Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:31 PM GMT

PDB ID	:	1KIU
Title	:	FimH adhesin Q133N mutant-FimC chaperone complex with methyl-alpha-D-mannose
Authors	:	Hung, C.S.; Bouckaert, J.
Deposited on	:	2001-12-03
Resolution	:	3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

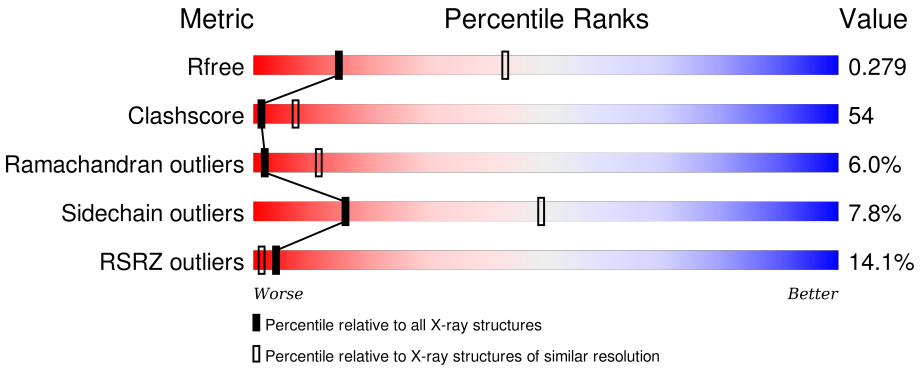
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	205	% 38% 53% 8% •
1	C	205	38% 53% 8% •
1	E	205	37% 55% 8% •
1	G	205	39% 53% 8% •
1	I	205	33% 22% 66% 12%

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Mol	Chain	Length	Quality of chain
1	K	205	45% 24% 65% 11%
1	M	205	38% 23% 65% 12%
1	O	205	37% 23% 65% 12%
2	B	279	49% 42% 10%
2	D	279	49% 42% 9%
2	F	279	48% 44% 8%
2	H	279	49% 42% 9%
2	J	279	20% 30% 62% 7%
2	L	279	21% 30% 62% 7%
2	N	279	19% 31% 62% 7%
2	P	279	21% 32% 61% 7%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	MMA	B	500	-	-	-	X
3	MMA	D	601	-	-	-	X
3	MMA	F	502	-	-	-	X
3	MMA	H	603	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 29657 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 CHAPERONE PROTEIN FimC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	205	Total	C	N	O	S	0	0	0
			1596	1010	276	304	6			
1	C	205	Total	C	N	O	S	0	0	0
			1596	1010	276	304	6			
1	E	205	Total	C	N	O	S	0	0	0
			1596	1010	276	304	6			
1	G	205	Total	C	N	O	S	0	0	0
			1596	1010	276	304	6			
1	I	205	Total	C	N	O	S	0	0	0
			1596	1010	276	304	6			
1	K	205	Total	C	N	O	S	0	0	0
			1596	1010	276	304	6			
1	M	205	Total	C	N	O	S	0	0	0
			1596	1010	276	304	6			
1	O	205	Total	C	N	O	S	0	0	0
			1596	1010	276	304	6			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	18	VAL	GLU	CONFLICT	UNP P31697
C	18	VAL	GLU	CONFLICT	UNP P31697
E	18	VAL	GLU	CONFLICT	UNP P31697
G	18	VAL	GLU	CONFLICT	UNP P31697
I	18	VAL	GLU	CONFLICT	UNP P31697
K	18	VAL	GLU	CONFLICT	UNP P31697
M	18	VAL	GLU	CONFLICT	UNP P31697
O	18	VAL	GLU	CONFLICT	UNP P31697

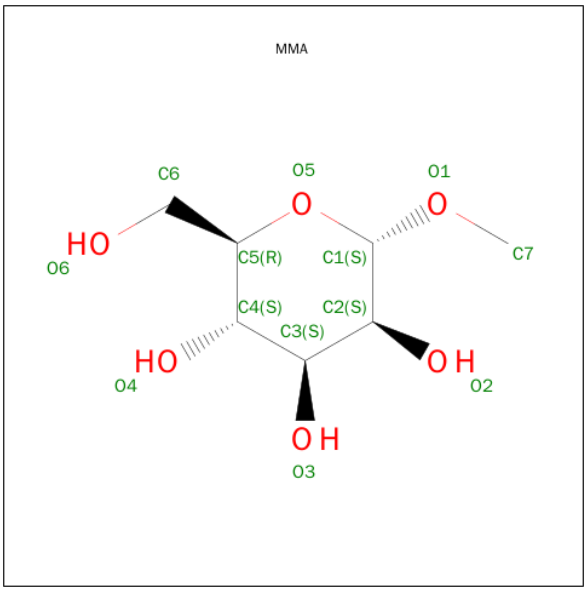
- Molecule 2 is a protein called FimH PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	279	Total	C	N	O	S	0	0	0
			2051	1296	342	409	4			
2	D	279	Total	C	N	O	S	0	0	0
			2051	1296	342	409	4			
2	F	279	Total	C	N	O	S	0	0	0
			2051	1296	342	409	4			
2	H	279	Total	C	N	O	S	0	0	0
			2051	1296	342	409	4			
2	J	279	Total	C	N	O	S	0	0	0
			2051	1296	342	409	4			
2	L	279	Total	C	N	O	S	0	0	0
			2051	1296	342	409	4			
2	N	279	Total	C	N	O	S	0	0	0
			2051	1296	342	409	4			
2	P	279	Total	C	N	O	S	0	0	0
			2051	1296	342	409	4			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	133	ASN	GLN	engineered	UNP P08191
D	133	ASN	GLN	engineered	UNP P08191
F	133	ASN	GLN	engineered	UNP P08191
H	133	ASN	GLN	engineered	UNP P08191
J	133	ASN	GLN	engineered	UNP P08191
L	133	ASN	GLN	engineered	UNP P08191
N	133	ASN	GLN	engineered	UNP P08191
P	133	ASN	GLN	engineered	UNP P08191

- Molecule 3 is SUGAR (O1-METHYL-MANNOSE) (three-letter code: MMA) (formula: $C_7H_{14}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C O 13 7 6	0	0
3	D	1	Total C O 13 7 6	0	0
3	F	1	Total C O 13 7 6	0	0
3	H	1	Total C O 13 7 6	0	0
3	J	1	Total C O 13 7 6	0	0
3	L	1	Total C O 13 7 6	0	0
3	N	1	Total C O 13 7 6	0	0
3	P	1	Total C O 13 7 6	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	19	Total O 19 19	0	0
4	B	58	Total O 58 58	0	0
4	C	20	Total O 20 20	0	0
4	D	54	Total O 54 54	0	0

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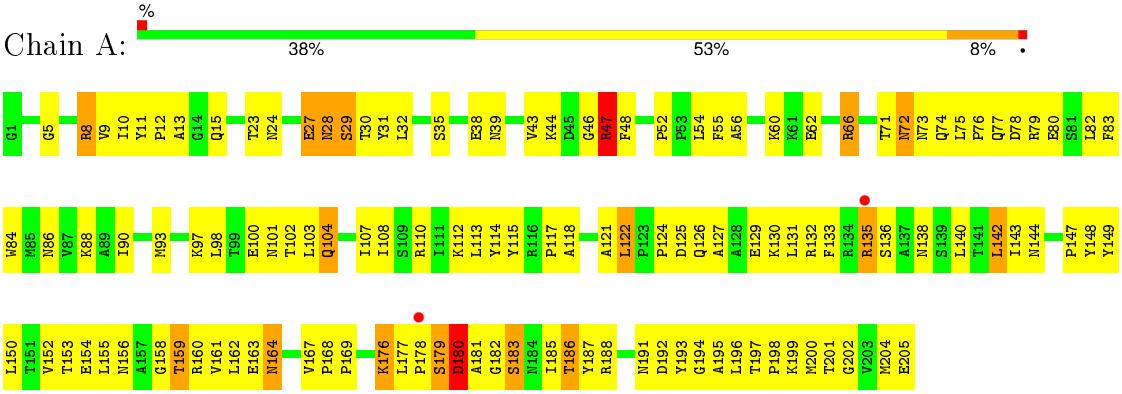
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	28	Total O 28 28	0	0
4	F	47	Total O 47 47	0	0
4	G	20	Total O 20 20	0	0
4	H	54	Total O 54 54	0	0
4	I	5	Total O 5 5	0	0
4	J	12	Total O 12 12	0	0
4	K	8	Total O 8 8	0	0
4	L	13	Total O 13 13	0	0
4	M	5	Total O 5 5	0	0
4	N	13	Total O 13 13	0	0
4	O	7	Total O 7 7	0	0
4	P	14	Total O 14 14	0	0

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.

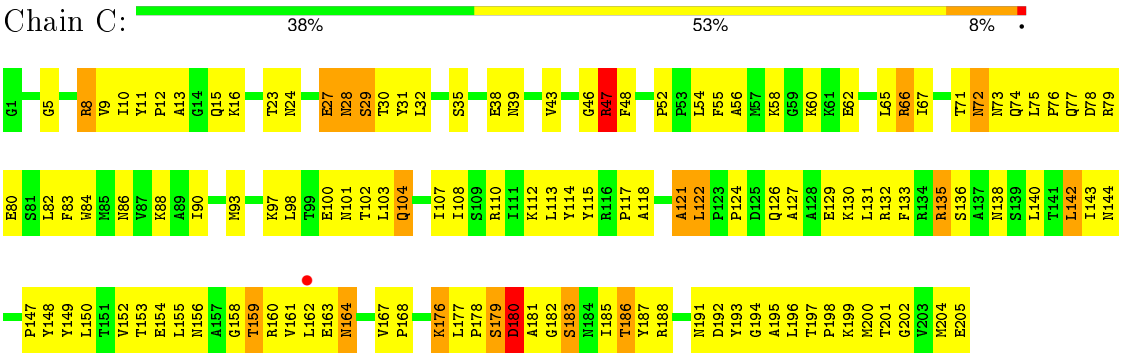
- Molecule 1: CHAPERONE PROTEIN FimC

Chain A:



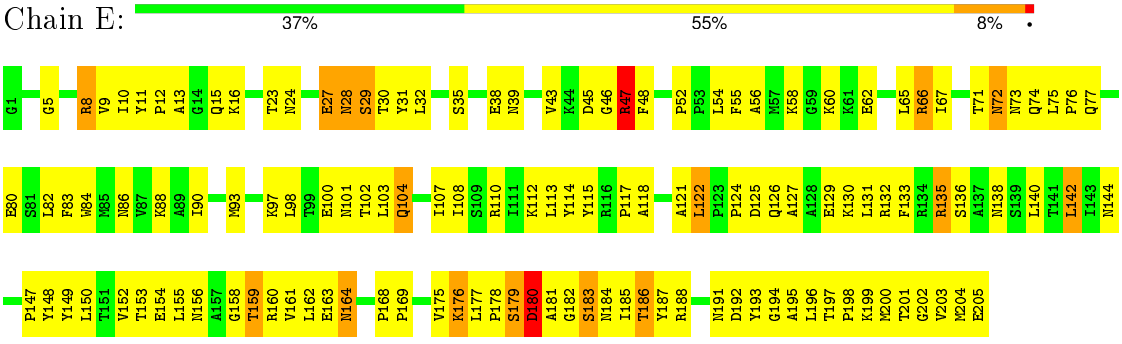
- Molecule 1: CHAPERONE PROTEIN FimC

Chain C:



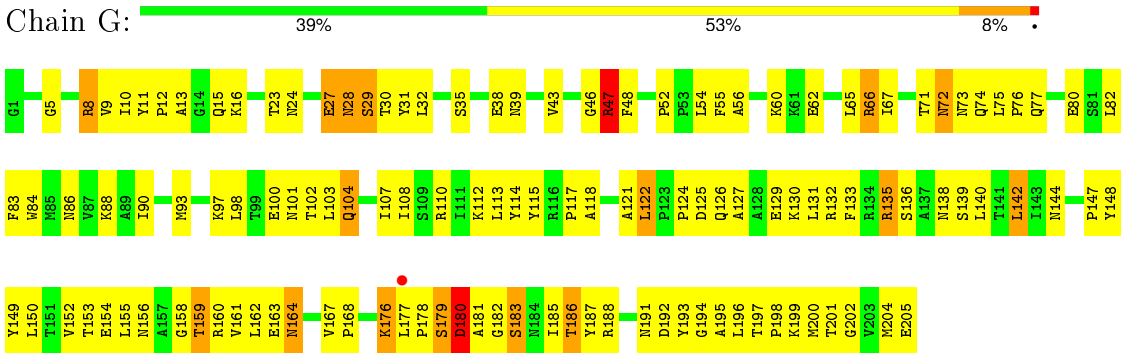
- Molecule 1: CHAPERONE PROTEIN FimC

Chain E:



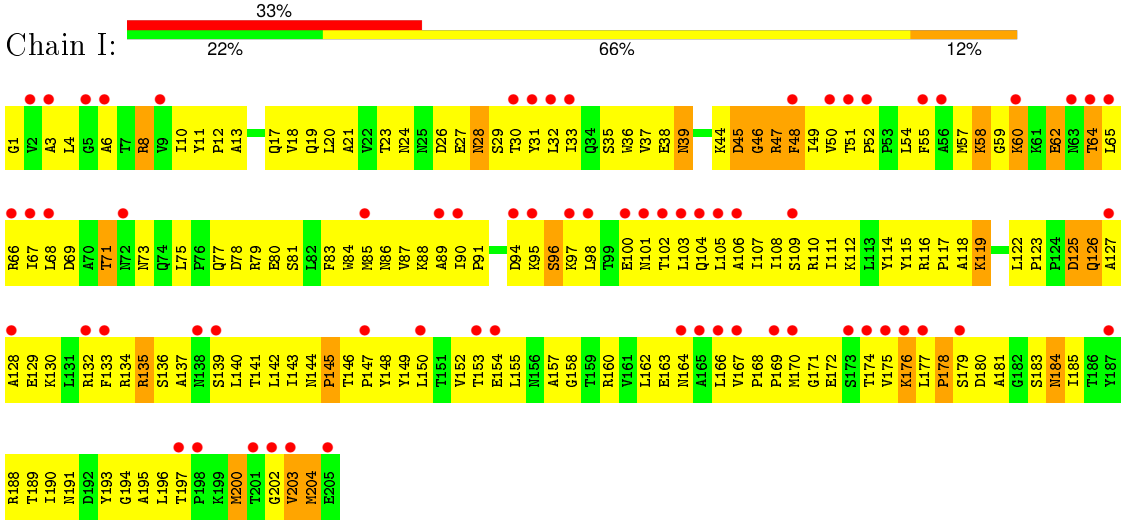
• Molecule 1: CHAPERONE PROTEIN FimC

Chain G:



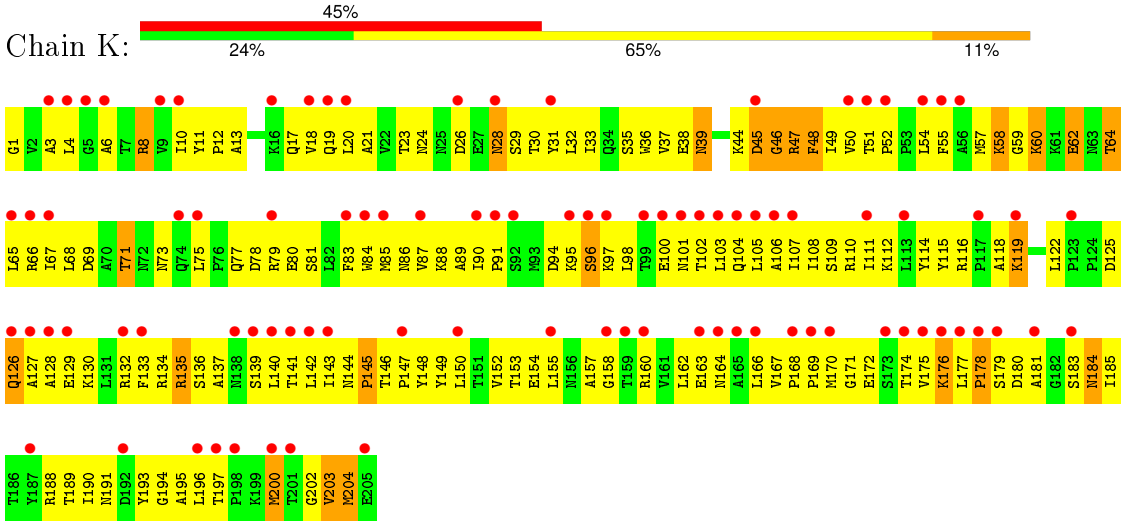
• Molecule 1: CHAPERONE PROTEIN FimC

Chain I:



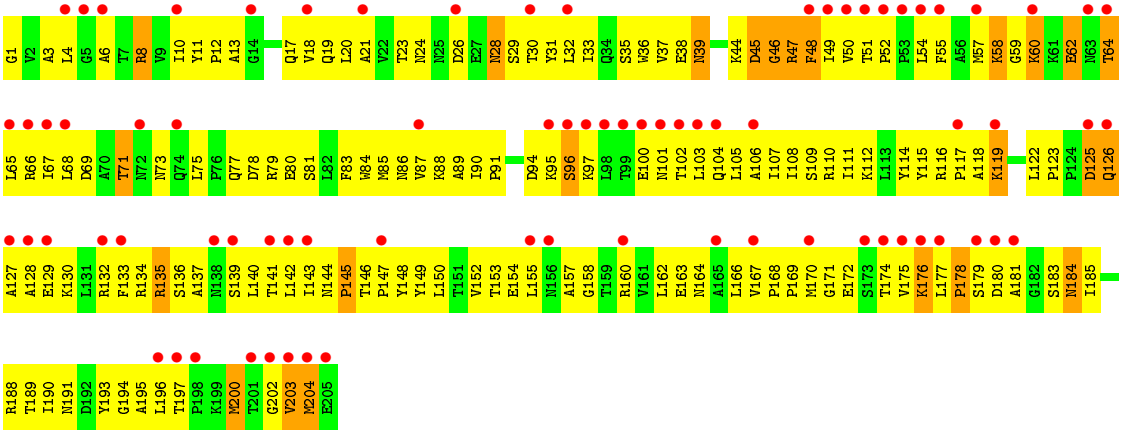
• Molecule 1: CHAPERONE PROTEIN FimC

Chain K:



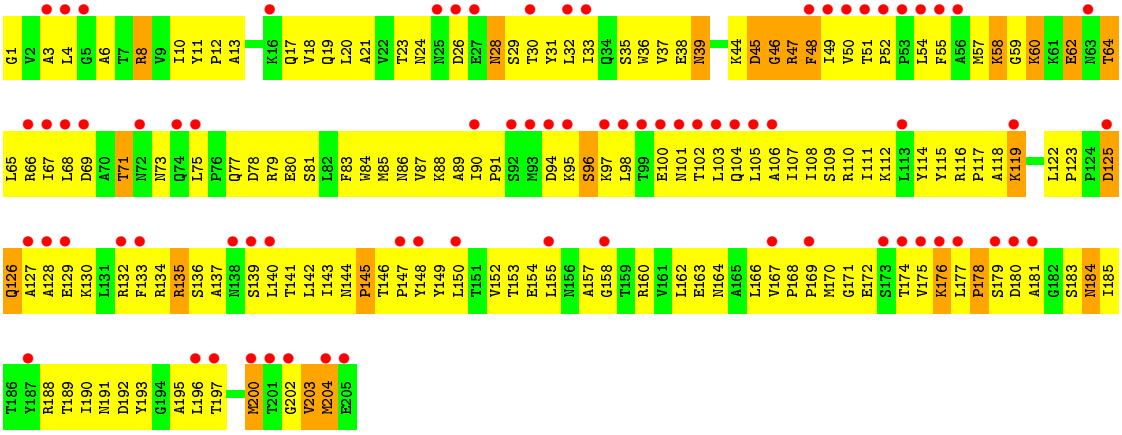
• Molecule 1: CHAPERONE PROTEIN FimC

Chain M:



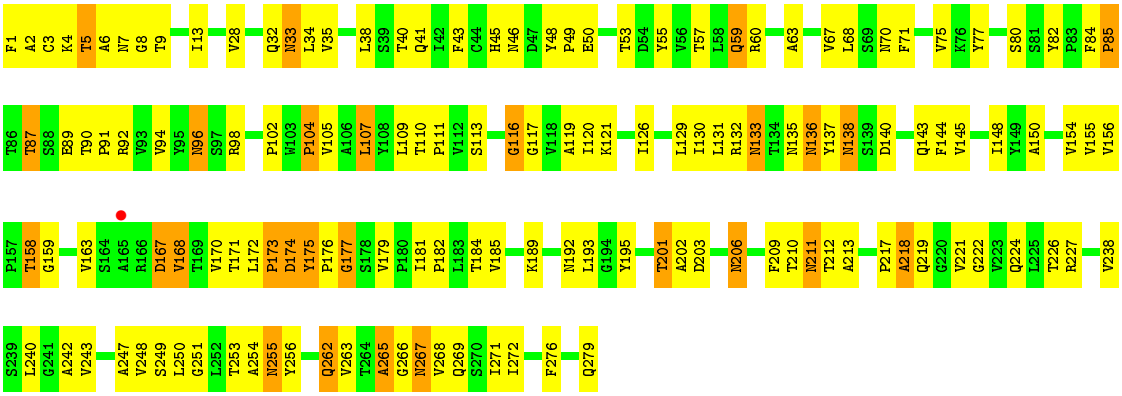
• Molecule 1: CHAPERONE PROTEIN FimC

Chain O:



