:119:GLY:HA2	1:J:15:GLN:O	2.14	0.47
1:J:22:VAL:HG21	1:J:157:GLU:HB2	1.95	0.47
1:K:75:TYR:C	1:K:77:LYS:H	2.17	0.47
1:A:197:ASN:C	1:A:197:ASN:ND2	2.67	0.47
1:B:24:PHE:HZ	1:B:154:ILE:HG23	1.79	0.47
1:F:180:SER:O	1:F:181:TYR:C	2.53	0.47
1:F:185:GLU:O	1:F:189:HIS:CD2	2.66	0.47
1:F:206:ILE:HD12	1:F:206:ILE:H	1.79	0.47
1:F:219:ASN:HD21	1:F:223:LYS:NZ	2.12	0.47
1:J:24:PHE:HA	1:J:27:MET:HE2	1.95	0.47
1:N:16:ALA:C	1:N:18:ALA:H	2.18	0.47
1:C:251:ILE:O	1:C:255:ASN:N	2.20	0.47
1:D:106:PHE:CD2	1:D:111:THR:HB	2.50	0.47
1:D:90:ASP:N	1:D:90:ASP:OD1	2.47	0.47
1:E:162:ILE:C	1:E:164:GLU:N	2.68	0.47
1:F:17:ALA:O	1:F:20:LYS:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:181:TYR:CD2	1:G:158:LYS:HG3	2.47	0.47
1:I:141:ILE:HG12	1:J:4:LEU:HD12	1.96	0.47
1:C:88:ASN:HD21	1:C:135:PHE:H	1.61	0.47
1:D:33:ASP:C	1:D:36:ASP:H	2.17	0.47
1:E:216:VAL:CB	1:G:19:GLY:HA2	2.44	0.47
1:E:35:ILE:O	1:E:36:ASP:HB2	2.15	0.47
1:L:10:ILE:HA	1:L:13:MET:HG2	1.95	0.47
1:L:174:MET:O	1:L:177:SER:OG	2.19	0.47
1:A:22:VAL:HG13	1:A:153:GLU:CG	2.45	0.47
1:A:4:LEU:HA	1:B:141:ILE:CG1	2.44	0.47
1:B:35:ILE:C	1:B:37:SER:H	2.17	0.47
1:B:35:ILE:HD13	1:B:128:LEU:HD22	1.96	0.47
1:D:117:ILE:CG2	1:D:118:GLY:N	2.71	0.47
1:E:103:ARG:C	1:E:105:LEU:N	2.66	0.47
1:A:79:LEU:O	1:A:122:ARG:NH1	2.46	0.47
1:E:117:ILE:HG13	1:E:122:ARG:HA	1.96	0.47
1:E:167:ARG:HE	1:G:227:ALA:HA	1.79	0.47
1:E:16:ALA:HB3	1:F:119:GLY:H	1.80	0.47
1:I:85:THR:H	1:I:115:PRO:HD2	1.79	0.47
1:I:11:ASN:HA	1:I:14:LEU:HB3	1.95	0.47
1:L:212:ILE:HG22	1:L:213:THR:H	1.80	0.47
1:C:35:ILE:O	1:C:130:ARG:NH2	2.48	0.47
1:D:130:ARG:HH21	1:D:135:PHE:HE1	1.63	0.47
1:F:66:LEU:HA	1:F:69:ARG:HD3	1.96	0.47
1:K:45:ARG:HB2	1:K:47:LYS:NZ	2.29	0.47
1:L:30:THR:O	1:L:31:LEU:HB2	2.15	0.47
1:A:75:TYR:CE1	1:A:102:ASN:HB3	2.50	0.47
1:C:43:SER:HB3	1:C:47:LYS:HG3	1.97	0.47
1:E:123:LEU:HD13	1:E:154:ILE:HG22	1.97	0.47
1:F:40:PHE:HB2	1:F:127:ILE:HB	1.95	0.47
1:G:42:VAL:HG13	1:G:46:GLY:HA2	1.97	0.47
1:G:76:THR:HG22	1:G:76:THR:O	2.15	0.47
1:H:178:SER:HB3	1:H:223:LYS:HD3	1.96	0.47
1:L:151:GLY:HA2	1:L:154:ILE:HD13	1.96	0.47
1:E:114:VAL:CG1	1:E:147:ALA:CB	2.93	0.47
1:H:192:GLU:N	1:H:192:GLU:CD	2.69	0.47
1:I:229:VAL:HG12	1:I:230:ILE:HG23	1.96	0.47
1:L:23:ASN:HD21	1:L:25:LYS:HB3	1.79	0.47
1:M:204:SER:HB3	1:M:214:ARG:HB3	1.96	0.47
1:A:222:ARG:C	1:A:224:LEU:N	2.67	0.47
1:A:145:TYR:CE1	1:B:145:TYR:CA	2.84	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:112:THR:N	1:C:128:LEU:O	2.48	0.47
1:D:31:LEU:CB	1:D:39:ILE:HD11	2.44	0.47
1:H:218:VAL:O	1:H:222:ARG:N	2.47	0.47
1:I:170:ALA:O	1:I:171:VAL:HG22	2.14	0.47
1:J:71:PHE:HA	1:J:72:PRO:HD3	1.75	0.47
1:K:221:LEU:C	1:K:223:LYS:H	2.19	0.47
1:A:136:ASN:C	1:A:138:ASP:H	2.15	0.47
1:A:116:ILE:CG2	1:A:151:GLY:CA	2.93	0.47
1:A:180:SER:O	1:A:183:GLU:N	2.48	0.47
1:D:20:LYS:C	1:D:22:VAL:H	2.18	0.47
1:F:75:TYR:HH	1:F:104:ASP:CG	2.18	0.47
1:J:15:GLN:HG3	1:J:20:LYS:CE	2.45	0.47
1:J:3:LEU:HA	1:J:6:LYS:HB2	1.97	0.47
1:M:172:VAL:O	1:M:172:VAL:HG12	2.13	0.47
1:M:31:LEU:HB3	1:M:35:ILE:HD12	1.97	0.47
1:B:233:ARG:H	1:B:242:ILE:HG13	1.79	0.46
1:C:7:THR:C	1:C:9:ILE:N	2.68	0.46
1:G:214:ARG:O	1:G:218:VAL:HG23	2.15	0.46
1:J:233:ARG:HG3	1:J:235:LEU:HD23	1.96	0.46
1:K:107:GLN:H	1:K:107:GLN:HG3	1.50	0.46
1:K:143:ALA:O	1:K:147:ALA:HB2	2.15	0.46
1:L:98:PHE:CD2	1:L:99:PRO:HD2	2.51	0.46
1:C:234:SER:HB3	1:C:240:THR:CA	2.44	0.46
1:D:126:LEU:HD22	1:D:147:ALA:CB	2.45	0.46
1:G:116:ILE:HG22	1:G:147:ALA:O	2.15	0.46
1:H:3:LEU:HD11	1:H:142:LEU:HD11	1.97	0.46
1:H:48:LEU:HD11	1:H:50:GLY:O	2.15	0.46
1:I:91:ILE:HA	1:I:107:GLN:HA	1.97	0.46
1:I:96:THR:O	1:I:97:ALA:CB	2.64	0.46
1:C:51:TYR:CD1	1:C:51:TYR:C	2.88	0.46
1:F:57:ILE:HD12	1:F:57:ILE:O	2.16	0.46
1:G:180:SER:O	1:G:181:TYR:C	2.53	0.46
1:J:244:VAL:HG12	1:J:246:ASN:H	1.79	0.46
1:N:106:PHE:HD1	1:N:111:THR:HG23	1.79	0.46
1:A:8:ARG:HA	1:A:11:ASN:HB2	1.97	0.46
1:C:7:THR:HG21	1:D:141:ILE:HG22	1.97	0.46
1:E:173:GLN:CG	1:H:169:LYS:HB3	2.28	0.46
1:J:187:ILE:HD11	1:J:220:ALA:CB	2.30	0.46
1:K:89:LEU:HD11	1:K:113:ILE:HD13	1.97	0.46
1:K:42:VAL:HG11	1:K:79:LEU:CD1	2.46	0.46
1:A:247:ASN:HD22	1:A:248:LYS:H	1.62	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:40:PHE:CD2	1:D:127:ILE:HG22	2.50	0.46
1:G:171:VAL:O	1:G:175:ALA:N	2.39	0.46
1:J:86:SER:O	1:J:112:THR:HG23	2.16	0.46
1:N:181:TYR:O	1:N:185:GLU:HG2	2.15	0.46
1:A:103:ARG:HD2	1:A:106:PHE:HE2	1.81	0.46
1:B:29:GLU:O	1:B:32:ARG:HB3	2.16	0.46
1:B:32:ARG:HD3	1:B:52:SER:HB3	1.97	0.46
1:C:90:ASP:O	1:C:106:PHE:CB	2.64	0.46
1:C:213:THR:O	1:C:216:VAL:HG13	2.16	0.46
1:C:75:TYR:O	1:C:79:LEU:N	2.40	0.46
1:J:191:PHE:HE1	1:J:242:ILE:HG21	1.81	0.46
1:L:25:LYS:O	1:L:29:GLU:N	2.36	0.46
1:A:38:ASN:O	1:A:128:LEU:HA	2.16	0.46
1:B:173:GLN:O	1:B:176:ILE:HB	2.16	0.46
1:D:219:ASN:HA	1:D:222:ARG:HD3	1.98	0.46
1:F:3:LEU:CD2	1:F:141:ILE:HD13	2.45	0.46
1:G:140:LEU:HG	1:H:4:LEU:HD11	1.97	0.46
1:H:187:ILE:HD13	1:H:187:ILE:HA	1.70	0.46
1:I:38:ASN:HB2	1:I:129:SER:O	2.16	0.46
1:I:212:ILE:HG21	1:I:216:VAL:HG11	1.97	0.46
1:L:55:GLN:O	1:L:56:GLN:HB2	2.16	0.46
1:A:116:ILE:HG22	1:A:151:GLY:CA	2.46	0.46
1:A:227:ALA:HA	1:C:167:ARG:NH2	2.31	0.46
1:A:46:GLY:HA3	1:A:76:THR:OG1	2.16	0.46
1:D:31:LEU:HB2	1:D:39:ILE:CG1	2.46	0.46
1:D:55:GLN:CG	1:D:56:GLN:N	2.78	0.46
1:F:8:ARG:HA	1:F:11:ASN:HB2	1.97	0.46
1:E:216:VAL:HB	1:G:19:GLY:CA	2.46	0.46
1:J:212:ILE:HG23	1:J:217:ILE:HD11	1.97	0.46
1:L:206:ILE:HG13	1:L:210:VAL:HB	1.98	0.46
1:M:24:PHE:C	1:M:26:GLU:H	2.19	0.46
1:B:187:ILE:HA	1:B:190:ILE:CG1	2.44	0.46
1:C:145:TYR:CE2	1:D:145:TYR:CB	2.79	0.46
1:C:61:ARG:HG3	1:C:105:LEU:CD1	2.38	0.46
1:D:159:ALA:O	1:D:160:GLU:HG3	2.16	0.46
1:E:106:PHE:HB3	1:E:111:THR:HG22	1.97	0.46
1:E:144:GLU:C	1:E:146:GLY:H	2.18	0.46
1:E:170:ALA:O	1:E:174:MET:HB2	2.16	0.46
1:G:145:TYR:HA	1:H:145:TYR:OH	2.05	0.46
1:G:187:ILE:HG12	1:G:220:ALA:HB1	1.97	0.46
1:J:163:GLU:O	1:J:167:ARG:HB3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:83:PRO:HB2	1:J:84:GLU:H	1.64	0.46
1:L:184:LEU:C	1:L:186:ALA:H	2.18	0.46
1:D:163:GLU:O	1:D:167:ARG:HB2	2.16	0.46
1:J:110:LEU:HD23	1:J:135:PHE:HD2	1.81	0.46
1:J:113:ILE:HG23	1:J:125:THR:CG2	2.45	0.46
1:L:249:PHE:O	1:L:253:LEU:N	2.47	0.46
1:A:7:THR:HG21	1:B:141:ILE:HG23	1.98	0.45
1:B:171:VAL:O	1:B:174:MET:HG3	2.16	0.45
1:E:140:LEU:HD22	1:F:4:LEU:HD21	1.98	0.45
1:F:4:LEU:C	1:F:6:LYS:H	2.17	0.45
1:G:113:ILE:O	1:G:113:ILE:HG22	2.16	0.45
1:A:155:LEU:O	1:A:159:ALA:N	2.46	0.45
1:C:204:SER:OG	1:C:205:LYS:N	2.48	0.45
1:E:90:ASP:HA	1:E:106:PHE:O	2.17	0.45
1:F:146:GLY:C	1:F:148:THR:N	2.66	0.45
1:J:15:GLN:HG3	1:J:20:LYS:NZ	2.31	0.45
1:L:176:ILE:HG23	1:L:179:LEU:HD23	1.98	0.45
1:L:38:ASN:OD1	1:L:54:ASN:N	2.42	0.45
1:M:167:ARG:HH21	1:N:227:ALA:HB2	1.80	0.45
1:A:41:VAL:O	1:A:48:LEU:HD12	2.16	0.45
1:C:93:SER:OG	1:C:94:GLU:N	2.50	0.45
1:F:202:VAL:H	1:F:206:ILE:HD11	1.81	0.45
1:F:210:VAL:HB	1:F:212:ILE:CD1	2.42	0.45
1:G:201:LEU:HB3	1:G:240:THR:HG22	1.98	0.45
1:G:225:GLU:C	1:G:227:ALA:H	2.18	0.45
1:H:232:SER:O	1:H:233:ARG:C	2.55	0.45
1:L:23:ASN:ND2	1:L:25:LYS:HB3	2.32	0.45
1:N:247:ASN:ND2	1:N:247:ASN:H	2.13	0.45
1:A:115:PRO:HA	1:A:125:THR:HA	1.99	0.45
1:A:208:ASP:OD1	1:A:208:ASP:C	2.54	0.45
1:C:187:ILE:HD13	1:C:190:ILE:HD12	1.99	0.45
1:C:40:PHE:CE1	1:C:62:MET:HE1	2.51	0.45
1:G:75:TYR:C	1:G:77:LYS:H	2.19	0.45
1:L:17:ALA:O	1:L:18:ALA:HB3	2.17	0.45
1:L:88:ASN:HB3	1:L:110:LEU:HD22	1.99	0.45
1:A:150:VAL:C	1:A:152:MET:N	2.70	0.45