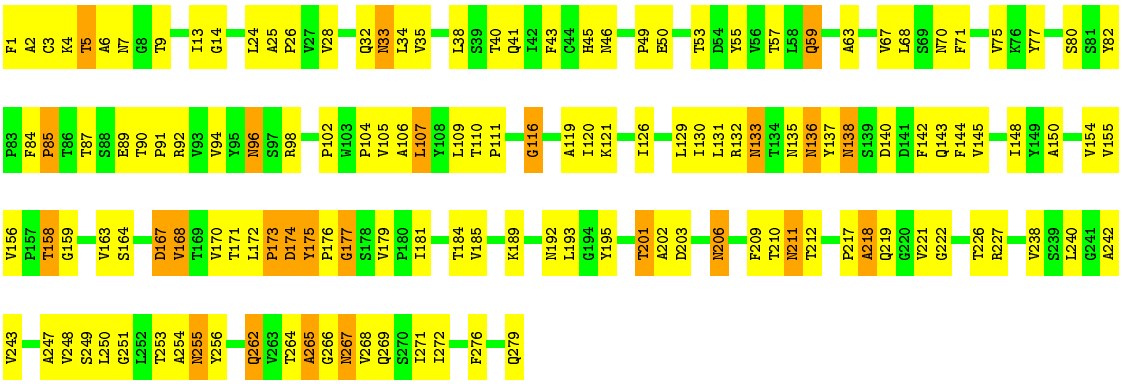
• Molecule 2: FimH PROTEIN

Chain B:



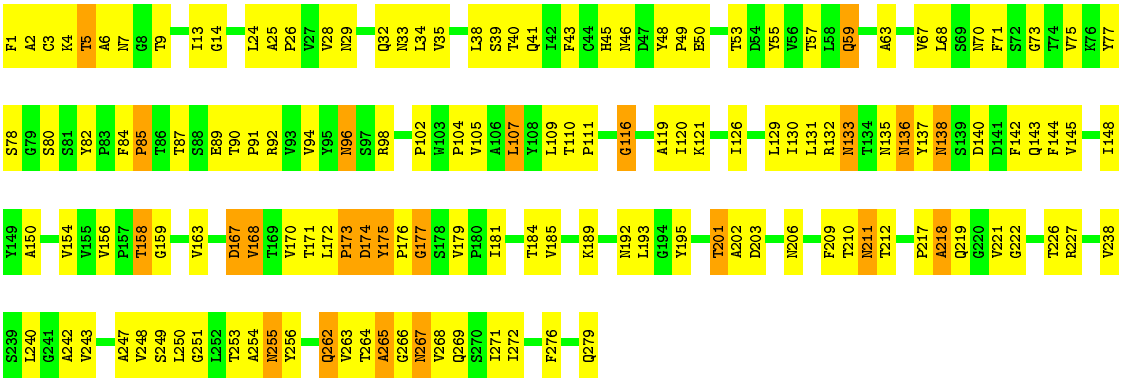
• Molecule 2: FimH PROTEIN

Chain D:



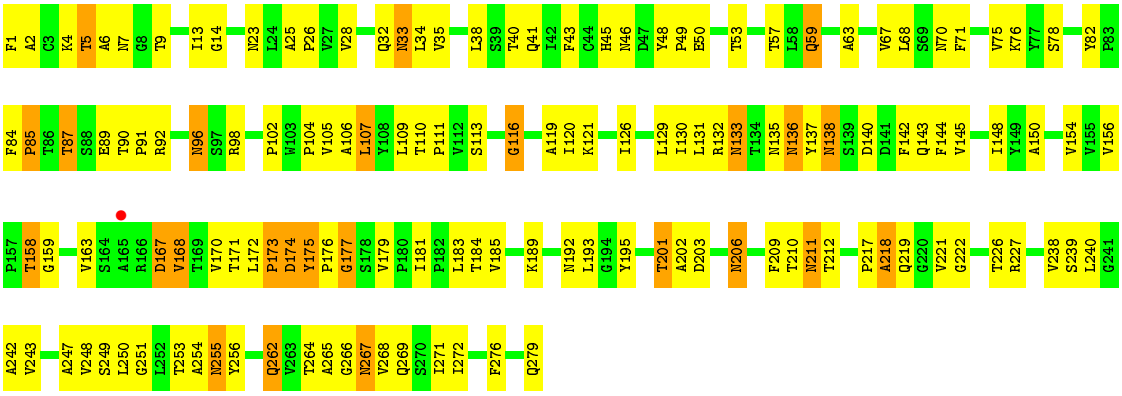
• Molecule 2: FimH PROTEIN

Chain F:



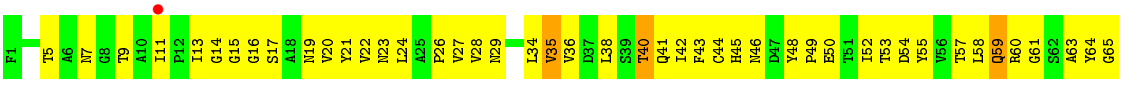
• Molecule 2: FimH PROTEIN

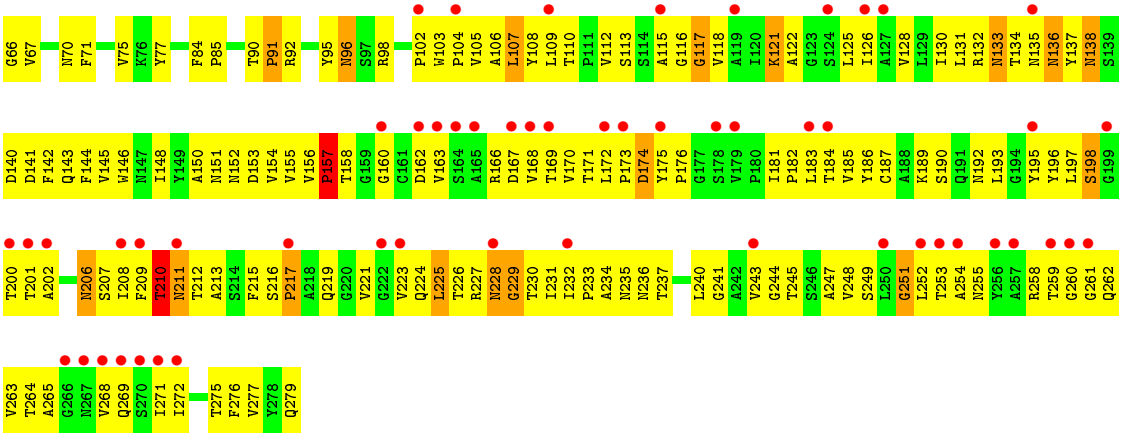
Chain H:



• Molecule 2: FimH PROTEIN

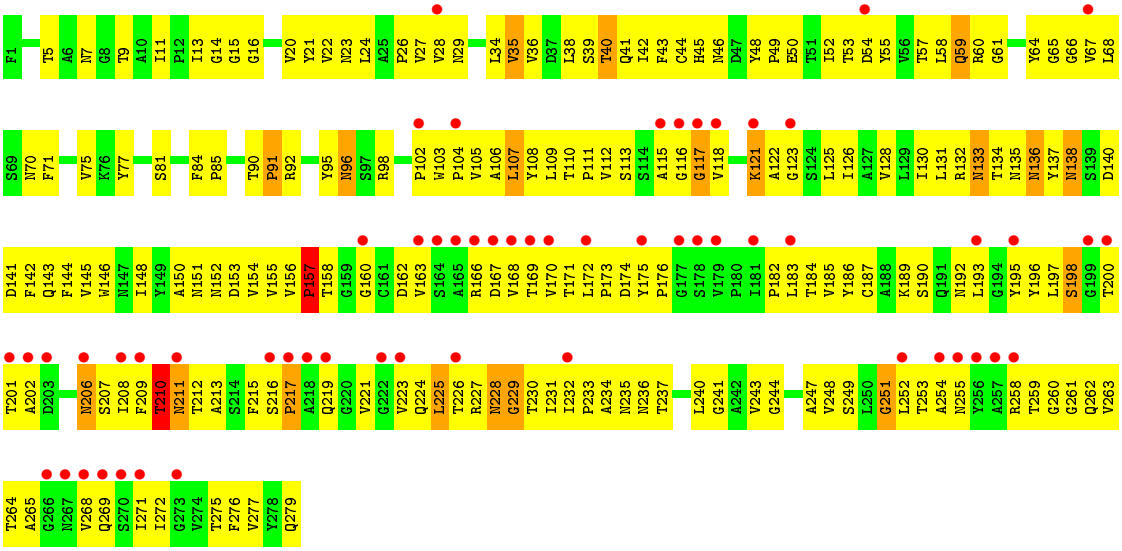
Chain J:





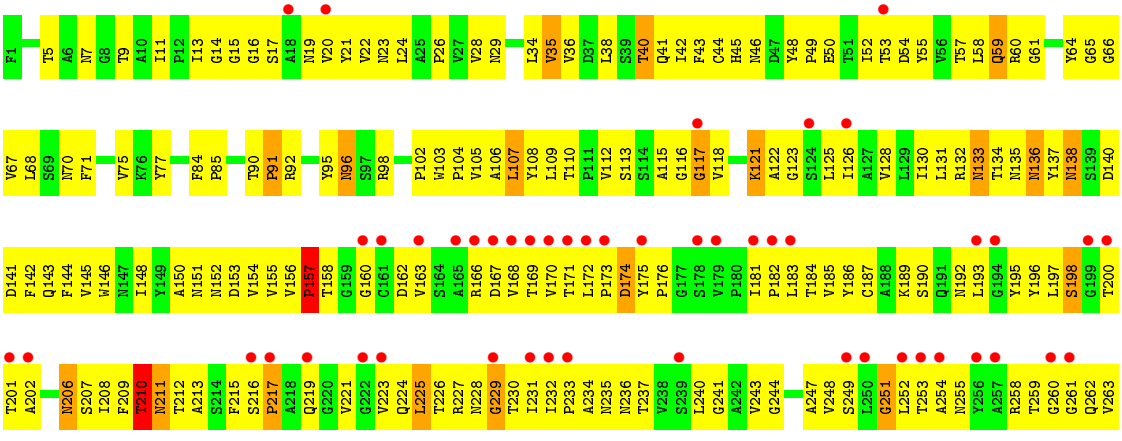
• Molecule 2: FimH PROTEIN

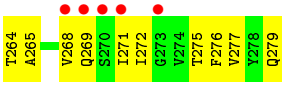
Chain L:



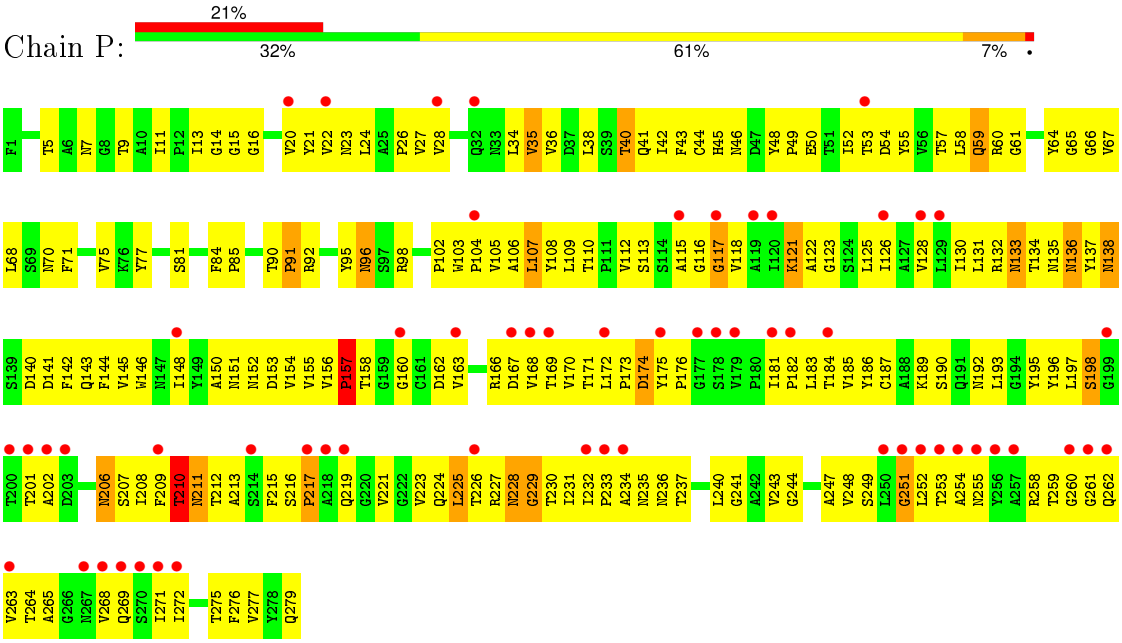
• Molecule 2: FimH PROTEIN

Chain N:





- Molecule 2: FimH PROTEIN



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	138.35Å 138.33Å 213.21Å 90.00° 89.98° 90.00°	Depositor
Resolution (Å)	45.00 – 3.00 44.46 – 3.00	Depositor EDS
% Data completeness (in resolution range)	89.1 (45.00-3.00) 89.2 (44.46-3.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	2.31 (at 3.01Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.236 , 0.278 0.236 , 0.279	Depositor DCC
R_{free} test set	7267 reflections (10.13%)	DCC
Wilson B-factor (Å^2)	59.9	Xtriage
Anisotropy	0.102	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 62.0	EDS
Estimated twinning fraction	0.457 for k,h,-l 0.457 for -k,-h,-l 0.447 for -h,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	1 of 71767 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	29657	wwPDB-VP
Average B, all atoms (Å^2)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.15% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MMA

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	0.42	0/1625	0.71	0/2209
1	C	0.42	0/1625	0.71	0/2209
1	E	0.42	0/1625	0.70	0/2209
1	G	0.42	0/1625	0.71	0/2209
1	I	0.29	0/1625	0.54	0/2209
1	K	0.29	0/1625	0.54	0/2209
1	M	0.29	0/1625	0.54	0/2209
1	O	0.29	0/1625	0.54	0/2209
2	B	0.48	0/2096	0.76	0/2880
2	D	0.49	0/2096	0.76	0/2880
2	F	0.49	0/2096	0.76	0/2880
2	H	0.49	0/2096	0.76	0/2880
2	J	0.33	0/2096	0.60	0/2880
2	L	0.33	0/2096	0.60	0/2880
2	N	0.33	0/2096	0.60	0/2880
2	P	0.33	0/2096	0.59	0/2880
All	All	0.39	0/29768	0.66	0/40712

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1596	0	1639	151	0
1	C	1596	0	1639	158	0
1	E	1596	0	1639	157	0
1	G	1596	0	1639	148	0
1	I	1596	0	1639	242	0
1	K	1596	0	1639	246	0
1	M	1596	0	1639	240	0
1	O	1596	0	1639	243	0
2	B	2051	0	2005	182	0
2	D	2051	0	2005	173	0
2	F	2051	0	2005	180	0
2	H	2051	0	2005	183	0
2	J	2051	0	2005	262	0
2	L	2051	0	2005	264	0
2	N	2051	0	2005	255	0
2	P	2051	0	2005	263	0
3	B	13	0	14	2	0
3	D	13	0	14	0	0
3	F	13	0	14	2	0
3	H	13	0	14	3	0
3	J	13	0	14	1	0
3	L	13	0	14	1	0
3	N	13	0	14	1	0
3	P	13	0	14	1	0
4	A	19	0	0	4	0
4	B	58	0	0	11	0
4	C	20	0	0	9	0
4	D	54	0	0	6	0
4	E	28	0	0	9	0
4	F	47	0	0	10	0
4	G	20	0	0	3	0
4	H	54	0	0	9	0
4	I	5	0	0	2	0
4	J	12	0	0	5	0
4	K	8	0	0	2	0
4	L	13	0	0	5	0
4	M	5	0	0	1	0
4	N	13	0	0	0	0
4	O	7	0	0	2	0
4	P	14	0	0	2	0
All	All	29657	0	29264	3137	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 54.

All (3137) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:141:THR:HA	1:K:174:THR:CG2	1.33	1.59
1:M:141:THR:HA	1:M:174:THR:CG2	1.32	1.55
1:O:141:THR:HA	1:O:174:THR:CG2	1.33	1.54
1:I:141:THR:HA	1:I:174:THR:CG2	1.33	1.54
1:O:141:THR:HA	1:O:174:THR:HG21	1.26	1.16
1:M:141:THR:CA	1:M:174:THR:HG22	1.76	1.15
1:O:141:THR:CA	1:O:174:THR:HG22	1.76	1.14
1:I:141:THR:CA	1:I:174:THR:HG22	1.76	1.14
1:K:141:THR:CA	1:K:174:THR:HG22	1.76	1.14
2:L:258:ARG:HD3	2:L:261:GLY:HA2	1.26	1.14
1:K:141:THR:HA	1:K:174:THR:HG21	1.26	1.13
1:I:141:THR:HA	1:I:174:THR:HG21	1.27	1.12
1:M:141:THR:HA	1:M:174:THR:HG21	1.25	1.10
1:I:141:THR:CA	1:I:174:THR:CG2	2.30	1.10
1:M:141:THR:CA	1:M:174:THR:CG2	2.29	1.10
1:K:141:THR:CA	1:K:174:THR:CG2	2.29	1.10
1:O:141:THR:CA	1:O:174:THR:CG2	2.29	1.10
2:P:258:ARG:HD3	2:P:261:GLY:HA2	1.27	1.09
2:J:258:ARG:HD3	2:J:261:GLY:HA2	1.26	1.08
2:N:258:ARG:HD3	2:N:261:GLY:HA2	1.26	1.08
1:I:140:LEU:HG	1:I:177:LEU:HD22	1.37	1.06
1:O:140:LEU:HG	1:O:177:LEU:HD22	1.38	1.05
1:K:140:LEU:HG	1:K:177:LEU:HD22	1.37	1.04
1:M:140:LEU:HG	1:M:177:LEU:HD22	1.38	1.03
1:A:122:LEU:HD11	1:A:130:LYS:HE3	1.43	1.00
1:G:122:LEU:HD11	1:G:130:LYS:HE3	1.41	0.99
2:B:113:SER:HB3	2:P:81:SER:H	1.28	0.99
2:J:210:THR:HG23	2:J:259:THR:HG21	1.45	0.99
1:E:122:LEU:HD11	1:E:130:LYS:HE3	1.41	0.98
2:L:210:THR:HG23	2:L:259:THR:HG21	1.44	0.98
2:P:210:THR:HG23	2:P:259:THR:HG21	1.45	0.98
1:E:160:ARG:HB2	1:E:180:ASP:HB2	1.46	0.97
2:H:113:SER:HB3	2:L:81:SER:H	1.30	0.97
1:C:122:LEU:HD11	1:C:130:LYS:HE3	1.43	0.97
1:A:160:ARG:HB2	1:A:180:ASP:HB2	1.46	0.96
2:H:173:PRO:HG3	2:H:179:VAL:HG13	1.48	0.96
2:F:173:PRO:HG3	2:F:179:VAL:HG13	1.47	0.95
2:B:173:PRO:HG3	2:B:179:VAL:HG13	1.48	0.95
1:K:163:GLU:H	1:K:175:VAL:HG11	1.31	0.95
1:O:97:LYS:HD2	2:P:170:VAL:HG21	1.49	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:210:THR:HG23	2:N:259:THR:HG21	1.45	0.95
1:G:160:ARG:HB2	1:G:180:ASP:HB2	1.46	0.95
1:K:97:LYS:HD2	2:L:170:VAL:HG21	1.49	0.95
2:D:173:PRO:HG3	2:D:179:VAL:HG13	1.47	0.94
1:M:97:LYS:HD2	2:N:170:VAL:HG21	1.49	0.94
1:I:163:GLU:H	1:I:175:VAL:HG11	1.31	0.94
1:C:160:ARG:HB2	1:C:180:ASP:HB2	1.46	0.94
1:I:141:THR:HA	1:I:174:THR:HG22	0.95	0.94
2:D:211:ASN:HD21	2:D:269:GLN:H	1.14	0.94
2:J:11:ILE:HG23	2:J:16:GLY:HA3	1.49	0.94
1:I:97:LYS:HD2	2:J:170:VAL:HG21	1.49	0.93
1:K:141:THR:HA	1:K:174:THR:HG22	0.96	0.93
1:O:163:GLU:H	1:O:175:VAL:HG11	1.30	0.93
2:H:211:ASN:HD21	2:H:269:GLN:H	1.13	0.93
1:O:141:THR:HA	1:O:174:THR:HG22	0.96	0.93
1:M:141:THR:HA	1:M:174:THR:HG22	0.96	0.93
1:M:163:GLU:H	1:M:175:VAL:HG11	1.31	0.93
2:B:211:ASN:HD21	2:B:269:GLN:H	1.14	0.92
2:P:11:ILE:HG23	2:P:16:GLY:HA3	1.49	0.92
2:L:11:ILE:HG23	2:L:16:GLY:HA3	1.50	0.91
2:N:11:ILE:HG23	2:N:16:GLY:HA3	1.49	0.90
1:O:102:THR:HG22	2:P:170:VAL:HG22	1.54	0.90
1:I:102:THR:HG22	2:J:170:VAL:HG22	1.53	0.90
1:K:4:LEU:HD21	1:K:87:VAL:HG21	1.53	0.89
2:F:211:ASN:HD21	2:F:269:GLN:H	1.14	0.89
1:O:4:LEU:HD21	1:O:87:VAL:HG21	1.52	0.89
1:M:102:THR:HG22	2:N:170:VAL:HG22	1.54	0.89
1:I:4:LEU:HD21	1:I:87:VAL:HG21	1.53	0.89
1:G:27:GLU:HG3	1:G:60:LYS:HZ2	1.38	0.89
1:I:21:ALA:HA	1:I:64:THR:HA	1.55	0.88
1:M:21:ALA:HA	1:M:64:THR:HA	1.55	0.88
1:K:21:ALA:HA	1:K:64:THR:HA	1.54	0.88
1:K:102:THR:HG22	2:L:170:VAL:HG22	1.54	0.88
1:M:4:LEU:HD21	1:M:87:VAL:HG21	1.52	0.87
1:O:21:ALA:HA	1:O:64:THR:HA	1.55	0.86
2:B:67:VAL:HG21	2:B:126:ILE:HG23	1.57	0.86
2:H:221:VAL:HG12	2:H:222:GLY:H	1.39	0.85
1:C:27:GLU:HG3	1:C:60:LYS:HZ2	1.40	0.85
2:F:67:VAL:HG21	2:F:126:ILE:HG23	1.58	0.85
2:H:201:THR:HG21	2:H:206:ASN:HD22	1.42	0.85
1:O:149:TYR:HB3	1:O:166:LEU:HD11	1.58	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:60:ARG:HG2	2:P:61:GLY:H	1.40	0.85
2:L:60:ARG:HG2	2:L:61:GLY:H	1.42	0.84
2:B:221:VAL:HG12	2:B:222:GLY:H	1.41	0.84
1:K:149:TYR:HB3	1:K:166:LEU:HD11	1.57	0.84
2:F:221:VAL:HG12	2:F:222:GLY:H	1.40	0.84
2:N:60:ARG:HG2	2:N:61:GLY:H	1.40	0.84
1:A:161:VAL:HG22	1:A:162:LEU:H	1.43	0.84
2:J:227:ARG:HH11	2:J:232:ILE:HG12	1.43	0.84
2:L:227:ARG:HH11	2:L:232:ILE:HG12	1.43	0.83
1:I:149:TYR:HB3	1:I:166:LEU:HD11	1.58	0.83
1:O:19:GLN:HG2	1:O:66:ARG:HG3	1.60	0.83
2:D:67:VAL:HG21	2:D:126:ILE:HG23	1.59	0.83
1:C:112:LYS:HG3	4:C:209:HOH:O	1.77	0.83
2:J:28:VAL:O	2:J:157:PRO:HD2	1.79	0.83
1:M:149:TYR:HB3	1:M:166:LEU:HD11	1.58	0.83
1:M:19:GLN:HG2	1:M:66:ARG:HG3	1.60	0.83
2:P:213:ALA:HB2	2:P:269:GLN:HB2	1.60	0.83
2:B:255:ASN:HD22	2:B:255:ASN:N	1.75	0.83
2:J:60:ARG:HG2	2:J:61:GLY:H	1.42	0.82
2:H:67:VAL:HG21	2:H:126:ILE:HG23	1.58	0.82
1:O:17:GLN:HB3	1:O:68:LEU:HD23	1.62	0.82
2:J:213:ALA:HB2	2:J:269:GLN:HB2	1.60	0.82
2:D:201:THR:HG21	2:D:206:ASN:HD22	1.44	0.82
2:P:227:ARG:HH11	2:P:232:ILE:HG12	1.43	0.82
2:D:221:VAL:HG12	2:D:222:GLY:H	1.41	0.82
1:K:17:GLN:HB3	1:K:68:LEU:HD23	1.62	0.82
2:D:255:ASN:N	2:D:255:ASN:HD22	1.77	0.82
1:E:161:VAL:HG22	1:E:162:LEU:H	1.44	0.82
1:E:27:GLU:HG3	1:E:60:LYS:NZ	1.94	0.82
2:N:227:ARG:HH11	2:N:232:ILE:HG12	1.44	0.82
1:I:17:GLN:HB3	1:I:68:LEU:HD23	1.62	0.82
2:P:28:VAL:O	2:P:157:PRO:HD2	1.80	0.82
1:E:27:GLU:HG3	1:E:60:LYS:HZ2	1.44	0.81
1:I:19:GLN:HG2	1:I:66:ARG:HG3	1.60	0.81
1:G:27:GLU:HG3	1:G:60:LYS:NZ	1.95	0.81
2:L:213:ALA:HB2	2:L:269:GLN:HB2	1.61	0.81
1:M:17:GLN:HB3	1:M:68:LEU:HD23	1.62	0.81
1:C:161:VAL:HG22	1:C:162:LEU:H	1.43	0.81
2:L:116:GLY:HA2	2:L:189:LYS:HG3	1.62	0.81
2:F:254:ALA:C	2:F:255:ASN:HD22	1.84	0.81
2:H:254:ALA:C	2:H:255:ASN:HD22	1.84	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:254:ALA:C	2:B:255:ASN:HD22	1.85	0.81
1:C:27:GLU:HG3	1:C:60:LYS:NZ	1.96	0.81
1:K:88:LYS:HG3	1:K:108:ILE:HG12	1.62	0.81
2:N:213:ALA:HB2	2:N:269:GLN:HB2	1.61	0.81
2:N:28:VAL:O	2:N:157:PRO:HD2	1.80	0.81
2:F:136:ASN:C	2:F:136:ASN:HD22	1.83	0.81
1:M:141:THR:CA	1:M:174:THR:HG21	2.04	0.81
2:D:254:ALA:C	2:D:255:ASN:HD22	1.83	0.81
1:I:88:LYS:HG3	1:I:108:ILE:HG12	1.62	0.81
2:L:28:VAL:O	2:L:157:PRO:HD2	1.80	0.80
2:B:32:GLN:O	2:B:110:THR:HG23	1.81	0.80
2:F:201:THR:HG21	2:F:206:ASN:HD22	1.44	0.80
2:F:240:LEU:HD11	2:F:250:LEU:CD2	2.10	0.80
1:A:27:GLU:HG3	1:A:60:LYS:HZ2	1.43	0.80
2:B:201:THR:HG21	2:B:206:ASN:HD22	1.46	0.80
1:K:19:GLN:HG2	1:K:66:ARG:HG3	1.61	0.80
2:H:255:ASN:HD22	2:H:255:ASN:N	1.76	0.80
2:B:59:GLN:HG2	2:B:132:ARG:HD2	1.64	0.80
2:N:116:GLY:HA2	2:N:189:LYS:HG3	1.62	0.80
2:P:264:THR:HG22	2:P:265:ALA:H	1.46	0.80
1:A:27:GLU:HG3	1:A:60:LYS:NZ	1.95	0.80
2:J:264:THR:HG22	2:J:265:ALA:H	1.47	0.80
2:H:240:LEU:HD11	2:H:250:LEU:CD2	2.11	0.80
1:M:88:LYS:HG3	1:M:108:ILE:HG12	1.62	0.80
2:N:227:ARG:HG3	2:N:230:THR:HB	1.64	0.80
1:G:161:VAL:HG22	1:G:162:LEU:H	1.45	0.79
1:O:88:LYS:HG3	1:O:108:ILE:HG12	1.62	0.79
1:G:13:ALA:HB3	1:G:118:ALA:H	1.46	0.79
2:F:120:ILE:HB	2:F:154:VAL:HB	1.64	0.79
2:J:116:GLY:HA2	2:J:189:LYS:HG3	1.62	0.79
1:I:190:ILE:HD12	2:J:279:GLN:HG2	1.64	0.79
2:H:120:ILE:HB	2:H:154:VAL:HB	1.64	0.79
2:B:136:ASN:HD22	2:B:136:ASN:C	1.83	0.79
2:B:240:LEU:HD11	2:B:250:LEU:CD2	2.12	0.79
2:H:136:ASN:C	2:H:136:ASN:HD22	1.84	0.79
2:P:116:GLY:HA2	2:P:189:LYS:HG3	1.61	0.79
1:K:190:ILE:HD12	2:L:279:GLN:HG2	1.63	0.79
2:H:32:GLN:O	2:H:110:THR:HG23	1.82	0.79
2:N:264:THR:HG22	2:N:265:ALA:H	1.46	0.79
1:E:13:ALA:HB3	1:E:118:ALA:H	1.47	0.79
2:D:240:LEU:HD11	2:D:250:LEU:CD2	2.13	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:32:GLN:O	2:D:110:THR:HG23	1.83	0.79
2:L:227:ARG:HG3	2:L:230:THR:HB	1.64	0.79
2:P:227:ARG:HG3	2:P:230:THR:HB	1.65	0.79
2:F:255:ASN:N	2:F:255:ASN:HD22	1.77	0.79
1:G:132:ARG:HG2	4:G:215:HOH:O	1.83	0.79
1:M:190:ILE:HD12	2:N:279:GLN:HG2	1.64	0.78
2:H:59:GLN:HG2	2:H:132:ARG:HD2	1.66	0.78
1:K:157:ALA:CB	1:K:181:ALA:HB1	2.13	0.78
1:G:176:LYS:HD2	1:G:176:LYS:H	1.48	0.78
1:O:157:ALA:CB	1:O:181:ALA:HB1	2.14	0.78
1:K:69:ASP:OD1	1:K:71:THR:HG22	1.84	0.78
2:D:138:ASN:C	2:D:138:ASN:HD22	1.85	0.78
1:M:157:ALA:CB	1:M:181:ALA:HB1	2.14	0.78
2:H:211:ASN:ND2	2:H:269:GLN:H	1.81	0.78
2:D:59:GLN:HG2	2:D:132:ARG:HD2	1.65	0.78
1:A:176:LYS:HD2	1:A:176:LYS:H	1.48	0.78
1:K:141:THR:CA	1:K:174:THR:HG21	2.06	0.78
1:A:132:ARG:HG2	4:A:215:HOH:O	1.82	0.78
1:M:69:ASP:OD1	1:M:71:THR:HG22	1.84	0.78
1:O:69:ASP:OD1	1:O:71:THR:HG22	1.84	0.78
2:J:227:ARG:HG3	2:J:230:THR:HB	1.65	0.78
1:C:13:ALA:HB3	1:C:118:ALA:H	1.48	0.78
1:C:136:SER:O	1:C:177:LEU:HD23	1.85	0.77
2:L:264:THR:HG22	2:L:265:ALA:H	1.46	0.77
2:F:32:GLN:O	2:F:110:THR:HG23	1.84	0.77
2:F:59:GLN:HG2	2:F:132:ARG:HD2	1.67	0.77
1:I:157:ALA:CB	1:I:181:ALA:HB1	2.14	0.77
2:P:226:THR:HG22	2:P:255:ASN:HD21	1.49	0.77
2:H:138:ASN:HD22	2:H:138:ASN:C	1.87	0.77
2:P:96:ASN:HD22	2:P:96:ASN:N	1.81	0.77
1:C:140:LEU:HD12	1:C:177:LEU:HD13	1.66	0.77
1:E:132:ARG:HG2	4:E:210:HOH:O	1.83	0.77
2:L:96:ASN:HD22	2:L:96:ASN:N	1.82	0.77
1:E:176:LYS:HD2	1:E:176:LYS:H	1.48	0.77
1:I:142:LEU:O	1:I:172:GLU:HB2	1.84	0.77
2:B:138:ASN:C	2:B:138:ASN:HD22	1.86	0.77
2:J:96:ASN:HD22	2:J:96:ASN:N	1.81	0.77
1:O:153:THR:HG21	1:O:196:LEU:HD22	1.67	0.77
1:O:190:ILE:HD12	2:P:279:GLN:HG2	1.64	0.77
1:G:140:LEU:HD12	1:G:177:LEU:HD13	1.67	0.77
1:K:160:ARG:HD3	1:K:180:ASP:HB2	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:226:THR:HG22	2:N:255:ASN:HD21	1.49	0.77
1:I:160:ARG:HD3	1:I:180:ASP:HB2	1.67	0.77
2:B:120:ILE:HB	2:B:154:VAL:HB	1.65	0.77
1:M:160:ARG:HD3	1:M:180:ASP:HB2	1.66	0.77
2:F:211:ASN:ND2	2:F:269:GLN:H	1.83	0.77
2:F:138:ASN:HD22	2:F:138:ASN:C	1.87	0.77
2:D:136:ASN:C	2:D:136:ASN:HD22	1.85	0.77
2:D:120:ILE:HB	2:D:154:VAL:HB	1.65	0.76
1:A:13:ALA:HB3	1:A:118:ALA:H	1.49	0.76
2:B:211:ASN:ND2	2:B:269:GLN:H	1.83	0.76
1:I:69:ASP:OD1	1:I:71:THR:HG22	1.84	0.76
1:O:142:LEU:O	1:O:172:GLU:HB2	1.85	0.76
2:D:211:ASN:ND2	2:D:269:GLN:H	1.83	0.76
2:L:226:THR:HG22	2:L:255:ASN:HD21	1.49	0.76
1:I:141:THR:CA	1:I:174:THR:HG21	2.06	0.76
1:G:16:LYS:HB3	4:G:210:HOH:O	1.86	0.76
1:E:140:LEU:HD12	1:E:177:LEU:HD13	1.67	0.76
1:M:153:THR:HG21	1:M:196:LEU:HD22	1.67	0.76
2:H:184:THR:HB	2:H:247:ALA:HB1	1.67	0.76
1:K:142:LEU:O	1:K:172:GLU:HB2	1.85	0.76
1:I:8:ARG:HB3	1:I:8:ARG:HH11	1.50	0.76
1:I:28:ASN:H	1:I:28:ASN:HD22	1.34	0.76
1:K:153:THR:HG21	1:K:196:LEU:HD22	1.67	0.76
1:I:153:THR:HG21	1:I:196:LEU:HD22	1.67	0.76
1:M:142:LEU:O	1:M:172:GLU:HB2	1.86	0.76
1:G:136:SER:O	1:G:177:LEU:HD23	1.86	0.75
2:J:213:ALA:HB1	4:J:610:HOH:O	1.85	0.75
2:N:96:ASN:N	2:N:96:ASN:HD22	1.82	0.75
1:O:28:ASN:HD22	1:O:28:ASN:H	1.34	0.75
2:B:217:PRO:O	2:B:219:GLN:N	2.20	0.75
1:C:176:LYS:HD2	1:C:176:LYS:H	1.50	0.75
1:A:136:SER:O	1:A:177:LEU:HD23	1.86	0.75
1:K:145:PRO:HA	1:K:170:MET:HA	1.68	0.75
1:M:8:ARG:HH11	1:M:8:ARG:HB3	1.52	0.75
1:O:160:ARG:HD3	1:O:180:ASP:HB2	1.67	0.75
2:D:218:ALA:HB2	2:D:266:GLY:C	2.07	0.75
1:I:145:PRO:HA	1:I:170:MET:HA	1.67	0.75
1:K:28:ASN:HD22	1:K:28:ASN:H	1.35	0.75
2:J:226:THR:HG22	2:J:255:ASN:HD21	1.50	0.75
1:A:140:LEU:HD12	1:A:177:LEU:HD13	1.69	0.75
1:G:52:PRO:HG2	1:G:55:PHE:CD1	2.22	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:120:ILE:HD13	2:B:126:ILE:HD12	1.68	0.74
2:F:120:ILE:HD13	2:F:126:ILE:HD12	1.69	0.74
2:H:120:ILE:HD13	2:H:126:ILE:HD12	1.69	0.74
2:N:172:LEU:N	2:N:173:PRO:HD2	2.01	0.74
1:O:71:THR:HG23	1:O:73:ASN:H	1.52	0.74
2:H:218:ALA:HB2	2:H:266:GLY:C	2.08	0.74
1:M:28:ASN:H	1:M:28:ASN:HD22	1.35	0.74
1:O:8:ARG:HH11	1:O:8:ARG:HB3	1.52	0.74
2:F:218:ALA:HB2	2:F:266:GLY:C	2.07	0.74
1:C:194:GLY:O	2:D:158:THR:HG21	1.87	0.74
1:I:71:THR:HG23	1:I:73:ASN:H	1.51	0.74