1:A:62:MET:O	1:A:65:MET:HB3	2.17	0.45
1:B:122:ARG:HH21	1:B:125:THR:HG23	1.81	0.45
1:A:145:TYR:CA	1:B:145:TYR:OH	2.65	0.45
1:D:90:ASP:HA	1:D:106:PHE:CB	2.39	0.45
1:J:176:ILE:HA	1:J:179:LEU:HD12	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:42:VAL:HG12	1:J:48:LEU:HB2	1.99	0.45
1:A:29:GLU:C	1:A:31:LEU:H	2.20	0.45
1:C:32:ARG:O	1:C:34:VAL:N	2.50	0.45
1:E:34:VAL:HG22	1:E:142:LEU:HD21	1.99	0.45
1:E:3:LEU:HA	1:E:6:LYS:HB2	1.98	0.45
1:G:111:THR:HA	1:G:128:LEU:O	2.17	0.45
1:F:215:SER:O	1:H:19:GLY:HA3	2.17	0.45
1:K:171:VAL:HA	1:K:174:MET:HB3	1.98	0.45
1:A:116:ILE:HD12	1:A:124:GLY:HA3	1.99	0.45
1:A:190:ILE:HG21	1:A:221:LEU:HD11	1.97	0.45
1:B:150:VAL:HG12	1:B:151:GLY:N	2.30	0.45
1:C:181:TYR:O	1:C:181:TYR:CD1	2.70	0.45
1:F:231:GLU:HB2	1:F:233:ARG:NH2	2.32	0.45
1:H:117:ILE:HG22	1:H:119:GLY:H	1.82	0.45
1:B:210:VAL:HG12	1:C:44:ARG:HH12	1.81	0.45
1:B:246:ASN:O	1:B:249:PHE:HB3	2.16	0.45
1:C:60:ASP:H	1:C:107:GLN:NE2	2.15	0.45
1:C:251:ILE:HG22	1:C:255:ASN:HB2	1.99	0.45
1:D:234:SER:HA	1:D:240:THR:HG21	1.99	0.45
1:D:90:ASP:C	1:D:92:ASN:H	2.20	0.45
1:E:10:ILE:HD13	1:E:145:TYR:O	2.16	0.45
1:E:4:LEU:HA	1:E:4:LEU:HD13	1.65	0.45
1:H:32:ARG:NH2	1:H:33:ASP:OD1	2.50	0.45
1:H:99:PRO:HB2	1:H:102:ASN:HB2	1.99	0.45
1:K:173:GLN:HA	1:K:176:ILE:HG22	1.99	0.45
1:L:89:LEU:HB2	1:L:111:THR:O	2.17	0.45
1:L:115:PRO:HA	1:L:125:THR:HG23	1.97	0.45
1:N:48:LEU:HB3	1:N:69:ARG:HD3	1.99	0.45
1:B:114:VAL:O	1:B:126:LEU:N	2.49	0.45
1:D:33:ASP:C	1:D:35:ILE:H	2.13	0.45
1:F:225:GLU:HG3	1:F:231:GLU:HA	1.99	0.45
1:F:66:LEU:C	1:F:68:ASP:H	2.20	0.45
1:E:155:LEU:CG	1:H:181:TYR:HB3	2.47	0.45
1:H:203:ALA:H	1:H:239:GLY:HA2	1.82	0.45
1:L:194:LEU:HD23	1:L:195:ASP:N	2.32	0.45
1:L:65:MET:SD	1:L:66:LEU:N	2.89	0.45
1:M:38:ASN:ND2	1:M:53:ILE:HG23	2.32	0.45
1:M:226:SER:OG	1:N:167:ARG:NH2	2.50	0.45
1:B:88:ASN:OD1	1:B:135:PHE:HB2	2.17	0.45
1:I:213:THR:HB	1:I:214:ARG:H	1.52	0.45
1:K:137:ASP:HA	1:K:140:LEU:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:172:VAL:HA	1:L:175:ALA:HB3	1.99	0.45
1:A:8:ARG:NE	1:B:144:GLU:OE2	2.51	0.44
1:B:98:PHE:HA	1:B:99:PRO:HD3	1.78	0.44
1:J:41:VAL:C	1:J:48:LEU:HD12	2.37	0.44
1:N:59:ASN:CG	1:N:62:MET:HB2	2.37	0.44
1:A:42:VAL:O	1:A:125:THR:HG23	2.17	0.44
1:A:57:ILE:HG12	1:A:131:LEU:HD13	1.99	0.44
1:A:31:LEU:HA	1:A:34:VAL:HG12	2.00	0.44
1:B:180:SER:OG	1:B:183:GLU:HG2	2.17	0.44
1:B:252:GLU:HA	1:B:255:ASN:HB2	1.98	0.44
1:C:90:ASP:O	1:C:106:PHE:HB2	2.17	0.44
1:D:91:ILE:O	1:D:103:ARG:NH2	2.51	0.44
1:D:118:GLY:C	1:D:120:GLY:N	2.68	0.44
1:J:115:PRO:HA	1:J:125:THR:CA	2.42	0.44
1:J:210:VAL:HB	1:J:212:ILE:HG22	1.98	0.44
1:J:216:VAL:HG12	1:L:19:GLY:N	2.32	0.44
1:J:35:ILE:O	1:J:36:ASP:CB	2.65	0.44
1:K:176:ILE:O	1:K:178:SER:N	2.49	0.44
1:J:119:GLY:O	1:K:182:SER:CB	2.65	0.44
1:K:234:SER:HB2	1:K:240:THR:CB	2.44	0.44
1:N:165:GLU:O	1:N:169:LYS:HE3	2.17	0.44
1:A:103:ARG:HD2	1:A:106:PHE:CE2	2.52	0.44
1:A:158:LYS:O	1:A:162:ILE:HG12	2.17	0.44
1:A:230:ILE:HD12	1:A:231:GLU:N	2.33	0.44
1:A:51:TYR:O	1:A:52:SER:CB	2.65	0.44
1:H:189:HIS:O	1:H:190:ILE:HG13	2.18	0.44
1:F:219:ASN:HB3	1:H:19:GLY:HA2	1.97	0.44
1:H:218:VAL:O	1:H:221:LEU:N	2.51	0.44
1:I:179:LEU:O	1:L:162:ILE:HD11	2.17	0.44
1:L:35:ILE:CD1	1:L:143:ALA:HB2	2.47	0.44
1:A:98:PHE:CD2	1:A:105:LEU:HD22	2.52	0.44
1:A:122:ARG:HH22	1:A:125:THR:HB	1.81	0.44
1:A:13:MET:HE1	1:A:27:MET:O	2.17	0.44
1:B:176:ILE:O	1:B:179:LEU:HB2	2.17	0.44
1:C:13:MET:HB3	1:C:14:LEU:H	1.67	0.44
1:D:20:LYS:HA	1:D:21:PRO:HD2	1.74	0.44
1:G:142:LEU:HA	1:G:145:TYR:HB3	1.99	0.44
1:H:173:GLN:O	1:H:176:ILE:HG22	2.18	0.44
1:H:46:GLY:O	1:H:70:GLN:HB2	2.16	0.44
1:J:115:PRO:HA	1:J:126:LEU:H	1.81	0.44
1:J:120:GLY:O	1:J:121:GLU:C	2.55	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:TYR:N	1:B:145:TYR:OH	2.50	0.44
1:A:179:LEU:HD13	1:A:184:LEU:HA	1.98	0.44
1:B:144:GLU:O	1:B:148:THR:OG1	2.33	0.44
1:C:172:VAL:HG22	1:C:229:VAL:HG22	1.99	0.44
1:C:99:PRO:O	1:C:102:ASN:HB2	2.18	0.44
1:C:9:ILE:O	1:C:11:ASN:N	2.51	0.44
1:D:157:GLU:HG3	1:D:158:LYS:N	2.31	0.44
1:E:3:LEU:O	1:E:6:LYS:HB2	2.17	0.44
1:J:130:ARG:HD2	1:J:133:ASP:CB	2.45	0.44
1:J:59:ASN:O	1:J:63:LYS:HB3	2.17	0.44
1:J:71:PHE:CG	1:J:79:LEU:HD11	2.53	0.44
1:L:131:LEU:HD12	1:L:132:GLN:HB2	1.98	0.44
1:C:106:PHE:N	1:C:106:PHE:CD1	2.84	0.44
1:C:233:ARG:O	1:C:241:TYR:N	2.44	0.44
1:C:41:VAL:HG12	1:C:116:ILE:HD11	1.99	0.44
1:C:48:LEU:HD11	1:C:51:TYR:HB3	2.00	0.44
1:D:31:LEU:CB	1:D:39:ILE:CD1	2.96	0.44
1:E:203:ALA:O	1:E:214:ARG:HG2	2.17	0.44
1:H:17:ALA:O	1:H:20:LYS:HB3	2.18	0.44
1:I:170:ALA:C	1:I:172:VAL:H	2.19	0.44
1:L:43:SER:OG	1:L:49:LEU:HD22	2.18	0.44
1:N:162:ILE:HG13	1:N:163:GLU:N	2.32	0.44
1:A:171:VAL:C	1:A:173:GLN:H	2.21	0.44
1:A:220:ALA:C	1:A:222:ARG:N	2.69	0.44
1:A:98:PHE:CE2	1:A:105:LEU:HD22	2.53	0.44
1:A:14:LEU:HD21	1:B:117:ILE:HG22	1.99	0.44
1:B:203:ALA:H	1:B:239:GLY:CA	2.17	0.44
1:B:53:ILE:HD12	1:B:53:ILE:O	2.18	0.44
1:D:206:ILE:HD12	1:D:206:ILE:H	1.83	0.44
1:F:167:ARG:HA	1:F:170:ALA:HB3	1.99	0.44
1:J:126:LEU:C	1:J:127:ILE:HG13	2.38	0.44
1:J:158:LYS:HA	1:J:161:GLU:HB3	2.00	0.44
1:K:43:SER:HB3	1:K:45:ARG:O	2.16	0.44
1:N:194:LEU:HG	1:N:199:GLY:HA3	2.00	0.44
1:A:159:ALA:HA	1:A:162:ILE:HG12	2.00	0.44
1:B:138:ASP:HA	1:B:141:ILE:CD1	2.48	0.44
1:G:185:GLU:HB3	1:G:189:HIS:CD2	2.53	0.44
1:J:32:ARG:HA	1:J:39:ILE:CG1	2.47	0.44
1:M:113:ILE:HG12	1:M:127:ILE:HG12	2.00	0.44
1:M:176:ILE:HA	1:M:179:LEU:HD12	2.00	0.44
1:A:126:LEU:HD12	1:A:127:ILE:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:ASN:CG	1:A:55:GLN:N	2.71	0.44
1:B:173:GLN:HA	1:B:176:ILE:HD12	2.00	0.44
1:C:116:ILE:HG13	1:C:116:ILE:H	1.69	0.44
1:C:224:LEU:O	1:C:226:SER:O	2.36	0.44
1:E:192:GLU:C	1:E:194:LEU:H	2.20	0.44
1:F:13:MET:HA	1:F:13:MET:CE	2.48	0.44
1:H:16:ALA:O	1:H:17:ALA:CB	2.65	0.44
1:H:184:LEU:O	1:H:188:GLU:N	2.46	0.44
1:H:230:ILE:CG2	1:H:244:VAL:HA	2.48	0.44
1:J:246:ASN:O	1:J:249:PHE:HB2	2.17	0.44
1:K:217:ILE:O	1:K:221:LEU:HD13	2.18	0.44
1:M:89:LEU:HB3	1:M:111:THR:HG23	2.00	0.44
1:N:32:ARG:HG2	1:N:37:SER:O	2.17	0.44
1:B:61:ARG:HB3	1:B:105:LEU:HA	2.00	0.43
1:B:47:LYS:HG2	1:B:69:ARG:O	2.18	0.43
1:C:10:ILE:CG2	1:C:31:LEU:HD21	2.48	0.43
1:E:92:ASN:O	1:E:93:SER:C	2.56	0.43
1:G:20:LYS:HA	1:G:21:PRO:HD2	1.76	0.43
1:A:123:LEU:HD22	1:A:154:ILE:HG21	1.99	0.43
1:B:103:ARG:NH1	1:B:103:ARG:CG	2.73	0.43
1:B:103:ARG:NH1	1:B:103:ARG:HG2	2.32	0.43
1:E:10:ILE:HD13	1:E:145:TYR:HB3	2.00	0.43
1:E:167:ARG:O	1:E:171:VAL:HG22	2.18	0.43
1:E:3:LEU:HA	1:E:6:LYS:HD2	1.99	0.43
1:E:169:LYS:CB	1:H:173:GLN:HG2	2.41	0.43
1:B:11:ASN:HD22	1:B:11:ASN:N	2.15	0.43
1:B:143:ALA:O	1:B:147:ALA:HB2	2.18	0.43
1:D:236:GLY:O	1:D:237:MET:HB2	2.17	0.43
1:F:32:ARG:C	1:F:34:VAL:N	2.72	0.43
1:G:214:ARG:HA	1:G:217:ILE:HD12	1.99	0.43
1:G:252:GLU:HA	1:G:255:ASN:CB	2.46	0.43
1:I:86:SER:O	1:I:112:THR:HA	2.19	0.43
1:I:19:GLY:CA	1:K:219:ASN:HB3	2.40	0.43
1:M:14:LEU:HD12	1:M:149:VAL:HG23	2.00	0.43
1:A:191:PHE:CE2	1:A:249:PHE:CE2	3.06	0.43
1:A:58:GLU:O	1:A:59:ASN:CB	2.66	0.43
1:B:233:ARG:H	1:B:242:ILE:HG12	1.82	0.43
1:C:103:ARG:HA	1:C:106:PHE:CE1	2.50	0.43
1:C:90:ASP:N	1:C:110:LEU:HD13	2.32	0.43
1:D:40:PHE:HD2	1:D:127:ILE:HG22	1.83	0.43
1:F:151:GLY:C	1:F:153:GLU:H	2.21	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:10:ILE:O	1:I:14:LEU:HB2	2.17	0.43
1:J:225:GLU:O	1:J:227:ALA:N	2.51	0.43
1:K:246:ASN:C	1:K:248:LYS:H	2.22	0.43
1:L:247:ASN:HB2	1:L:248:LYS:HD2	2.00	0.43
1:M:34:VAL:HG12	1:M:142:LEU:HD13	2.01	0.43
1:B:28:ALA:HB2	1:B:41:VAL:HG23	1.99	0.43
1:C:90:ASP:HA	1:C:109:GLY:O	2.18	0.43
1:C:111:THR:HA	1:C:129:SER:HA	1.99	0.43
1:D:115:PRO:C	1:D:116:ILE:HG13	2.39	0.43
1:D:143:ALA:O	1:D:147:ALA:HB3	2.19	0.43
1:E:140:LEU:HD23	1:F:8:ARG:HH21	1.83	0.43
1:E:35:ILE:HG12	1:E:142:LEU:HD13	2.00	0.43
1:E:207:ALA:HB3	1:E:214:ARG:HG3	2.00	0.43
1:G:167:ARG:O	1:G:170:ALA:HB3	2.18	0.43
1:G:83:PRO:HB2	1:G:84:GLU:H	1.62	0.43
1:I:116:ILE:HD11	1:I:126:LEU:HD13	1.99	0.43
1:J:148:THR:O	1:J:152:MET:N	2.46	0.43
1:L:159:ALA:O	1:L:160:GLU:HG3	2.18	0.43
1:M:247:ASN:N	1:M:247:ASN:HD22	2.06	0.43
1:N:157:GLU:OE2	1:N:158:LYS:HG2	2.18	0.43
1:N:201:LEU:HG	1:N:202:VAL:H	1.82	0.43
1:A:178:SER:HB2	1:C:164:GLU:OE2	2.18	0.43
1:D:106:PHE:HB3	1:D:111:THR:CB	2.49	0.43
1:D:114:VAL:HG21	1:D:143:ALA:HB1	2.00	0.43
1:D:17:ALA:H	1:D:20:LYS:HD2	1.83	0.43
1:H:98:PHE:HA	1:H:99:PRO:HD3	1.83	0.43
1:J:176:ILE:HA	1:J:179:LEU:HB2	1.99	0.43
1:K:131:LEU:H	1:K:131:LEU:HD12	1.84	0.43
1:M:198:GLU:HB3	1:M:199:GLY:H	1.70	0.43
1:E:74:GLU:HG3	1:E:77:LYS:HB3	2.00	0.43
1:E:4:LEU:HD12	1:E:8:ARG:HH22	1.84	0.43
1:F:81:ASN:C	1:F:83:PRO:HD3	2.38	0.43
1:I:185:GLU:HB3	1:I:189:HIS:CD2	2.53	0.43
1:L:60:ASP:H	1:L:107:GLN:NE2	2.16	0.43
1:L:90:ASP:C	1:L:92:ASN:N	2.71	0.43
1:M:55:GLN:O	1:M:57:ILE:HG13	2.18	0.43
1:B:164:GLU:O	1:B:168:SER:OG	2.19	0.43
1:C:173:GLN:C	1:C:175:ALA:H	2.22	0.43
1:C:214:ARG:C	1:C:216:VAL:H	2.21	0.43
1:C:7:THR:O	1:C:9:ILE:N	2.52	0.43
1:F:38:ASN:ND2	1:F:129:SER:O	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:109:GLY:O	1:G:111:THR:HG23	2.19	0.43
1:N:15:GLN:HB3	1:N:18:ALA:HA	2.01	0.43
1:D:113:ILE:N	1:D:113:ILE:HD12	2.33	0.43
1:D:190:ILE:CD1	1:D:221:LEU:CD1	2.96	0.43
1:F:24:PHE:CE1	1:F:41:VAL:HG21	2.53	0.43
1:H:82:VAL:O	1:H:122:ARG:NH1	2.52	0.43
1:M:230:ILE:HG22	1:M:244:VAL:HA	2.00	0.43
1:A:103:ARG:O	1:A:104:ASP:C	2.56	0.43
1:C:230:ILE:HG22	1:C:244:VAL:HG12	2.01	0.43
1:C:202:VAL:HA	1:C:239:GLY:CA	2.49	0.43
1:E:112:THR:O	1:E:128:LEU:HD12	2.19	0.43
1:E:145:TYR:HE2	1:F:145:TYR:C	2.21	0.43
1:E:114:VAL:HG12	1:E:147:ALA:CB	2.49	0.43
1:E:173:GLN:HE22	1:E:252:GLU:HB3	1.84	0.43
1:G:136:ASN:HD22	1:G:137:ASP:N	2.14	0.43
1:G:176:ILE:HD12	1:G:249:PHE:CE1	2.54	0.43
1:H:102:ASN:O	1:H:105:LEU:HB3	2.19	0.43
1:H:17:ALA:C	1:H:20:LYS:HB3	2.39	0.43
1:H:76:THR:O	1:H:78:ASN:N	2.51	0.43
1:H:98:PHE:CD2	1:H:103:ARG:HG3	2.54	0.43
1:J:136:ASN:HD22	1:J:137:ASP:H	1.66	0.43
1:J:214:ARG:O	1:J:218:VAL:HG23	2.19	0.43
1:I:19:GLY:CA	1:K:216:VAL:HA	2.48	0.43
1:K:53:ILE:HG23	1:K:55:GLN:O	2.19	0.43
1:L:65:MET:C	1:L:67:GLU:N	2.72	0.43
1:A:22:VAL:HG22	1:A:153:GLU:CD	2.39	0.42
1:B:187:ILE:HD12	1:B:224:LEU:HD11	2.01	0.42
1:C:20:LYS:HE3	1:C:20:LYS:HB2	1.67	0.42
1:C:82:VAL:HA	1:C:83:PRO:HD3	1.75	0.42
1:C:79:LEU:HA	1:C:98:PHE:CZ	2.54	0.42
1:F:247:ASN:HB2	1:F:248:LYS:HD2	2.01	0.42
1:H:24:PHE:HB2	1:H:49:LEU:HB3	2.01	0.42
1:L:28:ALA:O	1:L:31:LEU:HB3	2.18	0.42
1:N:200:LEU:HD13	1:N:241:TYR:HB2	2.00	0.42
1:A:222:ARG:O	1:A:225:GLU:N	2.51	0.42
1:A:55:GLN:H	1:A:55:GLN:HG3	1.76	0.42
1:B:25:LYS:O	1:B:29:GLU:N	2.52	0.42
1:C:204:SER:O	1:C:207:ALA:HB3	2.19	0.42
1:C:61:ARG:HA	1:C:64:LYS:HE2	2.00	0.42
1:E:141:ILE:HD13	1:F:141:ILE:HD11	2.02	0.42
1:E:141:ILE:O	1:E:145:TYR:N	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:202:VAL:CG2	1:G:206:ILE:HG12	2.48	0.42
1:H:16:ALA:O	1:H:17:ALA:HB3	2.19	0.42
1:L:91:ILE:CA	1:L:106:PHE:HD1	2.29	0.42
1:L:35:ILE:HD13	1:L:143:ALA:HB2	2.01	0.42
1:L:90:ASP:O	1:L:93:SER:N	2.52	0.42
1:L:79:LEU:HB2	1:L:98:PHE:HZ	1.83	0.42
1:B:105:LEU:HB2	1:B:106:PHE:CD2	2.54	0.42
1:C:155:LEU:C	1:C:157:GLU:H	2.23	0.42
1:C:29:GLU:HA	1:C:52:SER:HG	1.84	0.42
1:E:173:GLN:CD	1:H:169:LYS:HD3	2.39	0.42
1:F:154:ILE:H	1:F:154:ILE:HG13	1.56	0.42
1:G:111:THR:CG2	1:G:127:ILE:HG23	2.49	0.42
1:G:245:LEU:O	1:G:245:LEU:HD23	2.18	0.42
1:F:223:LYS:HD3	1:H:167:ARG:HH12	1.83	0.42
1:J:150:VAL:HG12	1:J:154:ILE:HD11	2.00	0.42
1:J:154:ILE:O	1:J:157:GLU:HB3	2.19	0.42
1:L:38:ASN:HB2	1:L:129:SER:H	1.84	0.42
1:C:19:GLY:O	1:C:20:LYS:O	2.37	0.42
1:C:234:SER:HB3	1:C:240:THR:CB	2.49	0.42
1:C:32:ARG:C	1:C:34:VAL:H	2.23	0.42
1:D:130:ARG:NH2	1:D:135:PHE:HE1	2.17	0.42
1:D:136:ASN:C	1:D:138:ASP:N	2.71	0.42
1:F:159:ALA:C	1:F:161:GLU:N	2.72	0.42
1:F:181:TYR:HD1	1:F:181:TYR:C	2.22	0.42
1:F:213:THR:C	1:F:215:SER:N	2.72	0.42
1:F:59:ASN:HB2	1:F:107:GLN:O	2.18	0.42
1:G:21:PRO:O	1:G:22:VAL:C	2.57	0.42
1:H:191:PHE:HD1	1:H:194:LEU:HD13	1.84	0.42
1:L:218:VAL:HG12	1:L:219:ASN:N	2.34	0.42
1:A:187:ILE:O	1:A:190:ILE:HG22	2.20	0.42
1:C:136:ASN:C	1:C:138:ASP:N	2.73	0.42
1:C:176:ILE:O	1:C:178:SER:N	2.53	0.42
1:D:114:VAL:O	1:D:126:LEU:N	2.47	0.42
1:D:90:ASP:C	1:D:92:ASN:N	2.72	0.42
1:F:159:ALA:C	1:F:161:GLU:H	2.21	0.42
1:F:157:GLU:C	1:F:159:ALA:H	2.22	0.42
1:H:98:PHE:CD2	1:H:99:PRO:HD2	2.54	0.42
1:I:39:ILE:HD13	1:I:128:LEU:HD21	2.02	0.42
1:J:173:GLN:HA	1:J:176:ILE:HD12	2.02	0.42
1:L:6:LYS:HB3	1:L:142:LEU:HD11	2.02	0.42
1:L:38:ASN:HB2	1:L:129:SER:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:61:ARG:HG2	1:L:105:LEU:CD1	2.49	0.42
1:N:76:THR:O	1:N:80:PHE:HB2	2.19	0.42
1:A:229:VAL:O	1:A:229:VAL:CG1	2.67	0.42
1:A:58:GLU:O	1:A:59:ASN:HB3	2.19	0.42
1:C:145:TYR:CZ	1:D:145:TYR:HB2	2.54	0.42
1:D:219:ASN:O	1:D:223:LYS:HG2	2.19	0.42
1:G:115:PRO:HB3	1:G:126:LEU:HB2	2.02	0.42
1:G:140:LEU:HA	1:G:143:ALA:HB3	2.01	0.42
1:G:154:ILE:HA	1:G:157:GLU:HG2	2.01	0.42
1:H:17:ALA:HA	1:H:20:LYS:HD3	2.00	0.42
1:J:38:ASN:O	1:J:128:LEU:HA	2.20	0.42
1:J:200:LEU:HG	1:J:201:LEU:N	2.34	0.42
1:K:187:ILE:H	1:K:187:ILE:HG12	1.62	0.42
1:L:65:MET:C	1:L:67:GLU:H	2.23	0.42
1:M:41:VAL:CG1	1:M:150:VAL:HG11	2.50	0.42
1:M:172:VAL:O	1:M:176:ILE:HD13	2.20	0.42
1:A:191:PHE:HE2	1:A:249:PHE:HE2	1.66	0.42
1:B:103:ARG:HG3	1:B:106:PHE:HE1	1.84	0.42
1:B:20:LYS:HB2	1:B:21:PRO:CD	2.47	0.42
1:C:89:LEU:N	1:C:110:LEU:HD12	2.35	0.42
1:F:155:LEU:C	1:F:157:GLU:N	2.73	0.42
1:I:115:PRO:HA	1:I:122:ARG:HD3	2.02	0.42
1:I:38:ASN:O	1:I:128:LEU:HA	2.20	0.42
1:A:220:ALA:O	1:A:222:ARG:N	2.52	0.42
1:A:250:LEU:N	1:A:250:LEU:CD2	2.75	0.42
1:A:250:LEU:O	1:A:254:GLU:HG2	2.20	0.42
1:A:2:ALA:O	1:A:5:GLN:HG3	2.19	0.42
1:A:4:LEU:HA	1:B:141:ILE:HD11	2.01	0.42
1:C:57:ILE:HB	1:C:108:ALA:HB1	2.01	0.42
1:E:117:ILE:HG22	1:F:14:LEU:HD12	2.01	0.42
1:F:86:SER:N	1:F:113:ILE:O	2.41	0.42
1:F:99:PRO:O	1:F:103:ARG:NH2	2.53	0.42
1:G:57:ILE:HG13	1:G:57:ILE:O	2.19	0.42
1:H:89:LEU:HB3	1:H:95:TYR:HE2	1.85	0.42
1:J:228:GLY:CA	1:L:228:GLY:HA3	2.49	0.42
1:A:150:VAL:O	1:A:152:MET:N	2.53	0.42
1:A:40:PHE:HD2	1:A:127:ILE:CG2	2.32	0.42
1:B:24:PHE:CD1	1:B:41:VAL:HG11	2.55	0.42
1:C:43:SER:OG	1:C:44:ARG:N	2.53	0.42
1:I:5:GLN:O	1:I:5:GLN:HG3	2.19	0.42
1:J:183:GLU:HB2	1:J:220:ALA:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:167:ARG:HG3	1:N:174:MET:HE1	2.01	0.42
1:D:17:ALA:H	1:D:20:LYS:CD	2.33	0.42
1:F:229:VAL:HG12	1:F:230:ILE:HG23	2.01	0.42
1:H:209:ARG:HG3	1:H:210:VAL:HG23	2.02	0.42
1:H:28:ALA:HB2	1:H:41:VAL:HG23	2.02	0.42
1:J:111:THR:HG23	1:J:129:SER:HB3	2.02	0.42
1:K:82:VAL:O	1:K:115:PRO:HG3	2.20	0.42
1:N:176:ILE:HA	1:N:179:LEU:HD12	2.00	0.42
1:A:218:VAL:O	1:A:222:ARG:HB2	2.20	0.41
1:B:25:LYS:O	1:B:29:GLU:HB2	2.20	0.41
1:D:25:LYS:HA	1:D:28:ALA:HB3	2.02	0.41
1:E:191:PHE:HD1	1:E:194:LEU:HD22	1.84	0.41
1:H:81:ASN:O	1:H:82:VAL:HB	2.20	0.41
1:I:40:PHE:HD2	1:I:48:LEU:HD12	1.84	0.41
1:J:131:LEU:HB3	1:J:132:GLN:H	1.60	0.41
1:N:135:PHE:CD2	1:N:140:LEU:HD13	2.55	0.41