1:E:86:ASN:HD21	1:E:110:ARG:HE	1.35	0.74
1:A:52:PRO:HG2	1:A:55:PHE:CD1	2.22	0.74
2:P:27:VAL:HG12	4:P:616:HOH:O	1.88	0.74
1:K:8:ARG:HB3	1:K:8:ARG:HH11	1.51	0.74
1:A:86:ASN:HD21	1:A:110:ARG:HE	1.35	0.74
2:L:172:LEU:N	2:L:173:PRO:HD2	2.02	0.74
2:F:184:THR:HB	2:F:247:ALA:HB1	1.69	0.74
2:B:184:THR:HB	2:B:247:ALA:HB1	1.69	0.74
1:C:52:PRO:HG2	1:C:55:PHE:CD1	2.22	0.74
2:N:135:ASN:HD21	2:N:138:ASN:HD21	1.34	0.74
2:D:184:THR:HB	2:D:247:ALA:HB1	1.69	0.74
2:J:172:LEU:N	2:J:173:PRO:HD2	2.02	0.74
1:M:71:THR:HG23	1:M:73:ASN:H	1.52	0.74
2:B:218:ALA:HB2	2:B:266:GLY:C	2.08	0.74
1:M:145:PRO:HA	1:M:170:MET:HA	1.68	0.74
1:G:88:LYS:HB2	1:G:108:ILE:HG12	1.70	0.74
1:E:136:SER:O	1:E:177:LEU:HD23	1.85	0.73
2:J:5:THR:HG22	2:J:9:THR:O	1.88	0.73
2:D:217:PRO:O	2:D:219:GLN:N	2.21	0.73
1:I:102:THR:HA	2:J:170:VAL:HA	1.70	0.73
2:N:226:THR:HG22	2:N:253:THR:HB	1.70	0.73
1:K:71:THR:HG23	1:K:73:ASN:H	1.52	0.73
1:K:157:ALA:HB3	1:K:181:ALA:HB1	1.70	0.73
2:F:217:PRO:O	2:F:219:GLN:N	2.21	0.73
1:K:102:THR:HA	2:L:170:VAL:HA	1.71	0.73
2:J:226:THR:HG22	2:J:253:THR:HB	1.69	0.73
2:P:226:THR:HG22	2:P:253:THR:HB	1.71	0.73
2:N:5:THR:HG22	2:N:9:THR:O	1.89	0.73
1:A:88:LYS:HB2	1:A:108:ILE:HG12	1.69	0.73
1:K:132:ARG:HG2	1:K:203:VAL:O	1.89	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:227:ARG:NH1	2:J:232:ILE:HG12	2.03	0.73
2:P:227:ARG:NH1	2:P:232:ILE:HG12	2.03	0.73
2:L:224:GLN:HG2	2:L:231:ILE:HD13	1.70	0.73
1:O:145:PRO:HA	1:O:170:MET:HA	1.68	0.73
2:P:135:ASN:HD21	2:P:138:ASN:HD21	1.33	0.73
1:M:157:ALA:HB3	1:M:181:ALA:HB1	1.71	0.73
2:L:227:ARG:NH1	2:L:232:ILE:HG12	2.03	0.73
2:H:217:PRO:O	2:H:219:GLN:N	2.22	0.73
1:E:52:PRO:HG2	1:E:55:PHE:CD1	2.24	0.73
2:L:5:THR:HG22	2:L:9:THR:O	1.89	0.73
2:L:219:GLN:HE21	2:L:262:GLN:HG2	1.54	0.73
1:M:102:THR:HA	2:N:170:VAL:HA	1.71	0.72
2:P:172:LEU:N	2:P:173:PRO:HD2	2.02	0.72
2:N:227:ARG:NH1	2:N:232:ILE:HG12	2.04	0.72
2:N:224:GLN:HG2	2:N:231:ILE:HD13	1.71	0.72
1:E:194:GLY:O	2:F:158:THR:HG21	1.90	0.72
1:E:88:LYS:HB2	1:E:108:ILE:HG12	1.72	0.72
2:L:226:THR:HG22	2:L:253:THR:HB	1.70	0.72
2:P:219:GLN:HE21	2:P:262:GLN:HG2	1.55	0.72
2:P:5:THR:HG22	2:P:9:THR:O	1.89	0.72
1:O:102:THR:HA	2:P:170:VAL:HA	1.71	0.72
2:N:219:GLN:HE21	2:N:262:GLN:HG2	1.54	0.72
2:J:190:SER:HB2	2:J:244:GLY:HA2	1.72	0.72
1:C:88:LYS:HB2	1:C:108:ILE:HG12	1.70	0.72
2:N:190:SER:HB2	2:N:244:GLY:HA2	1.72	0.72
2:J:219:GLN:HE21	2:J:262:GLN:HG2	1.54	0.72
2:P:224:GLN:HG2	2:P:231:ILE:HD13	1.72	0.72
1:O:141:THR:CA	1:O:174:THR:HG21	2.05	0.72
1:O:157:ALA:HB3	1:O:181:ALA:HB1	1.71	0.72
1:I:157:ALA:HB3	1:I:181:ALA:HB1	1.71	0.72
2:L:135:ASN:HD21	2:L:138:ASN:HD21	1.33	0.72
1:A:194:GLY:O	2:B:158:THR:HG21	1.90	0.72
1:G:9:VAL:HA	4:G:208:HOH:O	1.89	0.72
1:G:86:ASN:HD21	1:G:110:ARG:HE	1.38	0.72
2:D:120:ILE:HD13	2:D:126:ILE:HD12	1.71	0.72
2:L:190:SER:HB2	2:L:244:GLY:HA2	1.71	0.72
1:M:79:ARG:HA	1:M:147:PRO:HB2	1.72	0.72
2:B:28:VAL:HG21	2:B:34:LEU:HD13	1.70	0.72
1:M:132:ARG:HG2	1:M:203:VAL:O	1.89	0.71
2:J:224:GLN:HG2	2:J:231:ILE:HD13	1.71	0.71
2:D:172:LEU:O	2:D:173:PRO:C	2.28	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:218:ALA:HB2	2:F:266:GLY:CA	2.20	0.71
2:J:135:ASN:HD21	2:J:138:ASN:HD21	1.36	0.71
1:C:9:VAL:HA	4:C:208:HOH:O	1.91	0.71
2:H:59:GLN:HA	2:H:89:GLU:HG3	1.72	0.71
2:F:28:VAL:HG21	2:F:34:LEU:HD13	1.72	0.71
2:D:218:ALA:HB2	2:D:266:GLY:CA	2.20	0.71
1:O:79:ARG:HA	1:O:147:PRO:HB2	1.72	0.71
2:P:190:SER:HB2	2:P:244:GLY:HA2	1.72	0.71
1:I:132:ARG:HG2	1:I:203:VAL:O	1.90	0.71
1:O:132:ARG:HG2	1:O:203:VAL:O	1.89	0.71
1:M:97:LYS:HB3	1:M:102:THR:HG21	1.72	0.71
2:D:201:THR:HG21	2:D:206:ASN:HA	1.71	0.71
2:H:218:ALA:HB2	2:H:266:GLY:CA	2.21	0.71
1:I:97:LYS:HB3	1:I:102:THR:HG21	1.72	0.71
2:F:201:THR:HG21	2:F:206:ASN:HA	1.73	0.71
1:K:97:LYS:HB3	1:K:102:THR:HG21	1.72	0.70
2:F:240:LEU:HD11	2:F:250:LEU:HD22	1.73	0.70
1:G:135:ARG:HH22	1:G:181:ALA:HB1	1.56	0.70
2:F:59:GLN:HA	2:F:89:GLU:HG3	1.71	0.70
1:O:145:PRO:O	1:O:170:MET:HG3	1.91	0.70
1:K:79:ARG:HA	1:K:147:PRO:HB2	1.71	0.70
1:O:97:LYS:HB3	1:O:102:THR:HG21	1.72	0.70
1:K:163:GLU:O	1:K:175:VAL:HG21	1.91	0.70
1:I:107:ILE:H	1:I:107:ILE:HD12	1.56	0.70
2:L:166:ARG:HG2	2:L:182:PRO:HB2	1.74	0.70
2:H:201:THR:HG21	2:H:206:ASN:HA	1.74	0.70
2:H:28:VAL:HG21	2:H:34:LEU:HD13	1.72	0.70
2:D:28:VAL:HG21	2:D:34:LEU:HD13	1.74	0.70
2:P:162:ASP:HB3	2:P:186:TYR:CE1	2.27	0.70
2:H:136:ASN:HD22	2:H:137:TYR:N	1.89	0.70
1:G:194:GLY:O	2:H:158:THR:HG21	1.91	0.70
2:P:166:ARG:HG2	2:P:182:PRO:HB2	1.74	0.70
1:O:107:ILE:HD12	1:O:107:ILE:H	1.57	0.70
1:G:32:LEU:HD22	1:G:54:LEU:HD11	1.73	0.70
2:N:162:ASP:HB3	2:N:186:TYR:CE1	2.27	0.70
1:I:163:GLU:O	1:I:175:VAL:HG21	1.92	0.70
1:M:107:ILE:HD12	1:M:107:ILE:H	1.57	0.70
2:P:206:ASN:ND2	2:P:234:ALA:HB3	2.07	0.70
2:J:206:ASN:ND2	2:J:234:ALA:HB3	2.07	0.70
1:O:102:THR:HB	2:P:168:VAL:CG2	2.22	0.70
2:L:182:PRO:O	2:L:183:LEU:HG	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:59:GLN:HA	2:D:89:GLU:HG3	1.74	0.70
1:C:185:ILE:HB	1:C:202:GLY:HA3	1.74	0.70
2:B:172:LEU:O	2:B:173:PRO:C	2.30	0.69
2:B:218:ALA:HB2	2:B:266:GLY:CA	2.22	0.69
2:J:209:PHE:CE2	2:J:234:ALA:HB2	2.27	0.69
2:B:263:VAL:HG23	4:B:529:HOH:O	1.92	0.69
1:I:157:ALA:O	1:I:184:ASN:HB3	1.92	0.69
1:E:188:ARG:HE	1:E:196:LEU:HD22	1.56	0.69
2:N:182:PRO:O	2:N:183:LEU:HG	1.92	0.69
2:B:201:THR:HG21	2:B:206:ASN:HA	1.74	0.69
1:E:135:ARG:HH22	1:E:181:ALA:HB1	1.57	0.69
1:A:193:TYR:O	2:B:158:THR:HG22	1.92	0.69
1:K:157:ALA:O	1:K:184:ASN:HB3	1.92	0.69
1:M:145:PRO:O	1:M:170:MET:HG3	1.91	0.69
2:B:172:LEU:N	2:B:173:PRO:HD2	2.07	0.69
2:N:171:THR:C	2:N:173:PRO:HD2	2.13	0.69
2:B:59:GLN:HA	2:B:89:GLU:HG3	1.73	0.69
2:J:193:LEU:HB3	2:J:240:LEU:HD12	1.74	0.69
2:J:126:ILE:HB	2:J:148:ILE:HG22	1.74	0.69
2:J:166:ARG:HG2	2:J:182:PRO:HB2	1.74	0.69
1:I:102:THR:HB	2:J:168:VAL:CG2	2.22	0.69
2:N:193:LEU:HB3	2:N:240:LEU:HD12	1.75	0.69
2:N:209:PHE:CE2	2:N:234:ALA:HB2	2.27	0.69
2:J:162:ASP:HB3	2:J:186:TYR:CE1	2.27	0.69
2:J:182:PRO:O	2:J:183:LEU:HG	1.92	0.69
1:K:145:PRO:O	1:K:170:MET:HG3	1.92	0.69
2:N:126:ILE:HB	2:N:148:ILE:HG22	1.74	0.69
2:L:162:ASP:HB3	2:L:186:TYR:CE1	2.27	0.69
2:L:206:ASN:ND2	2:L:234:ALA:HB3	2.07	0.69
1:O:157:ALA:O	1:O:184:ASN:HB3	1.92	0.69
1:K:107:ILE:HD12	1:K:107:ILE:H	1.56	0.69
2:N:206:ASN:ND2	2:N:234:ALA:HB3	2.07	0.69
2:L:209:PHE:CE2	2:L:234:ALA:HB2	2.27	0.69
2:L:126:ILE:HB	2:L:148:ILE:HG22	1.74	0.69
1:M:157:ALA:O	1:M:184:ASN:HB3	1.93	0.69
1:M:102:THR:HB	2:N:168:VAL:CG2	2.22	0.69
1:I:91:PRO:HG3	1:I:105:LEU:O	1.93	0.69
1:I:145:PRO:O	1:I:170:MET:HG3	1.91	0.69
1:A:32:LEU:HD22	1:A:54:LEU:HD11	1.74	0.69
1:I:79:ARG:HA	1:I:147:PRO:HB2	1.72	0.69
1:K:102:THR:HB	2:L:168:VAL:CG2	2.21	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:135:ARG:HH22	1:C:181:ALA:HB1	1.57	0.69
2:L:193:LEU:HB3	2:L:240:LEU:HD12	1.75	0.69
2:F:5:THR:HG23	2:F:7:ASN:H	1.57	0.69
1:C:86:ASN:HD21	1:C:110:ARG:HE	1.39	0.69
2:N:166:ARG:HG2	2:N:182:PRO:HB2	1.75	0.69
2:L:59:GLN:HG3	2:L:143:GLN:HE21	1.57	0.69
1:G:185:ILE:HB	1:G:202:GLY:HA3	1.75	0.69
1:A:135:ARG:HH22	1:A:181:ALA:HB1	1.57	0.68
1:C:135:ARG:NH1	1:C:177:LEU:HD21	2.08	0.68
2:P:209:PHE:CE2	2:P:234:ALA:HB2	2.27	0.68
2:H:172:LEU:O	2:H:173:PRO:C	2.30	0.68
2:H:172:LEU:N	2:H:173:PRO:HD2	2.08	0.68
1:I:8:ARG:HB3	1:I:8:ARG:NH1	2.07	0.68
1:K:143:ILE:HG13	1:K:172:GLU:HB3	1.76	0.68
1:M:163:GLU:O	1:M:175:VAL:HG21	1.92	0.68
1:O:163:GLU:O	1:O:175:VAL:HG21	1.91	0.68
1:O:8:ARG:HB3	1:O:8:ARG:NH1	2.08	0.68
1:C:32:LEU:HD22	1:C:54:LEU:HD11	1.75	0.68
2:P:126:ILE:HB	2:P:148:ILE:HG22	1.74	0.68
2:L:71:PHE:HA	2:L:110:THR:O	1.93	0.68
2:J:171:THR:C	2:J:173:PRO:HD2	2.14	0.68
2:P:59:GLN:HG3	2:P:143:GLN:HE21	1.58	0.68
2:D:172:LEU:N	2:D:173:PRO:HD2	2.09	0.68
1:M:91:PRO:HG3	1:M:105:LEU:O	1.93	0.68
2:J:59:GLN:HG3	2:J:143:GLN:HE21	1.58	0.68
2:N:20:VAL:HG21	2:N:42:ILE:HD11	1.76	0.68
1:A:185:ILE:HB	1:A:202:GLY:HA3	1.75	0.68
2:F:136:ASN:HD22	2:F:137:TYR:N	1.92	0.68
2:F:263:VAL:HG23	4:F:546:HOH:O	1.93	0.68
2:N:59:GLN:HG3	2:N:143:GLN:HE21	1.59	0.68
2:P:182:PRO:O	2:P:183:LEU:HG	1.93	0.68
1:O:91:PRO:HG3	1:O:105:LEU:O	1.93	0.68
1:M:8:ARG:NH1	1:M:8:ARG:HB3	2.09	0.68
1:K:8:ARG:NH1	1:K:8:ARG:HB3	2.08	0.68
1:M:143:ILE:HG13	1:M:172:GLU:HB3	1.76	0.68
1:C:188:ARG:NH1	1:C:199:LYS:N	2.42	0.68
2:L:171:THR:C	2:L:173:PRO:HD2	2.13	0.68
2:B:136:ASN:HD22	2:B:137:TYR:N	1.91	0.68
1:C:126:GLN:HG2	1:C:126:GLN:O	1.94	0.68
2:H:267:ASN:HD22	2:H:267:ASN:N	1.92	0.67
1:G:188:ARG:HE	1:G:196:LEU:HD22	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:136:ASN:HD22	2:D:137:TYR:N	1.91	0.67
1:E:185:ILE:HB	1:E:202:GLY:HA3	1.76	0.67
1:A:126:GLN:O	1:A:126:GLN:HG2	1.93	0.67
1:I:77:GLN:HA	1:I:77:GLN:HE21	1.59	0.67
1:G:193:TYR:O	2:H:158:THR:HG22	1.95	0.67
1:A:188:ARG:HE	1:A:196:LEU:HD22	1.58	0.67
2:H:240:LEU:HD11	2:H:250:LEU:HD22	1.74	0.67
1:C:193:TYR:O	2:D:158:THR:HG22	1.95	0.67
2:J:71:PHE:HA	2:J:110:THR:O	1.95	0.67
1:O:143:ILE:HG13	1:O:172:GLU:HB3	1.76	0.67
1:E:188:ARG:NH1	1:E:199:LYS:N	2.42	0.67
2:N:5:THR:HG23	2:N:7:ASN:H	1.60	0.67
1:I:143:ILE:HG13	1:I:172:GLU:HB3	1.77	0.67
2:J:210:THR:HG22	2:J:221:VAL:O	1.95	0.67
1:C:188:ARG:HE	1:C:196:LEU:HD22	1.60	0.67
1:K:91:PRO:HG3	1:K:105:LEU:O	1.94	0.67
1:M:103:LEU:C	2:N:168:VAL:HG23	2.15	0.67
2:P:171:THR:C	2:P:173:PRO:HD2	2.13	0.67
2:P:5:THR:HG23	2:P:7:ASN:H	1.60	0.67
1:E:32:LEU:HD22	1:E:54:LEU:HD11	1.75	0.67
2:N:210:THR:HG22	2:N:221:VAL:O	1.95	0.67
2:D:240:LEU:HD11	2:D:250:LEU:HD22	1.75	0.67
1:M:177:LEU:HD11	1:M:181:ALA:HB3	1.77	0.67
1:G:188:ARG:NH1	1:G:199:LYS:N	2.42	0.67
2:B:67:VAL:CG2	2:B:126:ILE:HG23	2.25	0.67
2:F:193:LEU:HD12	2:F:243:VAL:HG21	1.77	0.67
1:O:103:LEU:C	2:P:168:VAL:HG23	2.15	0.67
2:P:193:LEU:HB3	2:P:240:LEU:HD12	1.76	0.67
2:N:71:PHE:HA	2:N:110:THR:O	1.94	0.67
1:G:154:GLU:OE1	1:G:188:ARG:HD3	1.95	0.66
2:P:210:THR:HG22	2:P:221:VAL:O	1.95	0.66
2:P:71:PHE:HA	2:P:110:THR:O	1.94	0.66
1:O:177:LEU:HD11	1:O:181:ALA:HB3	1.78	0.66
1:K:3:ALA:HB1	2:L:160:GLY:O	1.96	0.66
2:F:67:VAL:CG2	2:F:126:ILE:HG23	2.26	0.66
2:F:221:VAL:HG12	2:F:222:GLY:N	2.10	0.66
2:P:117:GLY:O	2:P:155:VAL:HA	1.96	0.66
1:A:188:ARG:NH1	1:A:199:LYS:N	2.43	0.66
2:F:172:LEU:N	2:F:173:PRO:HD2	2.09	0.66
2:L:117:GLY:O	2:L:155:VAL:HA	1.95	0.66
1:G:135:ARG:NH1	1:G:177:LEU:HD21	2.11	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:ARG:NH1	1:A:177:LEU:HD21	2.10	0.66
2:H:219:GLN:HB3	4:H:644:HOH:O	1.95	0.66
1:M:176:LYS:O	1:M:178:PRO:HD3	1.96	0.66
1:M:77:GLN:HA	1:M:77:GLN:HE21	1.60	0.66
1:E:193:TYR:O	2:F:158:THR:HG22	1.95	0.66
2:D:267:ASN:N	2:D:267:ASN:HD22	1.93	0.66
1:C:154:GLU:OE1	1:C:188:ARG:HD3	1.95	0.66
1:I:103:LEU:C	2:J:168:VAL:HG23	2.15	0.66
2:L:268:VAL:O	2:L:269:GLN:HG3	1.95	0.66
1:K:77:GLN:HA	1:K:77:GLN:HE21	1.61	0.66
2:F:172:LEU:O	2:F:173:PRO:C	2.32	0.66
1:K:103:LEU:C	2:L:168:VAL:HG23	2.16	0.66
2:D:67:VAL:CG2	2:D:126:ILE:HG23	2.26	0.66
2:J:117:GLY:O	2:J:155:VAL:HA	1.96	0.66
2:B:193:LEU:HD12	2:B:243:VAL:HG21	1.78	0.66
2:D:5:THR:HG23	2:D:7:ASN:H	1.59	0.66
2:N:21:TYR:HB3	2:N:151:ASN:HD21	1.60	0.66
2:P:64:TYR:HB2	2:P:125:LEU:O	1.96	0.66
2:L:20:VAL:HG21	2:L:42:ILE:HD11	1.77	0.66
2:P:21:TYR:HB3	2:P:151:ASN:HD21	1.60	0.66
2:B:221:VAL:HG12	2:B:222:GLY:N	2.11	0.66
2:B:240:LEU:HD11	2:B:250:LEU:HD22	1.76	0.66
2:J:183:LEU:O	2:J:249:SER:HA	1.96	0.66
2:P:20:VAL:HG21	2:P:42:ILE:HD11	1.77	0.66
2:B:5:THR:HG23	2:B:7:ASN:H	1.59	0.66