1:B:16:ALA:O	1:B:17:ALA:HB3	2.20	0.41
1:C:224:LEU:HB3	1:C:230:ILE:CG1	2.40	0.41
1:C:53:ILE:O	1:C:53:ILE:HG23	2.19	0.41
1:D:122:ARG:HG3	1:D:122:ARG:O	2.21	0.41
1:H:230:ILE:HG22	1:H:244:VAL:HA	2.02	0.41
1:K:35:ILE:O	1:K:36:ASP:CB	2.68	0.41
1:L:133:ASP:CG	1:L:134:GLN:N	2.71	0.41
1:N:162:ILE:HG13	1:N:163:GLU:H	1.84	0.41
1:N:175:ALA:HB1	1:N:224:LEU:CD1	2.51	0.41
1:N:198:GLU:HG2	1:N:241:TYR:HE1	1.85	0.41
1:A:100:VAL:HA	1:A:103:ARG:NE	2.36	0.41
1:A:16:ALA:HB1	1:A:153:GLU:OE2	2.20	0.41
1:B:91:ILE:HD12	1:B:91:ILE:H	1.85	0.41
1:D:10:ILE:HA	1:D:13:MET:HG3	2.03	0.41
1:D:17:ALA:O	1:D:18:ALA:HB3	2.21	0.41
1:D:31:LEU:HB3	1:D:39:ILE:HD11	2.02	0.41
1:E:117:ILE:HG23	1:E:118:GLY:N	2.36	0.41
1:E:205:LYS:HA	1:E:205:LYS:HE3	2.02	0.41
1:G:88:ASN:ND2	1:G:110:LEU:HB3	2.36	0.41
1:I:199:GLY:O	1:I:242:ILE:HB	2.19	0.41
1:I:55:GLN:HB2	1:I:131:LEU:HD21	2.02	0.41
1:L:28:ALA:HA	1:L:39:ILE:HG21	2.02	0.41
1:L:49:LEU:HG	1:L:50:GLY:N	2.35	0.41
1:M:152:MET:O	1:M:152:MET:HG3	2.19	0.41
1:A:181:TYR:HD1	1:A:181:TYR:C	2.24	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:35:ILE:HG23	1:B:37:SER:HB3	2.01	0.41
1:C:172:VAL:HA	1:C:175:ALA:HB3	2.02	0.41
1:D:218:VAL:HG12	1:D:219:ASN:OD1	2.21	0.41
1:E:37:SER:HA	1:E:130:ARG:HG3	2.02	0.41
1:F:130:ARG:HG3	1:F:135:PHE:CZ	2.56	0.41
1:F:99:PRO:HD2	1:F:102:ASN:OD1	2.20	0.41
1:J:126:LEU:HD23	1:J:128:LEU:HD11	2.03	0.41
1:I:119:GLY:CA	1:J:15:GLN:O	2.68	0.41
1:K:115:PRO:O	1:K:116:ILE:HG13	2.21	0.41
1:M:172:VAL:O	1:M:172:VAL:CG1	2.69	0.41
1:M:219:ASN:HA	1:M:222:ARG:HG3	2.03	0.41
1:M:51:TYR:O	1:M:52:SER:CB	2.68	0.41
1:N:71:PHE:HB3	1:N:75:TYR:HB2	2.02	0.41
1:A:231:GLU:OE1	1:A:245:LEU:HD11	2.19	0.41
1:C:179:LEU:HD23	1:C:183:GLU:CB	2.48	0.41
1:E:13:MET:O	1:E:13:MET:HG2	2.19	0.41
1:F:15:GLN:HA	1:F:15:GLN:HE21	1.85	0.41
1:H:237:MET:HG3	1:H:239:GLY:O	2.20	0.41
1:I:115:PRO:CB	1:I:122:ARG:HD3	2.50	0.41
1:I:144:GLU:HG2	1:J:8:ARG:HH22	1.84	0.41
1:I:187:ILE:HD13	1:I:187:ILE:HA	1.87	0.41
1:J:200:LEU:HB2	1:N:238:LYS:NZ	2.35	0.41
1:K:20:LYS:HA	1:K:21:PRO:HD2	1.87	0.41
1:K:247:ASN:C	1:K:247:ASN:HD22	2.24	0.41
1:L:98:PHE:O	1:L:103:ARG:NH2	2.54	0.41
1:A:146:GLY:C	1:A:148:THR:H	2.24	0.41
1:B:105:LEU:HD13	1:B:106:PHE:CZ	2.54	0.41
1:B:11:ASN:O	1:B:14:LEU:O	2.39	0.41
1:C:126:LEU:CD2	1:C:147:ALA:HB2	2.48	0.41
1:C:186:ALA:O	1:C:190:ILE:CG1	2.62	0.41
1:E:161:GLU:CG	1:E:162:ILE:N	2.77	0.41
1:F:201:LEU:HD12	1:F:201:LEU:HA	1.94	0.41
1:F:86:SER:HB3	1:F:113:ILE:N	2.24	0.41
1:G:239:GLY:O	1:G:240:THR:CB	2.66	0.41
1:I:86:SER:HB3	1:I:113:ILE:HB	2.03	0.41
1:I:24:PHE:CD2	1:I:41:VAL:HG11	2.55	0.41
1:I:37:SER:OG	1:I:128:LEU:HD23	2.20	0.41
1:J:59:ASN:HB3	1:J:62:MET:HB2	2.02	0.41
1:K:149:VAL:O	1:K:153:GLU:HB2	2.21	0.41
1:M:170:ALA:HB3	1:N:174:MET:SD	2.61	0.41
1:N:91:ILE:HG23	1:N:107:GLN:HA	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:MET:O	1:A:176:ILE:N	2.54	0.41
1:A:202:VAL:C	1:A:204:SER:H	2.23	0.41
1:F:162:ILE:C	1:F:164:GLU:N	2.72	0.41
1:F:35:ILE:O	1:F:130:ARG:NH2	2.53	0.41
1:F:59:ASN:HD22	1:F:62:MET:HB2	1.85	0.41
1:H:157:GLU:HG3	1:H:158:LYS:HG2	2.03	0.41
1:H:197:ASN:ND2	1:H:198:GLU:OE2	2.52	0.41
1:H:220:ALA:HB3	1:H:221:LEU:HD22	2.02	0.41
1:I:182:SER:HB2	1:I:212:ILE:HG12	2.03	0.41
1:I:190:ILE:HG23	1:I:201:LEU:HD22	2.03	0.41
1:I:74:GLU:C	1:I:76:THR:H	2.24	0.41
1:K:43:SER:CB	1:K:49:LEU:HD11	2.44	0.41
1:A:126:LEU:C	1:A:127:ILE:HD12	2.41	0.41
1:A:2:ALA:O	1:A:3:LEU:C	2.59	0.41
1:C:59:ASN:ND2	1:C:105:LEU:O	2.54	0.41
1:A:173:GLN:HE21	1:D:169:LYS:HD2	1.86	0.41
1:E:105:LEU:HG	1:E:106:PHE:HD2	1.85	0.41
1:E:116:ILE:O	1:E:117:ILE:HD12	2.21	0.41
1:E:202:VAL:HA	1:E:239:GLY:HA3	2.03	0.41
1:E:250:LEU:HA	1:E:253:LEU:CB	2.51	0.41
1:G:32:ARG:HG2	1:G:54:ASN:OD1	2.21	0.41
1:K:187:ILE:HG22	1:K:191:PHE:CZ	2.56	0.41
1:K:29:GLU:HG2	1:K:52:SER:OG	2.21	0.41
1:K:3:LEU:O	1:K:7:THR:HG23	2.21	0.41
1:L:172:VAL:HG11	1:L:249:PHE:HD1	1.86	0.41
1:L:203:ALA:HB3	1:L:238:LYS:O	2.21	0.41
1:L:2:ALA:O	1:L:3:LEU:HD12	2.21	0.41
1:B:71:PHE:HD1	1:B:72:PRO:HD2	1.85	0.41
1:C:126:LEU:HD23	1:C:147:ALA:CB	2.50	0.41
1:F:4:LEU:HA	1:F:7:THR:HG23	2.01	0.41
1:I:157:GLU:O	1:I:159:ALA:N	2.54	0.41
1:I:47:LYS:HA	1:I:69:ARG:O	2.19	0.41
1:K:121:GLU:HG3	1:K:123:LEU:HD21	2.02	0.41
1:J:181:TYR:CE2	1:K:123:LEU:HD22	2.52	0.41
1:M:10:ILE:HG22	1:M:149:VAL:HG21	2.03	0.41
1:A:176:ILE:HA	1:A:176:ILE:HD12	1.93	0.41
1:A:16:ALA:HA	1:A:20:LYS:HG2	2.03	0.41
1:B:207:ALA:O	1:B:211:GLY:HA2	2.21	0.41
1:C:246:ASN:C	1:C:248:LYS:H	2.23	0.41
1:B:19:GLY:HA3	1:D:215:SER:HB3	2.03	0.41
1:F:141:ILE:HG23	1:F:142:LEU:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:115:PRO:HB2	1:G:116:ILE:H	1.65	0.41
1:G:179:LEU:HD22	1:G:183:GLU:HB3	2.03	0.41
1:L:80:PHE:O	1:L:122:ARG:NH1	2.53	0.41
1:L:184:LEU:C	1:L:186:ALA:N	2.74	0.41
1:M:71:PHE:HA	1:M:72:PRO:HD3	1.79	0.41
1:E:213:THR:HB	1:E:215:SER:OG	2.21	0.41
1:H:14:LEU:HB3	1:H:15:GLN:H	1.67	0.41
1:J:47:LYS:HG2	1:J:70:GLN:HG3	2.03	0.41
1:L:8:ARG:HA	1:L:11:ASN:HB2	2.03	0.41
1:A:95:TYR:HB3	1:A:97:ALA:H	1.85	0.40
1:C:164:GLU:O	1:C:168:SER:HB2	2.21	0.40
1:E:103:ARG:O	1:E:105:LEU:N	2.54	0.40
1:G:197:ASN:ND2	1:G:244:VAL:HG22	2.36	0.40
1:A:122:ARG:HH21	1:A:125:THR:HB	1.83	0.40
1:A:135:PHE:CD1	1:A:135:PHE:N	2.89	0.40
1:A:247:ASN:ND2	1:A:247:ASN:H	2.17	0.40
1:B:178:SER:HB3	1:B:223:LYS:NZ	2.37	0.40
1:C:229:VAL:HG12	1:C:230:ILE:HG23	2.04	0.40
1:G:82:VAL:HG21	1:G:113:ILE:HG21	2.03	0.40
1:I:112:THR:O	1:I:127:ILE:HA	2.22	0.40
1:I:44:ARG:HD2	1:L:181:TYR:OH	2.21	0.40
1:A:194:LEU:HD11	1:A:199:GLY:HA2	2.03	0.40
1:B:122:ARG:C	1:B:124:GLY:N	2.74	0.40
1:B:173:GLN:NE2	1:C:166:ALA:HA	2.20	0.40
1:E:34:VAL:HG13	1:E:142:LEU:CD2	2.48	0.40
1:F:157:GLU:O	1:F:159:ALA:N	2.55	0.40
1:H:194:LEU:HD21	1:H:197:ASN:C	2.41	0.40
1:I:187:ILE:CD1	1:I:190:ILE:HD12	2.48	0.40
1:I:217:ILE:HG22	1:I:221:LEU:HD13	2.02	0.40
1:J:78:ASN:O	1:J:82:VAL:HG23	2.22	0.40
1:A:184:LEU:CG	1:A:185:GLU:N	2.83	0.40
1:B:204:SER:O	1:B:207:ALA:HB3	2.22	0.40
1:B:59:ASN:HD21	1:B:106:PHE:HA	1.86	0.40
1:F:180:SER:O	1:F:182:SER:N	2.53	0.40
1:G:116:ILE:HG22	1:G:148:THR:HA	2.03	0.40
1:G:82:VAL:HA	1:G:83:PRO:HD3	1.96	0.40
1:I:115:PRO:HB3	1:I:122:ARG:HD3	2.04	0.40
1:J:113:ILE:O	1:J:113:ILE:HG22	2.21	0.40
1:K:118:GLY:C	1:K:120:GLY:N	2.74	0.40
1:K:145:TYR:CE2	1:L:145:TYR:HB2	2.52	0.40
1:L:32:ARG:HD2	1:L:54:ASN:HA	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:216:VAL:O	1:D:220:ALA:N	2.47	0.40
1:D:48:LEU:HD22	1:D:69:ARG:HD2	2.03	0.40
1:D:98:PHE:HA	1:D:99:PRO:HD3	1.79	0.40
1:E:78:ASN:HB2	1:E:98:PHE:CE2	2.57	0.40
1:E:93:SER:O	1:E:94:GLU:C	2.60	0.40
1:I:22:VAL:HG21	1:I:157:GLU:HG3	2.02	0.40
1:I:96:THR:O	1:I:97:ALA:HB2	2.22	0.40
1:K:82:VAL:O	1:K:115:PRO:CG	2.69	0.40
1:L:122:ARG:NE	1:L:125:THR:HG23	2.34	0.40
1:L:180:SER:O	1:L:183:GLU:N	2.54	0.40
1:M:31:LEU:HD21	1:M:149:VAL:HG11	2.04	0.40
1:M:84:GLU:HB2	1:M:85:THR:H	1.81	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	255/263 (97%)	174 (68%)	56 (22%)	25 (10%)	1	14
1	B	255/263 (97%)	177 (69%)	54 (21%)	24 (9%)	1	15
1	C	255/263 (97%)	169 (66%)	59 (23%)	27 (11%)	0	11
1	D	255/263 (97%)	171 (67%)	55 (22%)	29 (11%)	0	10
1	E	255/263 (97%)	183 (72%)	53 (21%)	19 (8%)	1	21
1	F	255/263 (97%)	169 (66%)	60 (24%)	26 (10%)	1	13
1	G	255/263 (97%)	187 (73%)	55 (22%)	13 (5%)	2	31
1	H	255/263 (97%)	178 (70%)	59 (23%)	18 (7%)	1	23
1	I	255/263 (97%)	160 (63%)	74 (29%)	21 (8%)	1	18
1	J	255/263 (97%)	179 (70%)	51 (20%)	25 (10%)	1	14

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	K	255/263 (97%)	177 (69%)	58 (23%)	20 (8%)	1 20
1	L	255/263 (97%)	169 (66%)	67 (26%)	19 (8%)	1 21
1	M	255/263 (97%)	196 (77%)	48 (19%)	11 (4%)	3 35
1	N	255/263 (97%)	198 (78%)	50 (20%)	7 (3%)	6 47
All	All	3570/3682 (97%)	2487 (70%)	799 (22%)	284 (8%)	1 19

All (284) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	LEU
1	A	14	LEU
1	A	52	SER
1	A	59	ASN
1	A	97	ALA
1	A	107	GLN
1	A	137	ASP
1	B	47	LYS
1	B	91	ILE
1	B	92	ASN
1	B	195	ASP
1	B	212	ILE
1	C	16	ALA
1	C	20	LYS
1	C	25	LYS
1	C	97	ALA
1	C	204	SER
1	C	238	LYS
1	D	17	ALA
1	D	18	ALA
1	D	34	VAL
1	D	55	GLN
1	D	73	GLU
1	D	83	PRO
1	D	183	GLU
1	D	184	LEU
1	E	56	GLN
1	E	65	MET
1	E	83	PRO
1	E	93	SER
1	E	218	VAL
1	F	17	ALA

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Mol	Chain	Res	Type
1	F	72	PRO
1	F	88	ASN
1	F	131	LEU
1	G	22	VAL
1	G	83	PRO
1	G	240	THR
1	H	14	LEU
1	H	17	ALA
1	H	21	PRO
1	H	73	GLU
1	H	83	PRO
1	H	181	TYR
1	H	233	ARG
1	I	187	ILE
1	I	237	MET
1	I	247	ASN
1	J	65	MET
1	J	83	PRO
1	J	96	THR
1	J	100	VAL
1	J	115	PRO
1	J	204	SER
1	J	230	ILE
1	J	237	MET
1	K	66	LEU
1	K	131	LEU
1	K	197	ASN
1	K	206	ILE
1	L	16	ALA
1	L	31	LEU
1	L	56	GLN
1	L	96	THR
1	L	104	ASP
1	M	52	SER
1	M	196	GLY
1	N	14	LEU
1	A	57	ILE
1	A	85	THR
1	A	91	ILE
1	A	196	GLY
1	A	204	SER
1	A	223	LYS