2:P:38:LEU:C	2:P:40:THR:H	1.99	0.66
1:K:176:LYS:O	1:K:178:PRO:HD3	1.96	0.66
2:H:221:VAL:HG12	2:H:222:GLY:N	2.09	0.66
1:O:176:LYS:O	1:O:178:PRO:HD3	1.96	0.66
1:I:23:THR:OG1	1:I:62:GLU:HG2	1.96	0.65
1:K:112:LYS:NZ	1:K:166:LEU:HD22	2.11	0.65
2:J:268:VAL:O	2:J:269:GLN:HG3	1.96	0.65
2:N:117:GLY:O	2:N:155:VAL:HA	1.96	0.65
2:P:206:ASN:HD21	2:P:234:ALA:HB3	1.61	0.65
2:J:20:VAL:HG21	2:J:42:ILE:HD11	1.76	0.65
1:E:199:LYS:O	1:E:200:MET:HG3	1.96	0.65
2:N:268:VAL:O	2:N:269:GLN:HG3	1.96	0.65
1:O:3:ALA:HB1	2:P:160:GLY:O	1.96	0.65
2:J:206:ASN:HD21	2:J:234:ALA:HB3	1.61	0.65
1:K:177:LEU:HD11	1:K:181:ALA:HB3	1.78	0.65
1:K:23:THR:OG1	1:K:62:GLU:HG2	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:112:LYS:NZ	1:I:166:LEU:HD22	2.12	0.65
2:H:5:THR:HG23	2:H:7:ASN:H	1.60	0.65
2:L:21:TYR:HB3	2:L:151:ASN:HD21	1.60	0.65
2:P:268:VAL:O	2:P:269:GLN:HG3	1.95	0.65
1:M:193:TYR:CE2	2:N:155:VAL:HG21	2.32	0.65
1:I:3:ALA:HB1	2:J:160:GLY:O	1.95	0.65
1:A:199:LYS:O	1:A:200:MET:HG3	1.97	0.65
1:O:193:TYR:CE2	2:P:155:VAL:HG21	2.32	0.65
1:K:193:TYR:CE2	2:L:155:VAL:HG21	2.32	0.65
1:E:135:ARG:NH1	1:E:177:LEU:HD21	2.10	0.65
1:O:79:ARG:HD3	1:O:169:PRO:HB2	1.78	0.65
1:G:97:LYS:HD3	1:G:100:GLU:OE1	1.97	0.65
2:J:21:TYR:HB3	2:J:151:ASN:HD21	1.61	0.65
1:I:177:LEU:HD11	1:I:181:ALA:HB3	1.78	0.65
2:B:171:THR:C	2:B:173:PRO:HD2	2.17	0.65
2:L:183:LEU:O	2:L:249:SER:HA	1.97	0.65
1:M:23:THR:OG1	1:M:62:GLU:HG2	1.97	0.65
2:D:221:VAL:HG12	2:D:222:GLY:N	2.11	0.65
1:K:79:ARG:HD3	1:K:169:PRO:HB2	1.78	0.65
1:M:3:ALA:HB1	2:N:160:GLY:O	1.96	0.65
2:N:64:TYR:HB2	2:N:125:LEU:O	1.96	0.65
2:L:64:TYR:HB2	2:L:125:LEU:O	1.96	0.65
2:H:67:VAL:CG2	2:H:126:ILE:HG23	2.27	0.65
2:L:163:VAL:HA	2:L:185:VAL:HG12	1.79	0.65
1:M:79:ARG:HD3	1:M:169:PRO:HB2	1.78	0.65
2:N:38:LEU:C	2:N:40:THR:H	1.99	0.65
2:B:182:PRO:HG3	4:B:512:HOH:O	1.97	0.65
2:B:267:ASN:HD22	2:B:267:ASN:N	1.92	0.65
1:C:197:THR:HB	1:C:198:PRO:HD2	1.79	0.65
1:O:23:THR:OG1	1:O:62:GLU:HG2	1.97	0.65
2:P:183:LEU:O	2:P:249:SER:HA	1.97	0.64
1:K:97:LYS:HD2	2:L:170:VAL:CG2	2.26	0.64
1:K:149:TYR:HB3	1:K:166:LEU:CD1	2.27	0.64
2:J:163:VAL:HA	2:J:185:VAL:HG12	1.79	0.64
2:P:163:VAL:HA	2:P:185:VAL:HG12	1.79	0.64
2:J:5:THR:HG23	2:J:7:ASN:H	1.60	0.64
2:L:27:VAL:HG12	4:L:505:HOH:O	1.97	0.64
1:G:199:LYS:O	1:G:200:MET:HG3	1.97	0.64
1:A:155:LEU:O	1:A:162:LEU:HB2	1.97	0.64
2:L:38:LEU:C	2:L:40:THR:H	2.00	0.64
1:K:158:GLY:HA3	1:K:184:ASN:HD22	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:210:THR:HG22	2:L:221:VAL:O	1.96	0.64
1:E:101:ASN:HB3	2:F:171:THR:HG23	1.79	0.64
1:G:155:LEU:O	1:G:162:LEU:HB2	1.97	0.64
2:D:172:LEU:O	2:D:174:ASP:N	2.31	0.64
2:D:163:VAL:HG22	2:D:185:VAL:HG12	1.80	0.64
1:O:144:ASN:HB3	1:O:167:VAL:HG12	1.79	0.64
1:G:197:THR:HB	1:G:198:PRO:HD2	1.78	0.64
1:C:155:LEU:O	1:C:162:LEU:HB2	1.97	0.64
1:M:188:ARG:HH21	1:M:196:LEU:CD1	2.11	0.64
2:J:59:GLN:HG2	2:J:132:ARG:HD2	1.79	0.64
1:M:144:ASN:HB3	1:M:167:VAL:HG12	1.78	0.64
1:G:126:GLN:O	1:G:126:GLN:HG2	1.97	0.64
1:O:135:ARG:NH2	1:O:177:LEU:HD21	2.12	0.64
1:I:193:TYR:CE2	2:J:155:VAL:HG21	2.32	0.64
2:D:59:GLN:CG	2:D:132:ARG:HD2	2.28	0.64
2:L:206:ASN:HD21	2:L:234:ALA:HB3	1.61	0.64
1:E:97:LYS:HD3	1:E:100:GLU:OE1	1.97	0.64
2:F:171:THR:C	2:F:173:PRO:HD2	2.18	0.64
1:I:97:LYS:HD2	2:J:170:VAL:CG2	2.26	0.64
2:J:96:ASN:N	2:J:96:ASN:ND2	2.45	0.64
1:E:126:GLN:O	1:E:126:GLN:HG2	1.97	0.64
1:M:158:GLY:HA3	1:M:184:ASN:HD22	1.62	0.64
2:L:5:THR:HG23	2:L:7:ASN:H	1.61	0.64
2:N:59:GLN:HG2	2:N:132:ARG:HD2	1.79	0.64
1:I:176:LYS:O	1:I:178:PRO:HD3	1.96	0.64
1:O:158:GLY:HA3	1:O:184:ASN:HD22	1.62	0.64
1:C:101:ASN:HB3	2:D:171:THR:HG23	1.80	0.64
1:A:197:THR:HB	1:A:198:PRO:HD2	1.78	0.64
1:I:144:ASN:HB3	1:I:167:VAL:HG12	1.79	0.64
1:O:77:GLN:HA	1:O:77:GLN:HE21	1.62	0.64
1:A:154:GLU:OE1	1:A:188:ARG:HD3	1.97	0.64
1:E:154:GLU:OE1	1:E:188:ARG:HD3	1.98	0.64
2:B:172:LEU:O	2:B:174:ASP:N	2.31	0.64
2:N:183:LEU:O	2:N:249:SER:HA	1.97	0.64
2:L:163:VAL:HG13	2:L:185:VAL:HG12	1.80	0.64
2:N:163:VAL:HA	2:N:185:VAL:HG12	1.79	0.64
2:P:96:ASN:ND2	2:P:96:ASN:N	2.45	0.64
1:E:138:ASN:O	1:E:177:LEU:N	2.31	0.64
2:H:172:LEU:O	2:H:174:ASP:N	2.31	0.63
2:F:172:LEU:O	2:F:174:ASP:N	2.31	0.63
1:G:138:ASN:O	1:G:177:LEU:N	2.30	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:59:GLN:HG2	2:L:132:ARG:HD2	1.79	0.63
2:J:64:TYR:HB2	2:J:125:LEU:O	1.97	0.63
1:K:144:ASN:HB3	1:K:167:VAL:HG12	1.79	0.63
2:J:38:LEU:C	2:J:40:THR:H	2.01	0.63
1:K:135:ARG:NH2	1:K:177:LEU:HD21	2.13	0.63
1:I:158:GLY:HA3	1:I:184:ASN:HD22	1.63	0.63
1:E:155:LEU:O	1:E:162:LEU:HB2	1.97	0.63
1:M:97:LYS:HD2	2:N:170:VAL:CG2	2.26	0.63
2:N:96:ASN:N	2:N:96:ASN:ND2	2.46	0.63
1:O:126:GLN:HG3	4:O:207:HOH:O	1.97	0.63
1:C:58:LYS:HG3	4:C:224:HOH:O	1.97	0.63
1:C:199:LYS:O	1:C:200:MET:HG3	1.97	0.63
2:H:171:THR:C	2:H:173:PRO:HD2	2.19	0.63
1:M:112:LYS:NZ	1:M:166:LEU:HD22	2.12	0.63
2:P:20:VAL:HG12	2:P:22:VAL:HG13	1.81	0.63
1:M:135:ARG:NH2	1:M:177:LEU:HD21	2.13	0.63
1:O:97:LYS:HD2	2:P:170:VAL:CG2	2.26	0.63
1:I:149:TYR:HB3	1:I:166:LEU:CD1	2.27	0.63
1:G:32:LEU:HB2	1:G:90:ILE:HB	1.81	0.63
1:I:79:ARG:HD3	1:I:169:PRO:HB2	1.78	0.63
2:J:14:GLY:HA2	2:J:142:PHE:CE2	2.33	0.63
1:I:135:ARG:NH2	1:I:177:LEU:HD21	2.13	0.63
1:M:149:TYR:HB3	1:M:166:LEU:CD1	2.28	0.63
2:N:163:VAL:HG13	2:N:185:VAL:HG12	1.80	0.63
1:C:97:LYS:HD3	1:C:100:GLU:OE1	1.97	0.63
1:A:122:LEU:HD11	1:A:130:LYS:CE	2.26	0.63
2:D:171:THR:C	2:D:173:PRO:HD2	2.19	0.63
1:M:19:GLN:HA	1:M:65:LEU:O	1.98	0.63
1:O:112:LYS:NZ	1:O:166:LEU:HD22	2.12	0.63
1:A:97:LYS:HD3	1:A:100:GLU:OE1	1.98	0.63
2:D:38:LEU:C	2:D:40:THR:H	2.02	0.63
1:E:197:THR:HB	1:E:198:PRO:HD2	1.79	0.63
1:A:101:ASN:HB3	2:B:171:THR:HG23	1.81	0.63
1:A:138:ASN:O	1:A:177:LEU:N	2.31	0.63
2:B:163:VAL:HG22	2:B:185:VAL:HG12	1.80	0.63
1:I:140:LEU:HD12	1:I:162:LEU:CD1	2.29	0.63
1:K:19:GLN:HA	1:K:65:LEU:O	1.99	0.63
1:I:19:GLN:HA	1:I:65:LEU:O	1.98	0.63
1:C:138:ASN:O	1:C:177:LEU:N	2.31	0.63
2:D:193:LEU:HD12	2:D:243:VAL:HG21	1.81	0.63
2:N:206:ASN:HD21	2:N:234:ALA:HB3	1.61	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:188:ARG:HH21	1:I:196:LEU:CD1	2.12	0.63
2:P:133:ASN:OD1	2:P:142:PHE:HB2	1.99	0.63
2:F:267:ASN:HD22	2:F:267:ASN:N	1.94	0.63
1:O:19:GLN:HA	1:O:65:LEU:O	1.98	0.62
2:L:20:VAL:HG12	2:L:22:VAL:HG13	1.81	0.62
2:P:14:GLY:HA2	2:P:142:PHE:CE2	2.34	0.62
2:L:112:VAL:HA	4:L:509:HOH:O	1.99	0.62
2:H:163:VAL:HG22	2:H:185:VAL:HG12	1.79	0.62
1:C:97:LYS:HD3	1:C:100:GLU:CD	2.20	0.62
2:D:211:ASN:OD1	2:D:268:VAL:HA	2.00	0.62
2:P:59:GLN:HG2	2:P:132:ARG:HD2	1.79	0.62
2:F:116:GLY:HA2	2:F:189:LYS:HE2	1.80	0.62
1:K:140:LEU:HD12	1:K:162:LEU:CD1	2.30	0.62
1:I:107:ILE:N	1:I:107:ILE:HD12	2.14	0.62
1:C:72:ASN:O	1:C:74:GLN:HG3	1.98	0.62
1:M:185:ILE:HG21	1:M:202:GLY:HA3	1.82	0.62
1:O:149:TYR:HB3	1:O:166:LEU:CD1	2.27	0.62
2:B:255:ASN:N	2:B:255:ASN:ND2	2.47	0.62
2:J:163:VAL:HG13	2:J:185:VAL:HG12	1.81	0.62
1:K:185:ILE:HG21	1:K:202:GLY:HA3	1.82	0.62
2:B:67:VAL:HG21	2:B:126:ILE:CG2	2.30	0.62
2:F:67:VAL:HG21	2:F:126:ILE:CG2	2.30	0.62
2:P:163:VAL:HG13	2:P:185:VAL:HG12	1.81	0.62
1:E:122:LEU:HD11	1:E:130:LYS:CE	2.25	0.62
2:D:116:GLY:HA2	2:D:189:LYS:HE2	1.82	0.62
1:E:72:ASN:O	1:E:74:GLN:HG3	1.98	0.62
1:A:32:LEU:HB2	1:A:90:ILE:HB	1.82	0.62
2:N:133:ASN:OD1	2:N:142:PHE:HB2	2.00	0.62
2:H:185:VAL:HG11	2:H:276:PHE:CE2	2.35	0.62
1:K:188:ARG:HH21	1:K:196:LEU:CD1	2.13	0.62
1:A:97:LYS:HD3	1:A:100:GLU:CD	2.20	0.62
2:B:185:VAL:HG11	2:B:276:PHE:CE2	2.35	0.62
1:O:188:ARG:HH21	1:O:196:LEU:CD1	2.13	0.61
2:H:193:LEU:HD12	2:H:243:VAL:HG21	1.81	0.61
2:L:14:GLY:HA2	2:L:142:PHE:CE2	2.35	0.61
1:G:101:ASN:HB3	2:H:171:THR:HG23	1.81	0.61
2:B:59:GLN:CG	2:B:132:ARG:HD2	2.29	0.61
2:H:59:GLN:CG	2:H:132:ARG:HD2	2.29	0.61
2:J:20:VAL:HG12	2:J:22:VAL:HG13	1.81	0.61
1:E:97:LYS:HD3	1:E:100:GLU:CD	2.20	0.61
1:O:185:ILE:HG21	1:O:202:GLY:HA3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:226:THR:CG2	2:L:255:ASN:HD21	2.13	0.61
2:F:59:GLN:CG	2:F:132:ARG:HD2	2.29	0.61
1:G:97:LYS:HD3	1:G:100:GLU:CD	2.21	0.61
2:D:67:VAL:HG21	2:D:126:ILE:CG2	2.31	0.61
2:H:38:LEU:C	2:H:40:THR:H	2.02	0.61
1:O:107:ILE:HD12	1:O:107:ILE:N	2.15	0.61
2:F:163:VAL:HG22	2:F:185:VAL:HG12	1.81	0.61
2:H:201:THR:CG2	2:H:206:ASN:HD22	2.13	0.61
2:H:255:ASN:ND2	2:H:255:ASN:N	2.48	0.61
2:N:219:GLN:NE2	2:N:262:GLN:HG2	2.15	0.61
2:J:133:ASN:OD1	2:J:142:PHE:HB2	2.00	0.61
1:I:185:ILE:HG21	1:I:202:GLY:HA3	1.82	0.61
1:M:140:LEU:HD12	1:M:162:LEU:CD1	2.30	0.61
1:K:107:ILE:N	1:K:107:ILE:HD12	2.15	0.61
2:L:219:GLN:NE2	2:L:262:GLN:HG2	2.15	0.61
1:E:32:LEU:HB2	1:E:90:ILE:HB	1.83	0.61
2:N:226:THR:CG2	2:N:255:ASN:HD21	2.12	0.61
2:D:185:VAL:HG11	2:D:276:PHE:CE2	2.36	0.61
2:F:38:LEU:C	2:F:40:THR:H	2.03	0.61
2:B:38:LEU:C	2:B:40:THR:H	2.04	0.61
1:O:140:LEU:HD12	1:O:162:LEU:CD1	2.30	0.61
1:M:107:ILE:HD12	1:M:107:ILE:N	2.14	0.61
2:N:59:GLN:CG	2:N:132:ARG:HD2	2.31	0.61
1:A:72:ASN:O	1:A:74:GLN:HG3	2.00	0.61
1:K:162:LEU:HB3	1:K:175:VAL:HG11	1.82	0.61
1:G:122:LEU:HD11	1:G:130:LYS:CE	2.24	0.61
2:P:219:GLN:NE2	2:P:262:GLN:HG2	2.16	0.61
1:C:32:LEU:HB2	1:C:90:ILE:HB	1.81	0.61
1:I:162:LEU:HB3	1:I:175:VAL:HG11	1.83	0.60
1:G:188:ARG:HH12	1:G:199:LYS:N	1.99	0.60
2:N:212:THR:HG21	2:N:271:ILE:HD11	1.83	0.60
1:I:27:GLU:HG2	4:I:206:HOH:O	2.00	0.60
1:A:9:VAL:HG22	4:A:209:HOH:O	2.01	0.60
1:O:130:LYS:HA	1:O:203:VAL:HG21	1.83	0.60
1:O:162:LEU:HB3	1:O:175:VAL:HG11	1.82	0.60
1:C:122:LEU:HD11	1:C:130:LYS:CE	2.26	0.60
2:J:226:THR:CG2	2:J:255:ASN:HD21	2.13	0.60
2:F:185:VAL:HG11	2:F:276:PHE:CE2	2.36	0.60
2:J:59:GLN:CG	2:J:132:ARG:HD2	2.31	0.60
2:N:14:GLY:HA2	2:N:142:PHE:CE2	2.36	0.60
2:L:133:ASN:OD1	2:L:142:PHE:HB2	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:188:ARG:HH12	1:C:199:LYS:N	2.00	0.60
1:K:31:TYR:CB	1:K:89:ALA:HB1	2.32	0.60
2:D:138:ASN:C	2:D:138:ASN:ND2	2.54	0.60
1:G:72:ASN:O	1:G:74:GLN:HG3	2.00	0.60
2:H:138:ASN:ND2	2:H:140:ASP:H	2.00	0.60
2:P:59:GLN:CG	2:P:132:ARG:HD2	2.31	0.60
2:N:20:VAL:HG12	2:N:22:VAL:HG13	1.81	0.60
2:D:227:ARG:HA	2:D:251:GLY:O	2.01	0.60
2:H:116:GLY:HA2	2:H:189:LYS:HE2	1.82	0.60
1:I:102:THR:HB	2:J:168:VAL:HG22	1.82	0.60
2:J:212:THR:HG21	2:J:271:ILE:HD11	1.84	0.60
2:D:24:LEU:HA	4:D:648:HOH:O	2.02	0.60
1:K:130:LYS:HA	1:K:203:VAL:HG21	1.82	0.60
1:M:130:LYS:HA	1:M:203:VAL:HG21	1.82	0.60
1:E:188:ARG:HH12	1:E:199:LYS:N	1.99	0.60
1:K:28:ASN:H	1:K:28:ASN:ND2	2.00	0.60
2:B:184:THR:HG22	2:B:249:SER:HA	1.84	0.60
2:J:219:GLN:NE2	2:J:262:GLN:HG2	2.16	0.60
1:M:162:LEU:HB3	1:M:175:VAL:HG11	1.82	0.60
1:I:130:LYS:HA	1:I:203:VAL:HG21	1.82	0.60
1:O:102:THR:HB	2:P:168:VAL:HG22	1.83	0.60
2:P:226:THR:CG2	2:P:255:ASN:HD21	2.13	0.60
2:J:98:ARG:HH11	2:J:98:ARG:HG3	1.67	0.60
2:L:52:ILE:HG23	2:L:137:TYR:HB2	1.84	0.60
1:M:28:ASN:H	1:M:28:ASN:ND2	2.00	0.60
2:D:184:THR:HG22	2:D:249:SER:HA	1.84	0.60
2:P:212:THR:HG21	2:P:271:ILE:HD11	1.84	0.60
2:L:212:THR:HG21	2:L:271:ILE:HD11	1.84	0.60
2:L:96:ASN:ND2	2:L:96:ASN:N	2.46	0.60
2:B:49:PRO:HD2	2:B:98:ARG:CZ	2.32	0.60
1:K:160:ARG:HB3	1:K:181:ALA:HB2	1.84	0.60
1:A:188:ARG:HH12	1:A:199:LYS:N	1.99	0.60
1:O:101:ASN:HB2	2:P:172:LEU:HA	1.83	0.60
1:K:101:ASN:HB2	2:L:172:LEU:HA	1.83	0.60
2:L:122:ALA:HA	2:L:150:ALA:O	2.02	0.60
2:B:116:GLY:HA2	2:B:189:LYS:HE2	1.82	0.60
1:O:31:TYR:CB	1:O:89:ALA:HB1	2.31	0.59
1:C:66:ARG:HG2	1:C:66:ARG:HH11	1.67	0.59
1:I:31:TYR:CB	1:I:89:ALA:HB1	2.32	0.59