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Mol	Chain	Res	Type
1	B	48	LEU
1	B	85	THR
1	B	131	LEU
1	B	218	VAL
1	C	8	ARG
1	C	33	ASP
1	C	69	ARG
1	C	74	GLU
1	C	85	THR
1	C	90	ASP
1	C	100	VAL
1	C	107	GLN
1	C	119	GLY
1	C	139	ASP
1	C	156	ARG
1	C	177	SER
1	D	65	MET
1	D	117	ILE
1	D	137	ASP
1	D	144	GLU
1	E	17	ALA
1	E	59	ASN
1	E	94	GLU
1	E	100	VAL
1	E	104	ASP
1	E	256	LEU
1	F	43	SER
1	F	56	GLN
1	F	85	THR
1	F	96	THR
1	F	97	ALA
1	F	147	ALA
1	F	152	MET
1	F	194	LEU
1	F	203	ALA
1	G	100	VAL
1	H	82	VAL
1	H	212	ILE
1	H	247	ASN
1	I	8	ARG
1	I	22	VAL
1	I	85	THR

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Mol	Chain	Res	Type
1	I	92	ASN
1	I	97	ALA
1	I	119	GLY
1	I	132	GLN
1	I	158	LYS
1	I	171	VAL
1	I	188	GLU
1	J	52	SER
1	J	132	GLN
1	J	136	ASN
1	J	225	GLU
1	K	21	PRO
1	K	46	GLY
1	K	57	ILE
1	K	72	PRO
1	K	83	PRO
1	K	151	GLY
1	K	177	SER
1	K	194	LEU
1	K	227	ALA
1	L	72	PRO
1	L	73	GLU
1	L	87	SER
1	L	107	GLN
1	L	133	ASP
1	L	207	ALA
1	A	44	ARG
1	A	151	GLY
1	A	215	SER
1	A	221	LEU
1	A	234	SER
1	B	16	ALA
1	B	17	ALA
1	B	21	PRO
1	B	44	ARG
1	B	52	SER
1	B	58	GLU
1	B	123	LEU
1	B	145	TYR
1	B	196	GLY
1	C	172	VAL
1	C	211	GLY

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Mol	Chain	Res	Type
1	D	29	GLU
1	D	87	SER
1	D	97	ALA
1	D	148	THR
1	D	161	GLU
1	D	235	LEU
1	D	237	MET
1	D	240	THR
1	E	161	GLU
1	E	248	LYS
1	F	22	VAL
1	F	36	ASP
1	F	122	ARG
1	F	156	ARG
1	F	227	ALA
1	F	254	GLU
1	G	17	ALA
1	G	76	THR
1	G	118	GLY
1	G	131	LEU
1	G	203	ALA
1	H	72	PRO
1	H	77	LYS
1	I	28	ALA
1	I	93	SER
1	I	137	ASP
1	I	212	ILE
1	J	36	ASP
1	J	62	MET
1	J	94	GLU
1	J	95	TYR
1	J	121	GLU
1	K	36	ASP
1	L	17	ALA
1	L	18	ALA
1	L	29	GLU
1	M	44	ARG
1	M	72	PRO
1	M	131	LEU
1	M	207	ALA
1	A	22	VAL
1	A	65	MET

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Mol	Chain	Res	Type
1	A	99	PRO
1	A	175	ALA
1	A	257	LYS
1	B	88	ASN
1	B	172	VAL
1	B	211	GLY
1	C	94	GLU
1	C	137	ASP
1	C	171	VAL
1	C	181	TYR
1	D	20	LYS
1	D	21	PRO
1	D	44	ARG
1	D	46	GLY
1	D	75	TYR
1	D	143	ALA
1	E	16	ALA
1	E	72	PRO
1	E	84	GLU
1	F	44	ARG
1	F	181	TYR
1	F	214	ARG
1	G	115	PRO
1	H	18	ALA
1	H	200	LEU
1	I	57	ILE
1	I	227	ALA
1	J	16	ALA
1	J	72	PRO
1	J	131	LEU
1	K	85	THR
1	L	28	ALA
1	L	212	ILE
1	N	168	SER
1	N	207	ALA
1	N	247	ASN
1	A	30	THR
1	B	97	ALA
1	B	203	ALA
1	C	132	GLN
1	D	22	VAL
1	D	88	ASN

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Mol	Chain	Res	Type
1	E	22	VAL
1	F	225	GLU
1	F	230	ILE
1	G	20	LYS
1	G	95	TYR
1	H	93	SER
1	H	136	ASN
1	J	47	LYS
1	J	56	GLN
1	K	222	ARG
1	M	13	MET
1	M	26	GLU
1	M	255	ASN
1	N	21	PRO
1	N	88	ASN
1	A	132	GLN
1	C	82	VAL
1	E	19	GLY
1	F	257	LYS
1	H	190	ILE
1	J	34	VAL
1	J	254	GLU
1	K	22	VAL
1	K	73	GLU
1	L	34	VAL
1	L	185	GLU
1	N	83	PRO
1	B	146	GLY
1	G	21	PRO
1	J	162	ILE
1	K	20	LYS
1	L	115	PRO
1	C	10	ILE
1	K	228	GLY
1	D	119	GLY
1	H	230	ILE
1	I	46	GLY
1	E	217	ILE
1	F	242	ILE
1	I	251	ILE
1	M	21	PRO
1	M	119	GLY

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	222/229 (97%)	182 (82%)	40 (18%)	2 16
1	B	222/229 (97%)	176 (79%)	46 (21%)	1 11
1	C	222/229 (97%)	180 (81%)	42 (19%)	2 14
1	D	222/229 (97%)	179 (81%)	43 (19%)	2 14
1	E	222/229 (97%)	169 (76%)	53 (24%)	1 7
1	F	222/229 (97%)	173 (78%)	49 (22%)	1 10
1	G	222/229 (97%)	189 (85%)	33 (15%)	4 25
1	H	222/229 (97%)	182 (82%)	40 (18%)	2 16
1	I	222/229 (97%)	180 (81%)	42 (19%)	2 14
1	J	222/229 (97%)	190 (86%)	32 (14%)	4 27
1	K	222/229 (97%)	178 (80%)	44 (20%)	1 13
1	L	222/229 (97%)	181 (82%)	41 (18%)	2 15
1	M	222/229 (97%)	195 (88%)	27 (12%)	6 32
1	N	222/229 (97%)	189 (85%)	33 (15%)	4 25
All	All	3108/3206 (97%)	2543 (82%)	565 (18%)	2 16

All (565) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	7	THR
1	A	9	ILE
1	A	14	LEU
1	A	24	PHE
1	A	32	ARG
1	A	34	VAL
1	A	43	SER
1	A	55	GLN
1	A	57	ILE
1	A	91	ILE

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Mol	Chain	Res	Type
1	A	123	LEU
1	A	125	THR
1	A	126	LEU
1	A	133	ASP
1	A	135	PHE
1	A	136	ASN
1	A	138	ASP
1	A	139	ASP
1	A	161	GLU
1	A	176	ILE
1	A	181	TYR
1	A	182	SER
1	A	183	GLU
1	A	184	LEU
1	A	185	GLU
1	A	197	ASN
1	A	200	LEU
1	A	208	ASP
1	A	210	VAL
1	A	213	THR
1	A	214	ARG
1	A	216	VAL
1	A	241	TYR
1	A	243	LYS
1	A	247	ASN
1	A	248	LYS
1	A	250	LEU
1	A	251	ILE
1	A	257	LYS
1	B	3	LEU
1	B	5	GLN
1	B	11	ASN
1	B	15	GLN
1	B	37	SER
1	B	42	VAL
1	B	43	SER
1	B	44	ARG
1	B	55	GLN
1	B	67	GLU
1	B	70	GLN
1	B	76	THR
1	B	86	SER

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Mol	Chain	Res	Type
1	B	88	ASN
1	B	91	ILE
1	B	98	PHE
1	B	101	GLU
1	B	103	ARG
1	B	105	LEU
1	B	106	PHE
1	B	112	THR
1	B	125	THR
1	B	127	ILE
1	B	128	LEU
1	B	132	GLN
1	B	133	ASP
1	B	152	MET
1	B	155	LEU
1	B	157	GLU
1	B	163	GLU
1	B	169	LYS
1	B	171	VAL
1	B	184	LEU
1	B	204	SER
1	B	205	LYS
1	B	209	ARG
1	B	222	ARG
1	B	223	LYS
1	B	233	ARG
1	B	235	LEU
1	B	241	TYR
1	B	251	ILE
1	B	252	GLU
1	B	253	LEU
1	B	254	GLU
1	B	256	LEU
1	C	10	ILE
1	C	20	LYS
1	C	24	PHE
1	C	41	VAL
1	C	49	LEU
1	C	51	TYR
1	C	54	ASN
1	C	65	MET
1	C	80	PHE

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Mol	Chain	Res	Type
1	C	89	LEU
1	C	91	ILE
1	C	92	ASN
1	C	96	THR
1	C	103	ARG
1	C	106	PHE
1	C	110	LEU
1	C	116	ILE
1	C	125	THR
1	C	128	LEU
1	C	134	GLN
1	C	136	ASN
1	C	140	LEU
1	C	144	GLU
1	C	145	TYR
1	C	153	GLU
1	C	161	GLU
1	C	167	ARG
1	C	180	SER
1	C	184	LEU
1	C	192	GLU
1	C	202	VAL
1	C	205	LYS
1	C	210	VAL
1	C	222	ARG
1	C	226	SER
1	C	235	LEU
1	C	237	MET
1	C	243	LYS
1	C	247	ASN
1	C	248	LYS
1	C	250	LEU
1	C	256	LEU
1	D	3	LEU
1	D	4	LEU
1	D	14	LEU
1	D	35	ILE
1	D	42	VAL
1	D	49	LEU
1	D	51	TYR
1	D	52	SER
1	D	53	ILE

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Mol	Chain	Res	Type
1	D	55	GLN
1	D	67	GLU
1	D	86	SER
1	D	90	ASP
1	D	96	THR
1	D	98	PHE
1	D	105	LEU
1	D	106	PHE
1	D	117	ILE
1	D	125	THR
1	D	131	LEU
1	D	153	GLU
1	D	155	LEU
1	D	158	LYS
1	D	162	ILE
1	D	184	LEU
1	D	187	ILE
1	D	194	LEU
1	D	206	ILE
1	D	209	ARG
1	D	212	ILE
1	D	213	THR
1	D	226	SER
1	D	231	GLU
1	D	235	LEU
1	D	238	LYS
1	D	241	TYR
1	D	246	ASN
1	D	248	LYS
1	D	249	PHE
1	D	253	LEU
1	D	254	GLU
1	D	255	ASN
1	D	256	LEU
1	E	4	LEU
1	E	8	ARG
1	E	13	MET
1	E	14	LEU
1	E	15	GLN
1	E	25	LYS
1	E	26	GLU
1	E	32	ARG

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Mol	Chain	Res	Type
1	E	33	ASP
1	E	42	VAL
1	E	44	ARG
1	E	45	ARG
1	E	53	ILE
1	E	61	ARG
1	E	62	MET
1	E	63	LYS
1	E	68	ASP
1	E	80	PHE
1	E	81	ASN
1	E	94	GLU
1	E	95	TYR
1	E	101	GLU
1	E	104	ASP
1	E	107	GLN
1	E	110	LEU
1	E	113	ILE
1	E	117	ILE
1	E	122	ARG
1	E	128	LEU
1	E	136	ASN
1	E	137	ASP
1	E	138	ASP
1	E	139	ASP
1	E	153	GLU
1	E	154	ILE
1	E	155	LEU
1	E	157	GLU
1	E	167	ARG
1	E	173	GLN
1	E	177	SER
1	E	197	ASN
1	E	198	GLU
1	E	205	LYS
1	E	212	ILE
1	E	214	ARG
1	E	230	ILE
1	E	231	GLU
1	E	233	ARG
1	E	235	LEU
1	E	238	LYS

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Mol	Chain	Res	Type
1	E	248	LYS
1	E	253	LEU
1	E	256	LEU
1	F	4	LEU
1	F	5	GLN
1	F	8	ARG
1	F	11	ASN
1	F	13	MET
1	F	14	LEU
1	F	15	GLN
1	F	30	THR
1	F	33	ASP
1	F	41	VAL
1	F	44	ARG
1	F	45	ARG
1	F	55	GLN
1	F	61	ARG
1	F	64	LYS
1	F	65	MET
1	F	73	GLU
1	F	87	SER
1	F	103	ARG
1	F	110	LEU
1	F	114	VAL
1	F	126	LEU
1	F	128	LEU
1	F	133	ASP
1	F	148	THR
1	F	154	ILE
1	F	173	GLN
1	F	181	TYR
1	F	187	ILE
1	F	193	GLU
1	F	194	LEU
1	F	197	ASN
1	F	198	GLU
1	F	205	LYS
1	F	206	ILE
1	F	208	ASP
1	F	210	VAL
1	F	212	ILE
1	F	213	THR

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Mol	Chain	Res	Type
1	F	215	SER
1	F	216	VAL
1	F	221	LEU
1	F	231	GLU
1	F	242	ILE
1	F	247	ASN
1	F	250	LEU
1	F	252	GLU
1	F	255	ASN
1	F	256	LEU
1	G	3	LEU
1	G	25	LYS
1	G	31	LEU
1	G	40	PHE
1	G	54	ASN
1	G	59	ASN
1	G	80	PHE
1	G	81	ASN
1	G	89	LEU
1	G	92	ASN
1	G	98	PHE
1	G	102	ASN
1	G	103	ARG
1	G	117	ILE
1	G	132	GLN
1	G	136	ASN
1	G	150	VAL
1	G	157	GLU
1	G	161	GLU
1	G	165	GLU
1	G	182	SER
1	G	197	ASN
1	G	200	LEU
1	G	202	VAL
1	G	209	ARG
1	G	214	ARG
1	G	221	LEU
1	G	224	LEU
1	G	237	MET
1	G	242	ILE
1	G	245	LEU
1	G	247	ASN

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Mol	Chain	Res	Type
1	G	254	GLU
1	H	3	LEU
1	H	10	ILE
1	H	11	ASN
1	H	14	LEU
1	H	22	VAL
1	H	24	PHE
1	H	33	ASP
1	H	36	ASP
1	H	47	LYS
1	H	52	SER
1	H	61	ARG
1	H	68	ASP
1	H	75	TYR
1	H	76	THR
1	H	89	LEU
1	H	91	ILE
1	H	98	PHE
1	H	100	VAL
1	H	102	ASN
1	H	128	LEU
1	H	163	GLU
1	H	167	ARG
1	H	174	MET
1	H	176	ILE
1	H	184	LEU
1	H	187	ILE
1	H	193	GLU
1	H	204	SER
1	H	214	ARG
1	H	217	ILE
1	H	224	LEU
1	H	226	SER
1	H	230	ILE
1	H	235	LEU
1	H	241	TYR
1	H	242	ILE
1	H	247	ASN
1	H	250	LEU
1	H	254	GLU
1	H	256	LEU
1	I	8	ARG

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Mol	Chain	Res	Type
1	I	13	MET
1	I	20	LYS
1	I	25	LYS
1	I	27	MET
1	I	45	ARG
1	I	52	SER
1	I	54	ASN
1	I	56	GLN
1	I	58	GLU
1	I	60	ASP
1	I	61	ARG
1	I	77	LYS
1	I	90	ASP
1	I	91	ILE
1	I	103	ARG
1	I	111	THR
1	I	125	THR
1	I	130	ARG
1	I	131	LEU
1	I	136	ASN
1	I	137	ASP
1	I	140	LEU
1	I	165	GLU
1	I	167	ARG
1	I	172	VAL
1	I	183	GLU
1	I	184	LEU
1	I	187	ILE
1	I	192	GLU
1	I	197	ASN
1	I	201	LEU
1	I	202	VAL
1	I	212	ILE
1	I	217	ILE
1	I	231	GLU
1	I	234	SER
1	I	246	ASN
1	I	248	LYS
1	I	250	LEU
1	I	251	ILE
1	I	257	LYS
1	J	8	ARG