1:K:88:LYS:HE3	1:K:90:ILE:HG12	1.84	0.59
2:B:113:SER:HB3	2:P:81:SER:N	2.10	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:211:ASN:OD1	2:H:268:VAL:HA	2.02	0.59
2:F:179:VAL:O	2:F:253:THR:HG23	2.02	0.59
1:K:102:THR:HB	2:L:168:VAL:HG22	1.82	0.59
2:H:227:ARG:HA	2:H:251:GLY:O	2.02	0.59
2:N:15:GLY:HA2	2:N:144:PHE:CD1	2.37	0.59
1:E:66:ARG:HG2	1:E:66:ARG:HH11	1.68	0.59
1:O:160:ARG:HB3	1:O:181:ALA:HB2	1.84	0.59
2:H:170:VAL:C	2:H:172:LEU:H	2.06	0.59
1:M:101:ASN:HB2	2:N:172:LEU:HA	1.82	0.59
2:J:46:ASN:CB	2:J:96:ASN:HA	2.32	0.59
1:I:28:ASN:H	1:I:28:ASN:ND2	1.99	0.59
2:P:207:SER:OG	2:P:233:PRO:HB3	2.03	0.59
2:B:28:VAL:O	2:B:156:VAL:HA	2.03	0.59
2:J:15:GLY:HA2	2:J:144:PHE:CD1	2.37	0.59
1:I:160:ARG:HB3	1:I:181:ALA:HB2	1.85	0.59
1:I:26:ASP:O	1:I:60:LYS:HB3	2.02	0.59
2:F:28:VAL:O	2:F:156:VAL:HA	2.03	0.59
2:H:131:LEU:HD23	2:H:131:LEU:C	2.23	0.59
1:E:102:THR:CA	2:F:171:THR:HG22	2.33	0.59
1:M:102:THR:HB	2:N:168:VAL:HG22	1.83	0.59
1:C:24:ASN:O	1:C:60:LYS:HA	2.03	0.59
1:O:100:GLU:HG2	2:P:172:LEU:HD12	1.85	0.59
1:E:24:ASN:O	1:E:60:LYS:HA	2.03	0.59
2:L:98:ARG:HG3	2:L:98:ARG:HH11	1.67	0.59
2:J:46:ASN:HB2	2:J:96:ASN:HA	1.85	0.59
2:L:15:GLY:HA2	2:L:144:PHE:CD1	2.38	0.59
1:A:155:LEU:HD12	1:A:187:TYR:HB3	1.85	0.59
2:F:211:ASN:OD1	2:F:268:VAL:HA	2.02	0.59
1:O:88:LYS:HE3	1:O:90:ILE:HG12	1.83	0.59
2:L:207:SER:OG	2:L:233:PRO:HB3	2.03	0.59
2:H:34:LEU:HB3	2:H:109:LEU:HB2	1.84	0.59
2:B:213:ALA:HB3	4:B:527:HOH:O	2.02	0.59
2:H:63:ALA:HB3	2:H:68:LEU:HD13	1.85	0.59
1:K:33:ILE:CG1	1:K:57:MET:HB2	2.33	0.59
1:M:31:TYR:CB	1:M:89:ALA:HB1	2.32	0.59
2:P:46:ASN:CB	2:P:96:ASN:HA	2.32	0.59
2:L:46:ASN:CB	2:L:96:ASN:HA	2.33	0.59
2:L:59:GLN:CG	2:L:132:ARG:HD2	2.32	0.59
2:F:49:PRO:HD2	2:F:98:ARG:CZ	2.33	0.59
1:M:160:ARG:HB3	1:M:181:ALA:HB2	1.85	0.59
1:G:156:ASN:C	1:G:158:GLY:H	2.06	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:227:ARG:C	2:N:229:GLY:H	2.07	0.59
2:B:59:GLN:HG3	2:B:143:GLN:HE21	1.68	0.59
1:C:135:ARG:NH2	1:C:181:ALA:HB1	2.18	0.59
2:P:15:GLY:HA2	2:P:144:PHE:CD1	2.38	0.59
2:B:227:ARG:HA	2:B:251:GLY:O	2.03	0.59
1:O:158:GLY:HA3	1:O:184:ASN:ND2	2.18	0.59
1:O:26:ASP:O	1:O:60:LYS:HB3	2.03	0.59
1:M:26:ASP:O	1:M:60:LYS:HB3	2.02	0.59
1:I:100:GLU:HG2	2:J:172:LEU:HD12	1.85	0.59
1:I:101:ASN:HB2	2:J:172:LEU:HA	1.83	0.59
1:I:101:ASN:HA	2:J:268:VAL:O	2.03	0.59
2:N:207:SER:OG	2:N:233:PRO:HB3	2.03	0.59
2:J:122:ALA:HA	2:J:150:ALA:O	2.02	0.59
2:P:52:ILE:HG23	2:P:137:TYR:HB2	1.84	0.59
2:D:131:LEU:C	2:D:131:LEU:HD23	2.23	0.59
2:L:43:PHE:CE2	2:L:102:PRO:HG3	2.37	0.59
1:I:23:THR:HG22	1:I:24:ASN:N	2.18	0.58
2:B:136:ASN:ND2	2:B:136:ASN:C	2.54	0.58
1:G:135:ARG:NH2	1:G:181:ALA:HB1	2.17	0.58
2:L:46:ASN:HB2	2:L:96:ASN:HA	1.85	0.58
2:J:207:SER:OG	2:J:233:PRO:HB3	2.03	0.58
2:D:28:VAL:O	2:D:156:VAL:HA	2.02	0.58
1:K:143:ILE:HA	1:K:172:GLU:CB	2.33	0.58
1:M:158:GLY:CA	1:M:184:ASN:HD22	2.16	0.58
1:I:143:ILE:HA	1:I:172:GLU:CB	2.33	0.58
1:I:33:ILE:CG1	1:I:57:MET:HB2	2.33	0.58
2:L:226:THR:HA	2:L:230:THR:O	2.03	0.58
2:D:201:THR:CG2	2:D:206:ASN:HD22	2.15	0.58
2:D:136:ASN:C	2:D:136:ASN:ND2	2.56	0.58
1:O:28:ASN:ND2	1:O:28:ASN:H	1.99	0.58
1:E:86:ASN:ND2	1:E:110:ARG:HE	2.01	0.58
2:F:227:ARG:HA	2:F:251:GLY:O	2.03	0.58
1:G:66:ARG:HG2	1:G:66:ARG:HH11	1.68	0.58
1:K:158:GLY:HA3	1:K:184:ASN:ND2	2.18	0.58
1:O:143:ILE:HA	1:O:172:GLU:CB	2.32	0.58
1:O:104:GLN:N	2:P:168:VAL:HG23	2.19	0.58
1:O:23:THR:HG22	1:O:24:ASN:N	2.18	0.58
2:J:227:ARG:C	2:J:229:GLY:H	2.07	0.58
1:O:101:ASN:HA	2:P:268:VAL:O	2.03	0.58
1:I:88:LYS:HE3	1:I:90:ILE:HG12	1.84	0.58
1:M:36:TRP:HH2	1:M:88:LYS:HE2	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:143:ILE:HA	1:M:172:GLU:CB	2.34	0.58
2:F:170:VAL:C	2:F:172:LEU:H	2.06	0.58
1:G:24:ASN:O	1:G:60:LYS:HA	2.03	0.58
1:O:112:LYS:HZ2	1:O:166:LEU:HD22	1.69	0.58
2:L:227:ARG:HH12	2:L:232:ILE:HA	1.69	0.58
2:H:126:ILE:CG1	2:H:150:ALA:HB2	2.33	0.58
2:F:255:ASN:N	2:F:255:ASN:ND2	2.49	0.58
2:P:98:ARG:HG3	2:P:98:ARG:HH11	1.67	0.58
2:P:43:PHE:CE2	2:P:102:PRO:HG3	2.37	0.58
2:N:43:PHE:CE2	2:N:102:PRO:HG3	2.38	0.58
1:K:158:GLY:CA	1:K:184:ASN:HD22	2.16	0.58
1:C:156:ASN:C	1:C:158:GLY:H	2.07	0.58
1:C:155:LEU:HD12	1:C:187:TYR:HB3	1.85	0.58
1:M:101:ASN:HA	2:N:268:VAL:O	2.04	0.58
1:A:86:ASN:ND2	1:A:110:ARG:HE	2.00	0.58
2:D:49:PRO:HD2	2:D:98:ARG:CZ	2.34	0.58
2:F:24:LEU:HA	4:F:545:HOH:O	2.02	0.58
1:A:102:THR:CA	2:B:171:THR:HG22	2.34	0.58
2:D:170:VAL:C	2:D:172:LEU:H	2.06	0.58
1:I:36:TRP:HH2	1:I:88:LYS:HE2	1.69	0.58
2:N:98:ARG:HH11	2:N:98:ARG:HG3	1.68	0.58
1:G:86:ASN:ND2	1:G:110:ARG:HE	2.01	0.58
2:H:28:VAL:O	2:H:156:VAL:HA	2.03	0.58
2:N:122:ALA:HA	2:N:150:ALA:O	2.04	0.58
1:G:161:VAL:O	1:G:162:LEU:HG	2.03	0.58
1:M:97:LYS:HB3	1:M:102:THR:CG2	2.34	0.58
1:K:23:THR:HG22	1:K:24:ASN:N	2.19	0.58
1:M:23:THR:HG22	1:M:24:ASN:N	2.18	0.58
1:I:18:VAL:HB	1:I:67:ILE:HB	1.85	0.58
1:K:36:TRP:HH2	1:K:88:LYS:HE2	1.69	0.58
1:A:24:ASN:O	1:A:60:LYS:HA	2.04	0.58
2:B:8:GLY:HA3	4:B:514:HOH:O	2.03	0.58
2:H:262:GLN:NE2	2:H:262:GLN:HA	2.19	0.58
2:J:27:VAL:HG12	4:J:607:HOH:O	2.02	0.58
1:G:102:THR:CA	2:H:171:THR:HG22	2.34	0.58
1:C:161:VAL:O	1:C:162:LEU:HG	2.04	0.58
1:K:24:ASN:ND2	1:K:59:GLY:O	2.37	0.58
2:L:227:ARG:C	2:L:229:GLY:H	2.07	0.58
1:K:100:GLU:HG2	2:L:172:LEU:HD12	1.86	0.58
2:J:52:ILE:HG23	2:J:137:TYR:HB2	1.85	0.58
2:F:2:ALA:HB3	2:F:45:HIS:CE1	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:251:GLY:O	2:P:252:LEU:HD23	2.03	0.58
2:H:43:PHE:HE2	2:H:102:PRO:HG3	1.68	0.58
2:B:43:PHE:HE2	2:B:102:PRO:HG3	1.68	0.58
1:M:158:GLY:HA3	1:M:184:ASN:ND2	2.19	0.58
1:K:26:ASP:O	1:K:60:LYS:HB3	2.02	0.58
1:O:24:ASN:ND2	1:O:59:GLY:O	2.37	0.58
1:M:112:LYS:HZ2	1:M:166:LEU:HD22	1.69	0.58
2:P:227:ARG:C	2:P:229:GLY:H	2.07	0.58
1:O:193:TYR:CG	2:P:155:VAL:HG11	2.39	0.58
2:H:59:GLN:HE21	2:H:143:GLN:NE2	2.02	0.58
2:P:46:ASN:HB2	2:P:96:ASN:HA	1.85	0.58
2:B:34:LEU:HB3	2:B:109:LEU:HB2	1.85	0.58
2:F:262:GLN:HA	2:F:262:GLN:NE2	2.19	0.58
1:I:158:GLY:CA	1:I:184:ASN:HD22	2.17	0.58
1:E:155:LEU:HD12	1:E:187:TYR:HB3	1.85	0.58
2:B:126:ILE:CG1	2:B:150:ALA:HB2	2.34	0.58
2:F:126:ILE:CG1	2:F:150:ALA:HB2	2.34	0.58
1:O:18:VAL:HB	1:O:67:ILE:HB	1.85	0.58
2:B:131:LEU:C	2:B:131:LEU:HD23	2.24	0.58
2:D:63:ALA:HB3	2:D:68:LEU:HD13	1.86	0.58
2:F:63:ALA:HB3	2:F:68:LEU:HD13	1.86	0.58
2:J:251:GLY:O	2:J:252:LEU:HD23	2.04	0.58
1:I:158:GLY:HA3	1:I:184:ASN:ND2	2.19	0.57
2:B:211:ASN:OD1	2:B:268:VAL:HA	2.03	0.57
1:I:104:GLN:N	2:J:168:VAL:HG23	2.19	0.57
1:M:33:ILE:CG1	1:M:57:MET:HB2	2.33	0.57
1:E:13:ALA:HB3	1:E:118:ALA:N	2.19	0.57
1:E:28:ASN:O	1:E:29:SER:HB3	2.04	0.57
2:J:44:CYS:HB2	2:J:95:TYR:CE2	2.38	0.57
2:H:49:PRO:HD2	2:H:98:ARG:CZ	2.33	0.57
1:C:102:THR:CA	2:D:171:THR:HG22	2.33	0.57
2:J:226:THR:HA	2:J:230:THR:O	2.04	0.57
2:N:226:THR:HA	2:N:230:THR:O	2.04	0.57
2:B:138:ASN:ND2	2:B:140:ASP:H	2.00	0.57
1:E:135:ARG:NH2	1:E:181:ALA:HB1	2.18	0.57
2:N:46:ASN:CB	2:N:96:ASN:HA	2.32	0.57
2:P:122:ALA:HA	2:P:150:ALA:O	2.03	0.57
2:J:43:PHE:CE2	2:J:102:PRO:HG3	2.38	0.57
1:C:28:ASN:O	1:C:29:SER:HB3	2.03	0.57
1:O:158:GLY:CA	1:O:184:ASN:HD22	2.16	0.57
1:A:161:VAL:HG22	1:A:162:LEU:N	2.16	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:97:LYS:HB3	1:K:102:THR:CG2	2.34	0.57
2:P:75:VAL:HG23	2:P:107:LEU:HD12	1.85	0.57
2:D:84:PHE:HA	2:D:85:PRO:C	2.25	0.57
1:M:104:GLN:N	2:N:168:VAL:HG23	2.19	0.57
1:C:161:VAL:HG22	1:C:162:LEU:N	2.16	0.57
1:M:193:TYR:CG	2:N:155:VAL:HG11	2.40	0.57
2:F:201:THR:CG2	2:F:206:ASN:HD22	2.14	0.57
1:C:13:ALA:HB3	1:C:118:ALA:N	2.19	0.57
2:F:34:LEU:HB3	2:F:109:LEU:HB2	1.86	0.57
1:C:86:ASN:ND2	1:C:110:ARG:HE	2.02	0.57
2:H:84:PHE:HA	2:H:85:PRO:C	2.24	0.57
1:C:8:ARG:HB3	1:C:8:ARG:NH1	2.19	0.57
1:A:66:ARG:HG2	1:A:66:ARG:HH11	1.69	0.57
2:J:175:TYR:CE1	2:J:263:VAL:HG21	2.40	0.57
1:G:155:LEU:HD12	1:G:187:TYR:HB3	1.86	0.57
1:O:33:ILE:CG1	1:O:57:MET:HB2	2.34	0.57
2:P:227:ARG:HH12	2:P:232:ILE:HA	1.70	0.57
1:M:100:GLU:HG2	2:N:172:LEU:HD12	1.85	0.57
1:K:193:TYR:CG	2:L:155:VAL:HG11	2.39	0.57
2:N:46:ASN:HB2	2:N:96:ASN:HA	1.86	0.57
2:H:111:PRO:HB3	2:H:156:VAL:HG21	1.85	0.57
2:N:44:CYS:HB2	2:N:95:TYR:CE2	2.39	0.57
2:B:179:VAL:O	2:B:253:THR:HG23	2.04	0.57
1:M:24:ASN:ND2	1:M:59:GLY:O	2.37	0.57
1:I:193:TYR:CG	2:J:155:VAL:HG11	2.39	0.57
1:M:18:VAL:HB	1:M:67:ILE:HB	1.85	0.57
2:H:136:ASN:ND2	2:H:136:ASN:C	2.54	0.57
2:F:92:ARG:HH11	2:F:92:ARG:HG3	1.68	0.57
2:H:184:THR:HG22	2:H:249:SER:HA	1.86	0.57
2:B:111:PRO:HB3	2:B:156:VAL:HG21	1.86	0.57
2:L:67:VAL:HG22	2:L:109:LEU:HD13	1.87	0.57
2:P:44:CYS:HB2	2:P:95:TYR:CE2	2.39	0.57
2:L:44:CYS:HB2	2:L:95:TYR:CE2	2.39	0.57
1:A:159:THR:CG2	1:A:180:ASP:HB3	2.35	0.57
1:O:97:LYS:HB3	1:O:102:THR:CG2	2.34	0.57
1:I:24:ASN:ND2	1:I:59:GLY:O	2.37	0.57
1:M:88:LYS:HE3	1:M:90:ILE:HG12	1.85	0.57
1:A:135:ARG:NH2	1:A:181:ALA:HB1	2.18	0.57
1:C:140:LEU:HD12	1:C:177:LEU:CD1	2.35	0.57
2:F:184:THR:HG22	2:F:249:SER:HA	1.86	0.57
2:F:219:GLN:HG3	4:F:503:HOH:O	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:163:GLU:HA	1:G:163:GLU:OE1	2.05	0.57
1:E:161:VAL:O	1:E:162:LEU:HG	2.05	0.57
2:B:170:VAL:C	2:B:172:LEU:H	2.07	0.57
1:G:159:THR:CG2	1:G:180:ASP:HB3	2.35	0.57
2:N:227:ARG:HH12	2:N:232:ILE:HA	1.69	0.57
1:E:179:SER:O	1:E:181:ALA:N	2.38	0.57
1:O:176:LYS:HB2	1:O:176:LYS:HZ3	1.70	0.57
1:K:101:ASN:HA	2:L:268:VAL:O	2.04	0.57
1:K:47:ARG:HH12	1:K:71:THR:HA	1.70	0.57
1:C:179:SER:O	1:C:181:ALA:N	2.38	0.57
2:H:76:LYS:HB3	4:H:617:HOH:O	2.04	0.57
1:K:105:LEU:CD1	2:L:183:LEU:HD11	2.35	0.57
1:K:18:VAL:HB	1:K:67:ILE:HB	1.86	0.57
1:M:77:GLN:NE2	1:M:77:GLN:HA	2.20	0.57
1:A:147:PRO:HG2	1:A:148:TYR:CE1	2.40	0.57
2:N:52:ILE:HG23	2:N:137:TYR:HB2	1.86	0.57
3:F:502:MMA:H2	4:F:531:HOH:O	2.04	0.57
1:G:84:TRP:CZ3	1:G:112:LYS:HG2	2.40	0.57
1:M:142:LEU:N	1:M:174:THR:HG22	2.20	0.56
2:N:212:THR:HG21	2:N:271:ILE:CD1	2.35	0.56
1:I:112:LYS:HZ2	1:I:166:LEU:HD22	1.68	0.56
1:G:179:SER:O	1:G:181:ALA:N	2.38	0.56
2:H:59:GLN:HG3	2:H:143:GLN:HE21	1.70	0.56
2:D:138:ASN:ND2	2:D:140:ASP:H	2.02	0.56
1:M:47:ARG:HH12	1:M:71:THR:HA	1.70	0.56
1:A:71:THR:O	1:A:71:THR:HG23	2.05	0.56
2:B:2:ALA:HB3	2:B:45:HIS:CE1	2.40	0.56
2:L:175:TYR:CE1	2:L:263:VAL:HG21	2.40	0.56
2:D:126:ILE:CG1	2:D:150:ALA:HB2	2.35	0.56
2:P:226:THR:HA	2:P:230:THR:O	2.04	0.56
2:B:201:THR:CG2	2:B:206:ASN:HD22	2.16	0.56
2:D:59:GLN:HE21	2:D:143:GLN:NE2	2.03	0.56
1:A:179:SER:O	1:A:181:ALA:N	2.39	0.56
2:N:251:GLY:O	2:N:252:LEU:HD23	2.04	0.56
2:F:130:ILE:HG12	2:F:145:VAL:HG22	1.87	0.56
1:K:104:GLN:N	2:L:168:VAL:HG23	2.19	0.56
1:M:105:LEU:CD1	2:N:183:LEU:HD11	2.35	0.56
1:O:114:TYR:CZ	1:O:149:TYR:HB2	2.40	0.56
2:J:227:ARG:HH12	2:J:232:ILE:HA	1.69	0.56
1:I:114:TYR:CZ	1:I:149:TYR:HB2	2.40	0.56
2:D:111:PRO:HB3	2:D:156:VAL:HG21	1.85	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:40:THR:HG22	2:N:40:THR:O	2.04	0.56
1:M:129:GLU:HB3	1:M:200:MET:SD	2.45	0.56
1:E:71:THR:O	1:E:71:THR:HG23	2.05	0.56
2:N:67:VAL:HG22	2:N:109:LEU:HD13	1.86	0.56
1:E:84:TRP:CZ3	1:E:112:LYS:HG2	2.40	0.56
2:F:84:PHE:HA	2:F:85:PRO:C	2.26	0.56
2:H:2:ALA:HB3	2:H:45:HIS:CE1	2.41	0.56
2:B:262:GLN:HA	2:B:262:GLN:NE2	2.19	0.56
2:P:210:THR:CG2	2:P:259:THR:HG21	2.29	0.56
1:E:156:ASN:C	1:E:158:GLY:H	2.07	0.56
1:I:97:LYS:HB3	1:I:102:THR:CG2	2.34	0.56
1:I:88:LYS:HE3	1:I:90:ILE:CG1	2.36	0.56
1:O:36:TRP:HH2	1:O:88:LYS:HE2	1.69	0.56
2:L:53:THR:HG22	2:L:96:ASN:OD1	2.06	0.56