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Mol	Chain	Res	Type
1	J	9	ILE
1	J	26	GLU
1	J	30	THR
1	J	32	ARG
1	J	48	LEU
1	J	49	LEU
1	J	64	LYS
1	J	68	ASP
1	J	74	GLU
1	J	80	PHE
1	J	89	LEU
1	J	114	VAL
1	J	116	ILE
1	J	122	ARG
1	J	128	LEU
1	J	131	LEU
1	J	132	GLN
1	J	136	ASN
1	J	153	GLU
1	J	164	GLU
1	J	167	ARG
1	J	173	GLN
1	J	184	LEU
1	J	185	GLU
1	J	212	ILE
1	J	214	ARG
1	J	233	ARG
1	J	235	LEU
1	J	248	LYS
1	J	250	LEU
1	J	252	GLU
1	K	4	LEU
1	K	13	MET
1	K	14	LEU
1	K	25	LYS
1	K	31	LEU
1	K	32	ARG
1	K	56	GLN
1	K	63	LYS
1	K	66	LEU
1	K	78	ASN
1	K	81	ASN

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Mol	Chain	Res	Type
1	K	82	VAL
1	K	88	ASN
1	K	90	ASP
1	K	92	ASN
1	K	98	PHE
1	K	103	ARG
1	K	105	LEU
1	K	107	GLN
1	K	112	THR
1	K	114	VAL
1	K	122	ARG
1	K	125	THR
1	K	130	ARG
1	K	131	LEU
1	K	136	ASN
1	K	140	LEU
1	K	148	THR
1	K	149	VAL
1	K	162	ILE
1	K	164	GLU
1	K	168	SER
1	K	176	ILE
1	K	187	ILE
1	K	195	ASP
1	K	197	ASN
1	K	201	LEU
1	K	213	THR
1	K	237	MET
1	K	242	ILE
1	K	245	LEU
1	K	247	ASN
1	K	248	LYS
1	K	251	ILE
1	L	14	LEU
1	L	15	GLN
1	L	24	PHE
1	L	30	THR
1	L	31	LEU
1	L	36	ASP
1	L	41	VAL
1	L	44	ARG
1	L	45	ARG

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Mol	Chain	Res	Type
1	L	49	LEU
1	L	51	TYR
1	L	61	ARG
1	L	69	ARG
1	L	73	GLU
1	L	74	GLU
1	L	81	ASN
1	L	86	SER
1	L	95	TYR
1	L	96	THR
1	L	98	PHE
1	L	102	ASN
1	L	106	PHE
1	L	107	GLN
1	L	125	THR
1	L	140	LEU
1	L	162	ILE
1	L	179	LEU
1	L	181	TYR
1	L	183	GLU
1	L	194	LEU
1	L	200	LEU
1	L	202	VAL
1	L	212	ILE
1	L	214	ARG
1	L	216	VAL
1	L	231	GLU
1	L	235	LEU
1	L	242	ILE
1	L	248	LYS
1	L	254	GLU
1	L	255	ASN
1	M	5	GLN
1	M	13	MET
1	M	15	GLN
1	M	30	THR
1	M	32	ARG
1	M	54	ASN
1	M	55	GLN
1	M	57	ILE
1	M	68	ASP
1	M	85	THR

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Mol	Chain	Res	Type
1	M	90	ASP
1	M	95	TYR
1	M	103	ARG
1	M	104	ASP
1	M	126	LEU
1	M	157	GLU
1	M	181	TYR
1	M	184	LEU
1	M	193	GLU
1	M	202	VAL
1	M	208	ASP
1	M	214	ARG
1	M	224	LEU
1	M	233	ARG
1	M	247	ASN
1	M	251	ILE
1	M	257	LYS
1	N	5	GLN
1	N	15	GLN
1	N	30	THR
1	N	32	ARG
1	N	36	ASP
1	N	56	GLN
1	N	59	ASN
1	N	60	ASP
1	N	69	ARG
1	N	103	ARG
1	N	110	LEU
1	N	111	THR
1	N	113	ILE
1	N	132	GLN
1	N	139	ASP
1	N	148	THR
1	N	155	LEU
1	N	167	ARG
1	N	174	MET
1	N	176	ILE
1	N	195	ASP
1	N	198	GLU
1	N	200	LEU
1	N	208	ASP
1	N	224	LEU

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Mol	Chain	Res	Type
1	N	225	GLU
1	N	237	MET
1	N	241	TYR
1	N	242	ILE
1	N	247	ASN
1	N	250	LEU
1	N	251	ILE
1	N	257	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (91) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	ASN
1	A	59	ASN
1	A	81	ASN
1	A	88	ASN
1	A	102	ASN
1	A	107	GLN
1	A	189	HIS
1	A	197	ASN
1	A	247	ASN
1	B	11	ASN
1	B	15	GLN
1	B	136	ASN
1	B	173	GLN
1	C	38	ASN
1	C	54	ASN
1	C	55	GLN
1	C	70	GLN
1	C	78	ASN
1	C	92	ASN
1	C	102	ASN
1	C	107	GLN
1	C	136	ASN
1	C	197	ASN
1	C	247	ASN
1	C	255	ASN
1	D	15	GLN
1	D	23	ASN
1	D	38	ASN
1	D	78	ASN
1	D	189	HIS

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Mol	Chain	Res	Type
1	D	246	ASN
1	E	5	GLN
1	E	136	ASN
1	E	173	GLN
1	E	189	HIS
1	E	197	ASN
1	F	5	GLN
1	F	11	ASN
1	F	15	GLN
1	F	55	GLN
1	F	189	HIS
1	F	197	ASN
1	F	219	ASN
1	F	246	ASN
1	F	255	ASN
1	G	55	GLN
1	G	88	ASN
1	G	134	GLN
1	G	136	ASN
1	G	197	ASN
1	G	247	ASN
1	H	5	GLN
1	H	38	ASN
1	H	81	ASN
1	H	255	ASN
1	I	15	GLN
1	I	38	ASN
1	I	88	ASN
1	I	107	GLN
1	I	132	GLN
1	I	189	HIS
1	I	197	ASN
1	I	219	ASN
1	I	247	ASN
1	J	70	GLN
1	J	136	ASN
1	K	15	GLN
1	K	78	ASN
1	K	81	ASN
1	K	88	ASN
1	K	102	ASN
1	K	197	ASN

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Mol	Chain	Res	Type
1	K	247	ASN
1	L	11	ASN
1	L	15	GLN
1	L	23	ASN
1	L	55	GLN
1	L	107	GLN
1	L	132	GLN
1	L	197	ASN
1	M	54	ASN
1	M	88	ASN
1	M	102	ASN
1	M	132	GLN
1	M	134	GLN
1	N	55	GLN
1	N	78	ASN
1	N	102	ASN
1	N	132	GLN
1	N	189	HIS
1	N	197	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 carbohydrates 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	257/263 (97%)	-0.69	1 (0%) 93 90	91, 179, 227, 244	4 (1%)
1	B	257/263 (97%)	-0.51	1 (0%) 93 90	122, 204, 276, 293	4 (1%)
1	C	257/263 (97%)	-0.66	1 (0%) 93 90	106, 187, 236, 260	4 (1%)
1	D	257/263 (97%)	-0.67	1 (0%) 93 90	113, 186, 257, 273	4 (1%)
1	E	257/263 (97%)	-0.66	2 (0%) 87 82	130, 206, 259, 274	4 (1%)
1	F	257/263 (97%)	-0.57	0 100 100	141, 213, 271, 282	4 (1%)
1	G	257/263 (97%)	-0.36	3 (1%) 81 73	146, 251, 331, 356	4 (1%)
1	H	257/263 (97%)	-0.57	2 (0%) 87 82	140, 235, 281, 293	4 (1%)
1	I	257/263 (97%)	-0.47	2 (0%) 87 82	127, 228, 287, 311	4 (1%)
1	J	257/263 (97%)	-0.59	3 (1%) 81 73	141, 216, 287, 304	4 (1%)
1	K	257/263 (97%)	-0.59	1 (0%) 93 90	159, 227, 273, 313	4 (1%)
1	L	257/263 (97%)	-0.59	0 100 100	146, 211, 251, 269	4 (1%)
1	M	257/263 (97%)	0.33	28 (10%) 7 7	262, 391, 465, 485	4 (1%)
1	N	257/263 (97%)	0.00	16 (6%) 24 17	202, 354, 407, 416	4 (1%)
All	All	3598/3682 (97%)	-0.47	61 (1%) 73 64	91, 220, 391, 485	56 (1%)

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	85	THR	5.7
1	M	137	ASP	4.6
1	M	8	ARG	4.6
1	M	5	GLN	4.3
1	M	21	PRO	4.1
1	M	20	LYS	4.1
1	M	6	LYS	4.0
1	I	54	ASN	3.6

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Mol	Chain	Res	Type	RSRZ
1	G	136	ASN	3.5
1	H	92	ASN	3.4
1	N	119	GLY	3.4
1	M	50	GLY	3.3
1	M	38	ASN	3.3
1	M	99	PRO	3.2
1	J	72	PRO	3.2
1	M	136	ASN	3.2
1	N	118	GLY	3.1
1	M	12	SER	3.0
1	M	48	LEU	3.0
1	M	7	THR	3.0
1	N	5	GLN	2.9
1	M	108	ALA	2.9
1	N	83	PRO	2.9
1	G	137	ASP	2.9
1	N	195	ASP	2.8
1	N	61	ARG	2.8
1	N	201	LEU	2.8
1	N	54	ASN	2.7
1	J	100	VAL	2.7
1	H	132	GLN	2.6
1	M	133	ASP	2.6
1	M	148	THR	2.6
1	M	70	GLN	2.6
1	N	58	GLU	2.5
1	G	69	ARG	2.5
1	M	138	ASP	2.5
1	M	86	SER	2.5
1	M	96	THR	2.4
1	E	134	GLN	2.4
1	N	6	LYS	2.4
1	N	92	ASN	2.4
1	M	84	GLU	2.4
1	N	59	ASN	2.4
1	N	130	ARG	2.3
1	E	54	ASN	2.3
1	M	74	GLU	2.3
1	A	132	GLN	2.3
1	M	13	MET	2.3
1	M	97	ALA	2.3
1	I	95	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	M	59	ASN	2.2
1	M	49	LEU	2.2
1	N	100	VAL	2.2
1	C	21	PRO	2.1
1	B	237	MET	2.1
1	M	107	GLN	2.1
1	K	118	GLY	2.1
1	N	101	GLU	2.1
1	N	55	GLN	2.0
1	D	94	GLU	2.0
1	J	73	GLU	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.