1:I:47:ARG:HH12	1:I:71:THR:HA	1.70	0.56
2:L:251:GLY:O	2:L:252:LEU:HD23	2.05	0.56
1:A:28:ASN:O	1:A:29:SER:HB3	2.05	0.56
1:C:163:GLU:HA	1:C:163:GLU:OE1	2.05	0.56
2:P:175:TYR:CE1	2:P:263:VAL:HG21	2.40	0.56
1:E:161:VAL:HG22	1:E:162:LEU:N	2.16	0.56
1:A:178:PRO:O	1:A:180:ASP:N	2.39	0.56
1:C:178:PRO:O	1:C:180:ASP:N	2.39	0.56
1:O:24:ASN:O	1:O:60:LYS:HB2	2.06	0.56
1:K:88:LYS:HE3	1:K:90:ILE:CG1	2.36	0.56
2:F:138:ASN:ND2	2:F:140:ASP:H	2.03	0.56
1:O:176:LYS:NZ	1:O:176:LYS:HB2	2.21	0.56
1:C:73:ASN:HA	4:C:213:HOH:O	2.06	0.56
1:G:147:PRO:HG2	1:G:148:TYR:CE1	2.40	0.56
1:K:129:GLU:HB3	1:K:200:MET:SD	2.46	0.56
2:P:197:LEU:HD11	2:P:225:LEU:HD12	1.88	0.56
1:I:107:ILE:H	1:I:107:ILE:CD1	2.19	0.56
2:B:138:ASN:ND2	2:B:138:ASN:C	2.56	0.56
2:F:59:GLN:HG3	2:F:143:GLN:HE21	1.70	0.56
1:I:77:GLN:NE2	1:I:77:GLN:HA	2.20	0.56
2:P:67:VAL:HG22	2:P:109:LEU:HD13	1.88	0.56
2:L:40:THR:O	2:L:40:THR:HG22	2.05	0.56
2:J:75:VAL:HG23	2:J:107:LEU:HD12	1.86	0.56
2:N:75:VAL:HG23	2:N:107:LEU:HD12	1.87	0.56
1:C:159:THR:CG2	1:C:180:ASP:HB3	2.36	0.56
1:K:114:TYR:CZ	1:K:149:TYR:HB2	2.40	0.56
1:O:88:LYS:HE3	1:O:90:ILE:CG1	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:34:LEU:HB3	2:D:109:LEU:HB2	1.86	0.56
2:P:40:THR:O	2:P:40:THR:HG22	2.05	0.56
1:M:24:ASN:O	1:M:60:LYS:HB2	2.06	0.56
2:P:135:ASN:HD21	2:P:138:ASN:ND2	2.03	0.56
2:L:135:ASN:HD21	2:L:138:ASN:ND2	2.02	0.56
2:F:111:PRO:HB3	2:F:156:VAL:HG21	1.87	0.56
1:O:129:GLU:HB3	1:O:200:MET:SD	2.45	0.56
1:C:147:PRO:HG2	1:C:148:TYR:CE1	2.41	0.56
1:O:35:SER:HB2	1:O:50:VAL:HG11	1.88	0.56
1:A:156:ASN:C	1:A:158:GLY:H	2.08	0.56
1:A:161:VAL:O	1:A:162:LEU:HG	2.06	0.56
1:O:105:LEU:CD1	2:P:183:LEU:HD11	2.35	0.56
1:O:107:ILE:CD1	1:O:107:ILE:H	2.19	0.56
1:A:176:LYS:N	1:A:176:LYS:HD2	2.20	0.56
1:O:47:ARG:HH12	1:O:71:THR:HA	1.71	0.56
1:M:176:LYS:NZ	1:M:176:LYS:HB2	2.21	0.56
1:K:176:LYS:NZ	1:K:176:LYS:HB2	2.21	0.56
1:C:71:THR:HG23	1:C:71:THR:O	2.06	0.56
2:J:44:CYS:HB2	2:J:95:TYR:HE2	1.71	0.56
1:C:10:ILE:O	1:C:12:PRO:HD3	2.06	0.56
1:O:142:LEU:N	1:O:174:THR:HG22	2.21	0.56
1:G:129:GLU:HA	1:G:200:MET:CE	2.36	0.56
1:I:105:LEU:CD1	2:J:183:LEU:HD11	2.35	0.56
1:K:24:ASN:O	1:K:60:LYS:HB2	2.06	0.56
1:K:52:PRO:HD2	1:K:65:LEU:HA	1.88	0.56
1:M:107:ILE:H	1:M:107:ILE:CD1	2.18	0.56
1:A:13:ALA:HB3	1:A:118:ALA:N	2.20	0.56
2:J:126:ILE:HD13	4:J:614:HOH:O	2.04	0.56
1:A:8:ARG:NH1	1:A:8:ARG:HB3	2.21	0.56
2:B:113:SER:CB	2:P:81:SER:H	2.11	0.55
1:E:159:THR:CG2	1:E:180:ASP:HB3	2.36	0.55
2:P:212:THR:HG21	2:P:271:ILE:CD1	2.36	0.55
2:J:196:TYR:HB3	2:J:237:THR:HA	1.88	0.55
2:N:197:LEU:HD11	2:N:225:LEU:HD12	1.88	0.55
2:N:135:ASN:HD21	2:N:138:ASN:ND2	2.03	0.55
2:F:43:PHE:HE2	2:F:102:PRO:HG3	1.70	0.55
1:G:71:THR:O	1:G:71:THR:HG23	2.05	0.55
1:E:102:THR:HA	2:F:171:THR:HG22	1.88	0.55
1:K:103:LEU:HB3	2:L:169:THR:HB	1.89	0.55
2:J:184:THR:HA	2:J:248:VAL:O	2.06	0.55
2:D:262:GLN:NE2	2:D:262:GLN:HA	2.20	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:142:LEU:N	1:K:174:THR:HG22	2.21	0.55
2:N:175:TYR:CE1	2:N:263:VAL:HG21	2.41	0.55
2:L:212:THR:HG21	2:L:271:ILE:CD1	2.35	0.55
2:D:179:VAL:O	2:D:253:THR:HG23	2.06	0.55
1:K:112:LYS:HZ2	1:K:166:LEU:HD22	1.71	0.55
2:B:59:GLN:HG3	2:B:143:GLN:NE2	2.21	0.55
2:J:40:THR:HG22	2:J:40:THR:O	2.05	0.55
1:E:8:ARG:NH1	1:E:8:ARG:HB3	2.22	0.55
1:I:142:LEU:N	1:I:174:THR:HG22	2.21	0.55
1:G:178:PRO:O	1:G:180:ASP:N	2.39	0.55
2:J:212:THR:HG21	2:J:271:ILE:CD1	2.35	0.55
1:M:114:TYR:CZ	1:M:149:TYR:HB2	2.41	0.55
1:G:140:LEU:HD12	1:G:177:LEU:CD1	2.36	0.55
1:A:75:LEU:HB2	4:A:218:HOH:O	2.07	0.55
1:I:35:SER:HB2	1:I:50:VAL:HG11	1.89	0.55
1:G:8:ARG:NH1	1:G:8:ARG:HB3	2.21	0.55
1:E:178:PRO:O	1:E:180:ASP:N	2.39	0.55
2:N:184:THR:HA	2:N:248:VAL:O	2.07	0.55
1:I:24:ASN:O	1:I:60:LYS:HB2	2.06	0.55
1:I:52:PRO:HD2	1:I:65:LEU:HA	1.88	0.55
1:K:107:ILE:CD1	1:K:107:ILE:H	2.19	0.55
2:D:59:GLN:HG3	2:D:143:GLN:HE21	1.71	0.55
1:C:176:LYS:N	1:C:176:LYS:HD2	2.21	0.55
2:N:145:VAL:HG12	2:N:146:TRP:N	2.21	0.55
2:J:67:VAL:HG22	2:J:109:LEU:HD13	1.87	0.55
1:I:176:LYS:NZ	1:I:176:LYS:HB2	2.22	0.55
2:B:84:PHE:HA	2:B:85:PRO:C	2.27	0.55
1:K:30:THR:OG1	1:K:58:LYS:HE3	2.06	0.55
1:E:163:GLU:OE1	1:E:163:GLU:HA	2.07	0.55
1:O:107:ILE:HG21	2:P:163:VAL:HG11	1.89	0.55
1:M:154:GLU:OE1	1:M:188:ARG:HD3	2.07	0.55
1:I:79:ARG:HA	1:I:147:PRO:CB	2.37	0.55
1:I:169:PRO:C	1:I:171:GLY:H	2.10	0.55
1:O:126:GLN:HA	1:O:129:GLU:CD	2.27	0.55
1:I:129:GLU:HB3	1:I:200:MET:SD	2.46	0.55
1:I:30:THR:OG1	1:I:58:LYS:HE3	2.06	0.55
1:G:161:VAL:HG22	1:G:162:LEU:N	2.18	0.55
1:I:103:LEU:HB3	2:J:169:THR:HB	1.88	0.55
2:P:196:TYR:HB3	2:P:237:THR:HA	1.88	0.55
1:M:188:ARG:HH21	1:M:196:LEU:HD12	1.71	0.55
1:K:126:GLN:HA	1:K:129:GLU:CD	2.27	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:122:LEU:CD2	1:I:146:THR:HG22	2.36	0.55
2:L:75:VAL:HG23	2:L:107:LEU:HD12	1.87	0.55
1:E:144:ASN:ND2	1:E:150:LEU:HG	2.22	0.55
1:E:129:GLU:HA	1:E:200:MET:CE	2.37	0.55
1:E:140:LEU:HD12	1:E:177:LEU:CD1	2.35	0.55
2:L:44:CYS:HB2	2:L:95:TYR:HE2	1.72	0.55
2:D:2:ALA:HB3	2:D:45:HIS:CE1	2.41	0.55
1:O:52:PRO:HD2	1:O:65:LEU:HA	1.87	0.55
1:O:6:ALA:HB3	1:O:20:LEU:CD2	2.37	0.55
1:M:88:LYS:HE3	1:M:90:ILE:CG1	2.37	0.55
1:A:140:LEU:HD12	1:A:177:LEU:CD1	2.36	0.55
1:K:122:LEU:CD2	1:K:146:THR:HG22	2.37	0.55
2:J:17:SER:HB2	2:L:262:GLN:OE1	2.07	0.55
2:P:44:CYS:HB2	2:P:95:TYR:HE2	1.72	0.55
1:M:126:GLN:HA	1:M:129:GLU:CD	2.27	0.55
2:F:131:LEU:C	2:F:131:LEU:HD23	2.27	0.55
1:A:129:GLU:HA	1:A:200:MET:CE	2.37	0.55
1:O:103:LEU:HB3	2:P:169:THR:HB	1.88	0.55
2:L:172:LEU:O	2:L:172:LEU:HD23	2.07	0.55
1:I:126:GLN:HA	1:I:129:GLU:CD	2.27	0.55
1:K:107:ILE:HG21	2:L:163:VAL:HG11	1.89	0.54
1:I:188:ARG:HH21	1:I:196:LEU:HD12	1.72	0.54
1:M:79:ARG:HA	1:M:147:PRO:CB	2.37	0.54
2:D:43:PHE:HE2	2:D:102:PRO:HG3	1.72	0.54
1:O:46:GLY:HA2	4:O:206:HOH:O	2.07	0.54
2:J:172:LEU:O	2:J:172:LEU:HD23	2.08	0.54
1:G:136:SER:C	1:G:138:ASN:H	2.10	0.54
1:O:188:ARG:HH21	1:O:196:LEU:HD12	1.72	0.54
1:O:77:GLN:HA	1:O:77:GLN:NE2	2.22	0.54
1:E:82:LEU:O	4:E:213:HOH:O	2.18	0.54
1:C:191:ASN:HD21	1:C:195:ALA:HB3	1.73	0.54
1:M:52:PRO:HD2	1:M:65:LEU:HA	1.88	0.54
1:C:84:TRP:CZ3	1:C:112:LYS:HG2	2.42	0.54
1:I:107:ILE:HG21	2:J:163:VAL:HG11	1.90	0.54
2:B:135:ASN:HD22	2:B:137:TYR:HB3	1.72	0.54
2:D:53:THR:HB	2:D:136:ASN:OD1	2.07	0.54
2:J:53:THR:HG22	2:J:96:ASN:OD1	2.07	0.54
2:L:145:VAL:HG12	2:L:146:TRP:N	2.22	0.54
2:H:262:GLN:HE21	2:H:262:GLN:HA	1.73	0.54
2:J:197:LEU:HD11	2:J:225:LEU:HD12	1.89	0.54
2:L:196:TYR:HB3	2:L:237:THR:HA	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:59:GLN:HE21	2:F:143:GLN:NE2	2.04	0.54
1:O:169:PRO:C	1:O:171:GLY:H	2.10	0.54
1:K:77:GLN:NE2	1:K:77:GLN:HA	2.21	0.54
2:P:22:VAL:HG12	2:P:41:GLN:HG3	1.90	0.54
1:M:122:LEU:CD2	1:M:146:THR:HG22	2.37	0.54
1:K:157:ALA:HA	1:K:184:ASN:O	2.08	0.54
2:N:53:THR:HG22	2:N:96:ASN:OD1	2.08	0.54
2:J:22:VAL:HG12	2:J:41:GLN:HG3	1.90	0.54
2:B:130:ILE:HG12	2:B:145:VAL:HG22	1.90	0.54
1:G:28:ASN:O	1:G:29:SER:HB3	2.05	0.54
1:M:35:SER:HB2	1:M:50:VAL:HG11	1.89	0.54
1:O:30:THR:OG1	1:O:58:LYS:HE3	2.06	0.54
1:O:142:LEU:H	1:O:174:THR:HG22	1.73	0.54
2:P:172:LEU:HD23	2:P:172:LEU:O	2.07	0.54
2:F:138:ASN:ND2	2:F:138:ASN:C	2.57	0.54
1:A:133:PHE:O	1:A:205:GLU:HG2	2.08	0.54
2:F:209:PHE:CD1	2:F:272:ILE:HD12	2.43	0.54
2:H:6:ALA:HB2	2:H:41:GLN:HA	1.90	0.54
1:M:142:LEU:H	1:M:174:THR:HG22	1.71	0.54
2:P:184:THR:HA	2:P:248:VAL:O	2.07	0.54
2:J:195:TYR:O	2:J:237:THR:HA	2.08	0.54
2:J:197:LEU:O	2:J:198:SER:HB3	2.08	0.54
1:M:107:ILE:HG21	2:N:163:VAL:HG11	1.90	0.54
1:M:169:PRO:C	1:M:171:GLY:H	2.10	0.54
2:P:42:ILE:HD13	2:P:146:TRP:CD2	2.43	0.54
2:P:38:LEU:C	2:P:40:THR:N	2.61	0.54
1:G:71:THR:O	1:G:73:ASN:N	2.41	0.54
1:M:30:THR:OG1	1:M:58:LYS:HE3	2.06	0.54
2:B:63:ALA:HB3	2:B:68:LEU:HD13	1.90	0.54
1:A:163:GLU:OE1	1:A:163:GLU:HA	2.06	0.54
1:O:157:ALA:HA	1:O:184:ASN:O	2.08	0.54
2:F:67:VAL:CG2	2:F:120:ILE:HD11	2.38	0.54
2:L:197:LEU:HD11	2:L:225:LEU:HD12	1.89	0.54
2:N:196:TYR:HB3	2:N:237:THR:HA	1.88	0.54
2:F:53:THR:HB	2:F:136:ASN:OD1	2.08	0.54
1:K:188:ARG:HH21	1:K:196:LEU:HD12	1.72	0.54
2:P:145:VAL:HG12	2:P:146:TRP:N	2.22	0.54
1:A:71:THR:O	1:A:73:ASN:N	2.40	0.54
1:I:122:LEU:HD23	1:I:146:THR:HG22	1.90	0.54
1:K:35:SER:HB2	1:K:50:VAL:HG11	1.89	0.54
1:O:140:LEU:HD12	1:O:162:LEU:HD11	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:6:ALA:HB3	1:M:20:LEU:CD2	2.38	0.54
1:G:176:LYS:HD2	1:G:176:LYS:N	2.20	0.54
2:D:92:ARG:HH11	2:D:92:ARG:HG3	1.72	0.54
2:P:71:PHE:HB3	2:P:110:THR:H	1.73	0.54
2:L:42:ILE:HD13	2:L:146:TRP:CD2	2.43	0.54
1:C:71:THR:O	1:C:73:ASN:N	2.41	0.54
1:K:133:PHE:HB2	1:K:204:MET:SD	2.48	0.54
2:B:43:PHE:CE2	2:B:102:PRO:HG3	2.43	0.54
2:H:113:SER:CB	2:L:81:SER:H	2.13	0.54
1:M:103:LEU:HB3	2:N:169:THR:HB	1.88	0.54
2:H:135:ASN:HD22	2:H:137:TYR:HB3	1.72	0.54
1:C:132:ARG:HG2	4:C:212:HOH:O	2.07	0.54
1:E:176:LYS:HD2	1:E:176:LYS:N	2.20	0.54
1:I:154:GLU:OE1	1:I:188:ARG:HD3	2.08	0.54
1:K:169:PRO:C	1:K:171:GLY:H	2.10	0.54
2:L:184:THR:HA	2:L:248:VAL:O	2.07	0.53
2:L:195:TYR:O	2:L:237:THR:HA	2.09	0.53
2:P:197:LEU:O	2:P:198:SER:HB3	2.09	0.53
2:N:42:ILE:HD13	2:N:146:TRP:CD2	2.43	0.53
2:H:192:ASN:HA	2:H:242:ALA:HA	1.89	0.53
1:I:140:LEU:HD12	1:I:162:LEU:HD11	1.89	0.53
2:D:126:ILE:HB	2:D:148:ILE:HG22	1.91	0.53
2:F:135:ASN:HD22	2:F:137:TYR:HB3	1.72	0.53
1:O:1:GLY:HA3	2:P:162:ASP:OD1	2.08	0.53
2:N:22:VAL:HG12	2:N:41:GLN:HG3	1.90	0.53
2:H:5:THR:HG22	2:H:9:THR:H	1.74	0.53
1:I:133:PHE:HB2	1:I:204:MET:SD	2.48	0.53
2:L:103:TRP:O	2:L:105:VAL:N	2.41	0.53
2:N:44:CYS:HB2	2:N:95:TYR:HE2	1.73	0.53
1:O:81:SER:O	1:O:83:PHE:HD1	1.91	0.53
1:M:157:ALA:HA	1:M:184:ASN:O	2.08	0.53
1:O:136:SER:HB2	1:O:139:SER:HB2	1.90	0.53
1:O:91:PRO:HD2	1:O:106:ALA:HB2	1.90	0.53
2:P:11:ILE:HG23	2:P:16:GLY:CA	2.32	0.53
1:I:6:ALA:HB3	1:I:20:LEU:CD2	2.38	0.53
2:P:172:LEU:N	2:P:173:PRO:CD	2.71	0.53
2:J:172:LEU:N	2:J:173:PRO:CD	2.72	0.53
1:G:133:PHE:O	1:G:205:GLU:HG2	2.08	0.53
1:E:136:SER:C	1:E:138:ASN:H	2.11	0.53
1:K:154:GLU:OE1	1:K:188:ARG:HD3	2.09	0.53
1:K:122:LEU:HD23	1:K:146:THR:HG22	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:184:THR:HG22	2:D:249:SER:CA	2.38	0.53
2:L:22:VAL:HG12	2:L:41:GLN:HG3	1.91	0.53
2:L:38:LEU:C	2:L:40:THR:N	2.62	0.53
2:H:48:TYR:H	3:H:603:MMA:H62	1.73	0.53
1:I:157:ALA:HA	1:I:184:ASN:O	2.08	0.53
1:C:129:GLU:HA	1:C:200:MET:CE	2.38	0.53
1:G:102:THR:HA	2:H:171:THR:HG22	1.90	0.53
1:M:91:PRO:HD2	1:M:106:ALA:HB2	1.91	0.53
1:K:6:ALA:HB3	1:K:20:LEU:CD2	2.38	0.53
1:O:122:LEU:CD2	1:O:146:THR:HG22	2.38	0.53
1:K:79:ARG:HA	1:K:147:PRO:CB	2.36	0.53
2:N:38:LEU:C	2:N:40:THR:N	2.61	0.53
2:J:14:GLY:HA2	2:J:142:PHE:CD2	2.44	0.53
2:H:43:PHE:CE2	2:H:102:PRO:HG3	2.44	0.53
1:A:144:ASN:ND2	1:A:150:LEU:HG	2.24	0.53
2:F:90:THR:HB	2:F:91:PRO:HD2	1.91	0.53
1:A:84:TRP:CZ3	1:A:112:LYS:HG2	2.43	0.53
1:K:142:LEU:H	1:K:174:THR:HG22	1.73	0.53
1:O:135:ARG:HH21	1:O:177:LEU:HD21	1.73	0.53
2:L:197:LEU:O	2:L:198:SER:HB3	2.08	0.53
2:P:197:LEU:CD1	2:P:225:LEU:HD12	2.38	0.53
1:O:154:GLU:OE1	1:O:188:ARG:HD3	2.07	0.53
2:B:184:THR:HG22	2:B:249:SER:CA	2.38	0.53
1:O:122:LEU:HD23	1:O:146:THR:HG22	1.91	0.53
1:O:79:ARG:HA	1:O:147:PRO:CB	2.37	0.53
1:M:1:GLY:HA3	2:N:162:ASP:OD1	2.09	0.53
2:J:103:TRP:O	2:J:105:VAL:N	2.42	0.53
1:E:71:THR:O	1:E:73:ASN:N	2.42	0.53
2:D:6:ALA:HB2	2:D:41:GLN:HA	1.90	0.53
1:I:95:LYS:HD2	1:I:95:LYS:N	2.23	0.53
2:H:67:VAL:HG21	2:H:126:ILE:CG2	2.32	0.53
2:N:195:TYR:O	2:N:237:THR:HA	2.08	0.53
2:D:135:ASN:HD22	2:D:137:TYR:HB3	1.73	0.53
1:E:133:PHE:O	1:E:205:GLU:HG2	2.08	0.53
2:J:145:VAL:HG12	2:J:146:TRP:N	2.23	0.53
2:F:262:GLN:HA	2:F:262:GLN:HE21	1.73	0.53
1:M:122:LEU:HD23	1:M:146:THR:HG22	1.90	0.53
1:I:136:SER:HB2	1:I:139:SER:HB2	1.90	0.53
1:A:136:SER:C	1:A:138:ASN:H	2.10	0.53
2:P:53:THR:HG22	2:P:96:ASN:OD1	2.08	0.53
1:O:28:ASN:N	1:O:28:ASN:HD22	1.98	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:1:GLY:HA3	2:L:162:ASP:OD1	2.08	0.53
2:L:148:ILE:N	2:L:148:ILE:HD12	2.23	0.53
2:P:21:TYR:HB3	2:P:151:ASN:ND2	2.24	0.53
2:J:21:TYR:HB3	2:J:151:ASN:ND2	2.24	0.53
2:P:103:TRP:O	2:P:105:VAL:N	2.41	0.53
1:E:147:PRO:HG2	1:E:148:TYR:CE1	2.43	0.53
2:B:90:THR:HB	2:B:91:PRO:HD2	1.91	0.53
1:A:104:GLN:HG3	2:B:168:VAL:HB	1.91	0.53
2:D:130:ILE:HG12	2:D:145:VAL:HG22	1.90	0.53
1:K:140:LEU:HD12	1:K:162:LEU:HD11	1.89	0.53
1:I:142:LEU:H	1:I:174:THR:HG22	1.73	0.53
1:I:91:PRO:HD3	4:I:207:HOH:O	2.07	0.53
2:J:155:VAL:O	2:J:157:PRO:HD3	2.08	0.53
2:N:172:LEU:HD23	2:N:172:LEU:O	2.08	0.53
2:J:135:ASN:HD21	2:J:138:ASN:ND2	2.06	0.53
2:J:71:PHE:HB3	2:J:110:THR:H	1.73	0.53
2:F:262:GLN:HB3	4:F:510:HOH:O	2.07	0.53
1:M:81:SER:O	1:M:83:PHE:HD1	1.92	0.53
1:C:133:PHE:O	1:C:205:GLU:HG2	2.08	0.53
2:H:262:GLN:HB3	4:H:607:HOH:O	2.08	0.53
2:B:262:GLN:HA	2:B:262:GLN:HE21	1.73	0.53
2:D:262:GLN:HB3	4:D:604:HOH:O	2.09	0.53
2:D:192:ASN:HA	2:D:242:ALA:HA	1.90	0.53
1:M:136:SER:HB2	1:M:139:SER:HB2	1.90	0.53
1:I:135:ARG:HH21	1:I:177:LEU:HD21	1.74	0.53
2:B:174:ASP:O	2:B:176:PRO:CD	2.56	0.53
2:B:210:THR:HG22	2:B:211:ASN:N	2.24	0.53
2:L:197:LEU:CD1	2:L:225:LEU:HD12	2.39	0.53
2:H:126:ILE:HG13	2:H:150:ALA:HB2	1.91	0.53
1:O:85:MET:HB2	1:O:111:ILE:CG1	2.39	0.53
2:N:197:LEU:O	2:N:198:SER:HB3	2.08	0.53
2:N:71:PHE:HB3	2:N:110:THR:H	1.74	0.53
2:J:42:ILE:HD13	2:J:146:TRP:CD2	2.44	0.53
1:A:191:ASN:HD21	1:A:195:ALA:HB3	1.73	0.53
1:K:81:SER:O	1:K:83:PHE:HD1	1.91	0.53
1:C:104:GLN:HG3	2:D:168:VAL:HB	1.91	0.53
1:M:140:LEU:HD12	1:M:162:LEU:HD11	1.90	0.52
1:C:102:THR:HA	2:D:171:THR:HG22	1.90	0.52
2:P:155:VAL:O	2:P:157:PRO:HD3	2.09	0.52
2:B:53:THR:HB	2:B:136:ASN:OD1	2.09	0.52
1:C:136:SER:C	1:C:138:ASN:H	2.11	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:107:ILE:N	1:C:107:ILE:HD12	2.25	0.52
2:N:17:SER:HB2	2:P:262:GLN:OE1	2.09	0.52
1:O:79:ARG:HB2	1:O:169:PRO:HB3	1.91	0.52
1:A:144:ASN:ND2	1:A:148:TYR:O	2.39	0.52
2:F:192:ASN:HA	2:F:242:ALA:HA	1.90	0.52
2:F:6:ALA:HB2	2:F:41:GLN:HA	1.91	0.52
1:K:135:ARG:HH21	1:K:177:LEU:HD21	1.73	0.52
2:H:67:VAL:CG2	2:H:120:ILE:HD11	2.39	0.52
2:P:195:TYR:O	2:P:237:THR:HA	2.08	0.52
1:I:85:MET:HB2	1:I:111:ILE:CG1	2.39	0.52
2:L:155:VAL:O	2:L:157:PRO:HD3	2.10	0.52
1:K:190:ILE:CD1	2:L:279:GLN:HG2	2.37	0.52
1:I:28:ASN:HD22	1:I:28:ASN:N	1.98	0.52
1:I:1:GLY:HA3	2:J:162:ASP:OD1	2.09	0.52
2:B:209:PHE:CD1	2:B:272:ILE:HD12	2.44	0.52
2:B:6:ALA:HB2	2:B:41:GLN:HA	1.90	0.52
1:K:136:SER:HB2	1:K:139:SER:HB2	1.90	0.52
1:A:102:THR:HA	2:B:171:THR:HG22	1.90	0.52
2:H:126:ILE:HB	2:H:148:ILE:HG22	1.91	0.52
2:N:155:VAL:O	2:N:157:PRO:HD3	2.09	0.52
1:I:80:GLU:HG3	1:I:147:PRO:O	2.10	0.52
1:C:144:ASN:ND2	1:C:150:LEU:HG	2.25	0.52
2:F:90:THR:HB	2:F:91:PRO:CD	2.38	0.52
1:O:95:LYS:HD2	1:O:95:LYS:N	2.24	0.52
1:K:91:PRO:HD2	1:K:106:ALA:HB2	1.91	0.52
2:D:174:ASP:O	2:D:176:PRO:CD	2.58	0.52
1:M:85:MET:HB2	1:M:111:ILE:CG1	2.39	0.52
1:G:107:ILE:HD12	1:G:107:ILE:N	2.25	0.52
2:B:5:THR:HG22	2:B:9:THR:H	1.74	0.52
1:E:104:GLN:HG3	2:F:168:VAL:HB	1.91	0.52
1:M:95:LYS:N	1:M:95:LYS:HD2	2.24	0.52
2:H:179:VAL:O	2:H:253:THR:HG23	2.09	0.52
2:B:92:ARG:HG3	2:B:92:ARG:HH11	1.73	0.52
2:J:192:ASN:HA	2:J:241:GLY:O	2.10	0.52
1:M:190:ILE:CD1	2:N:279:GLN:HG2	2.38	0.52
2:H:92:ARG:HH11	2:H:92:ARG:HG3	1.73	0.52
2:D:184:THR:HA	2:D:248:VAL:O	2.10	0.52
2:N:207:SER:O	2:N:224:GLN:HG3	2.09	0.52
2:P:14:GLY:HA2	2:P:142:PHE:CD2	2.44	0.52
2:L:14:GLY:HA2	2:L:142:PHE:CD2	2.45	0.52
1:O:133:PHE:HB2	1:O:204:MET:SD	2.49	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:55:TYR:HB3	2:J:92:ARG:HB2	1.92	0.52
2:J:11:ILE:CG2	2:J:16:GLY:HA3	2.34	0.52
2:D:255:ASN:N	2:D:255:ASN:ND2	2.50	0.52
2:F:59:GLN:HG3	2:F:143:GLN:NE2	2.25	0.52
1:O:190:ILE:CD1	2:P:279:GLN:HG2	2.38	0.52
1:I:28:ASN:N	1:I:28:ASN:ND2	2.57	0.52
2:J:59:GLN:HE21	2:J:143:GLN:NE2	2.07	0.52
1:I:13:ALA:HB3	1:I:118:ALA:CB	2.40	0.52
1:O:128:ALA:HA	1:O:150:LEU:HD22	1.91	0.52
1:E:191:ASN:HD21	1:E:195:ALA:HB3	1.75	0.52
1:G:104:GLN:HG3	2:H:168:VAL:HB	1.92	0.52
1:G:191:ASN:HD21	1:G:195:ALA:HB3	1.75	0.52
1:I:38:GLU:HA	1:I:44:LYS:HA	1.91	0.52
1:M:135:ARG:HH21	1:M:177:LEU:HD21	1.73	0.52
1:I:31:TYR:HB2	1:I:89:ALA:HB1	1.91	0.52
2:N:197:LEU:CD1	2:N:225:LEU:HD12	2.39	0.52
2:F:135:ASN:ND2	2:F:137:TYR:HB3	2.25	0.52
2:L:53:THR:HG22	2:L:96:ASN:CB	2.39	0.52
1:K:147:PRO:HA	1:K:169:PRO:HB3	1.92	0.52
2:N:103:TRP:O	2:N:105:VAL:N	2.43	0.52
1:A:47:ARG:NH1	1:A:47:ARG:HG3	2.25	0.52
2:F:43:PHE:CE2	2:F:102:PRO:HG3	2.44	0.52
1:I:30:THR:OG1	1:I:58:LYS:HG2	2.10	0.52
2:H:130:ILE:HG12	2:H:145:VAL:HG22	1.90	0.52
2:D:90:THR:HB	2:D:91:PRO:HD2	1.91	0.52
1:E:131:LEU:HD23	1:E:187:TYR:CE2	2.45	0.52
1:C:158:GLY:HA2	4:C:221:HOH:O	2.09	0.52
2:J:11:ILE:HG23	2:J:16:GLY:CA	2.32	0.52
2:B:67:VAL:CG2	2:B:120:ILE:HD11	2.39	0.52
2:B:67:VAL:HG23	2:B:120:ILE:HD11	1.92	0.52
1:C:9:VAL:HG22	4:C:208:HOH:O	2.10	0.52
1:A:47:ARG:CB	1:A:83:PHE:HE2	2.23	0.52
2:J:210:THR:CG2	2:J:259:THR:HG21	2.30	0.52
2:N:130:ILE:HD12	2:N:130:ILE:N	2.25	0.52
2:F:136:ASN:ND2	2:F:136:ASN:C	2.54	0.52
2:B:59:GLN:HE21	2:B:143:GLN:NE2	2.07	0.52
1:E:203:VAL:HB	4:E:210:HOH:O	2.10	0.52
2:P:192:ASN:HA	2:P:241:GLY:O	2.10	0.52
2:H:184:THR:HA	2:H:248:VAL:O	2.10	0.52
1:M:79:ARG:HB2	1:M:169:PRO:HB3	1.91	0.52
1:I:79:ARG:HB2	1:I:169:PRO:HB3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:71:PHE:HB3	2:L:110:THR:H	1.74	0.52
2:N:48:TYR:CE1	3:N:506:MMA:H73	2.45	0.52
2:B:48:TYR:H	3:B:500:MMA:H62	1.74	0.52
1:K:95:LYS:HD2	1:K:95:LYS:N	2.23	0.52
1:O:163:GLU:HB3	1:O:175:VAL:HG13	1.92	0.52
2:J:197:LEU:CD1	2:J:225:LEU:HD12	2.39	0.52
2:J:130:ILE:N	2:J:130:ILE:HD12	2.24	0.52
1:G:13:ALA:HB3	1:G:118:ALA:N	2.18	0.52
1:E:144:ASN:ND2	1:E:148:TYR:O	2.39	0.52
2:B:90:THR:HB	2:B:91:PRO:CD	2.39	0.52
1:O:13:ALA:HB3	1:O:118:ALA:CB	2.40	0.52
1:M:38:GLU:HA	1:M:44:LYS:HA	1.91	0.52
1:K:128:ALA:HA	1:K:150:LEU:HD22	1.91	0.52
1:E:188:ARG:HG2	1:E:188:ARG:HH11	1.76	0.51
1:K:31:TYR:HB2	1:K:89:ALA:HB1	1.91	0.51
1:O:31:TYR:HB2	1:O:89:ALA:HB1	1.92	0.51
2:N:268:VAL:HG12	2:N:269:GLN:N	2.25	0.51
2:D:90:THR:HB	2:D:91:PRO:CD	2.39	0.51
1:E:175:VAL:HG12	4:E:230:HOH:O	2.09	0.51
1:A:12:PRO:HB2	1:A:15:GLN:HG2	1.92	0.51
1:A:10:ILE:O	1:A:12:PRO:HD3	2.10	0.51
2:F:35:VAL:HA	2:F:107:LEU:O	2.10	0.51
2:D:209:PHE:CD1	2:D:272:ILE:HD12	2.45	0.51
2:B:174:ASP:O	2:B:176:PRO:HD2	2.09	0.51
2:P:268:VAL:HG12	2:P:269:GLN:N	2.25	0.51
2:H:135:ASN:ND2	2:H:137:TYR:HB3	2.25	0.51
2:H:59:GLN:HG3	2:H:143:GLN:NE2	2.24	0.51
1:O:80:GLU:HG3	1:O:147:PRO:O	2.10	0.51
1:K:79:ARG:HB2	1:K:169:PRO:HB3	1.91	0.51
2:N:59:GLN:HE21	2:N:143:GLN:NE2	2.08	0.51
1:C:12:PRO:HB2	1:C:15:GLN:HG2	1.91	0.51
2:D:43:PHE:CE2	2:D:102:PRO:HG3	2.46	0.51
1:I:81:SER:O	1:I:83:PHE:HD1	1.92	0.51
2:B:192:ASN:HA	2:B:242:ALA:HA	1.91	0.51
2:L:210:THR:CG2	2:L:259:THR:HG21	2.29	0.51
2:H:174:ASP:O	2:H:176:PRO:CD	2.58	0.51
1:K:6:ALA:HB3	1:K:20:LEU:HD21	1.93	0.51
2:N:53:THR:HG22	2:N:96:ASN:CB	2.41	0.51
1:M:147:PRO:HA	1:M:169:PRO:HB3	1.93	0.51
2:N:148:ILE:HD12	2:N:148:ILE:N	2.26	0.51
2:P:131:LEU:HD22	2:P:144:PHE:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:144:ASN:ND2	1:G:150:LEU:HG	2.24	0.51
2:D:262:GLN:HE21	2:D:262:GLN:HA	1.74	0.51
1:G:10:ILE:O	1:G:12:PRO:HD3	2.10	0.51
1:A:114:TYR:CE1	1:A:149:TYR:HB2	2.46	0.51
1:G:129:GLU:HA	1:G:200:MET:HE2	1.92	0.51
1:I:91:PRO:HD2	1:I:106:ALA:HB2	1.91	0.51
1:I:6:ALA:HB3	1:I:20:LEU:HD21	1.93	0.51
2:L:172:LEU:N	2:L:173:PRO:CD	2.71	0.51
1:I:86:ASN:HA	1:I:109:SER:O	2.11	0.51
2:J:264:THR:HG22	2:J:265:ALA:N	2.21	0.51
2:P:53:THR:HG22	2:P:96:ASN:CB	2.40	0.51
2:H:184:THR:HG22	2:H:249:SER:CA	2.40	0.51
2:J:148:ILE:N	2:J:148:ILE:HD12	2.24	0.51
2:L:102:PRO:HB2	4:L:508:HOH:O	2.11	0.51
1:K:30:THR:OG1	1:K:58:LYS:HG2	2.11	0.51
1:M:30:THR:OG1	1:M:58:LYS:HG2	2.10	0.51
1:G:12:PRO:HB2	1:G:15:GLN:HG2	1.93	0.51
1:A:188:ARG:CZ	1:A:197:THR:O	2.59	0.51
2:H:113:SER:HB3	2:L:81:SER:N	2.12	0.51
1:C:188:ARG:CZ	1:C:197:THR:O	2.58	0.51
2:F:174:ASP:O	2:F:176:PRO:CD	2.59	0.51
1:O:6:ALA:HB3	1:O:20:LEU:HD21	1.92	0.51
1:I:55:PHE:HE1	1:I:57:MET:HG3	1.76	0.51
2:P:130:ILE:HD12	2:P:130:ILE:N	2.24	0.51
1:K:85:MET:HB2	1:K:111:ILE:CG1	2.40	0.51
2:N:172:LEU:N	2:N:173:PRO:CD	2.71	0.51
2:H:138:ASN:C	2:H:138:ASN:ND2	2.56	0.51
2:J:53:THR:HG22	2:J:96:ASN:CB	2.40	0.51
2:H:219:GLN:HA	4:H:631:HOH:O	2.09	0.51
1:M:80:GLU:HG3	1:M:147:PRO:O	2.11	0.51
2:P:122:ALA:HB1	2:P:151:ASN:O	2.11	0.51
1:C:16:LYS:HB3	4:C:223:HOH:O	2.10	0.51
1:M:163:GLU:HB3	1:M:175:VAL:HG13	1.92	0.51
1:G:188:ARG:CZ	1:G:197:THR:O	2.58	0.51
1:G:156:ASN:OD1	1:G:161:VAL:HG23	2.10	0.51
1:C:156:ASN:OD1	1:C:161:VAL:HG23	2.10	0.51
1:K:60:LYS:HD3	1:K:60:LYS:O	2.11	0.51
2:L:130:ILE:HD12	2:L:130:ILE:N	2.26	0.51
2:F:184:THR:HG22	2:F:249:SER:CA	2.41	0.51
1:A:107:ILE:HD12	1:A:107:ILE:N	2.26	0.51
2:N:224:GLN:CG	2:N:231:ILE:HD13	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:207:SER:O	2:J:224:GLN:HG3	2.09	0.51
1:K:38:GLU:HA	1:K:44:LYS:HA	1.91	0.51
1:I:128:ALA:HA	1:I:150:LEU:HD22	1.92	0.51
1:E:45:ASP:HB2	4:E:214:HOH:O	2.10	0.51
2:B:35:VAL:HA	2:B:107:LEU:O	2.10	0.51
2:H:271:ILE:O	2:H:272:ILE:HD13	2.10	0.51
1:E:156:ASN:OD1	1:E:161:VAL:HG23	2.10	0.51
2:F:173:PRO:HB2	2:F:177:GLY:HA3	1.92	0.51
1:K:104:GLN:HG3	2:L:168:VAL:HB	1.93	0.51
2:L:192:ASN:HA	2:L:241:GLY:O	2.10	0.51
1:M:153:THR:HG21	1:M:196:LEU:CD2	2.39	0.51
1:K:176:LYS:HB2	1:K:176:LYS:HZ3	1.76	0.51
2:J:122:ALA:HB1	2:J:151:ASN:O	2.10	0.51
1:C:97:LYS:HD3	1:C:100:GLU:OE2	2.11	0.51
1:C:47:ARG:CB	1:C:83:PHE:HE2	2.24	0.51
2:D:35:VAL:HA	2:D:107:LEU:O	2.10	0.51
2:F:210:THR:HG22	2:F:211:ASN:N	2.25	0.51
2:F:67:VAL:HG23	2:F:120:ILE:HD11	1.91	0.51
2:D:67:VAL:CG2	2:D:120:ILE:HD11	2.41	0.51
2:J:163:VAL:HG13	2:J:185:VAL:CG1	2.41	0.51
2:N:192:ASN:HA	2:N:241:GLY:O	2.10	0.51
2:P:96:ASN:H	2:P:96:ASN:HD22	1.58	0.51
1:O:153:THR:HG21	1:O:196:LEU:CD2	2.39	0.51
2:F:184:THR:HA	2:F:248:VAL:O	2.10	0.51
2:L:201:THR:HA	2:L:209:PHE:HA	1.93	0.51
1:E:97:LYS:HD3	1:E:100:GLU:OE2	2.11	0.51
2:N:14:GLY:HA2	2:N:142:PHE:CD2	2.46	0.51
1:A:47:ARG:HH11	1:A:47:ARG:HG3	1.76	0.51
2:N:84:PHE:HA	2:N:85:PRO:C	2.31	0.51
2:F:271:ILE:O	2:F:272:ILE:HD13	2.10	0.51
2:P:55:TYR:HB3	2:P:92:ARG:HB2	1.92	0.51
1:K:13:ALA:HB3	1:K:118:ALA:CB	2.40	0.51
1:O:38:GLU:HA	1:O:44:LYS:HA	1.91	0.51
2:L:207:SER:O	2:L:224:GLN:HG3	2.11	0.51
2:N:193:LEU:HD12	2:N:243:VAL:HG21	1.93	0.51
2:P:148:ILE:N	2:P:148:ILE:HD12	2.26	0.51
2:J:38:LEU:C	2:J:40:THR:N	2.62	0.51
1:M:133:PHE:HB2	1:M:204:MET:SD	2.50	0.51
2:H:131:LEU:HB3	2:H:144:PHE:HB2	1.93	0.51
2:H:106:ALA:HB3	4:H:617:HOH:O	2.10	0.51
1:G:47:ARG:NH1	1:G:47:ARG:HG3	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:29:ASN:HA	4:F:526:HOH:O	2.09	0.51
1:A:156:ASN:HD22	1:A:186:THR:HB	1.76	0.51
2:B:173:PRO:HB2	2:B:177:GLY:HA3	1.92	0.51
2:D:173:PRO:HB2	2:D:177:GLY:HA3	1.93	0.51
2:P:11:ILE:CG2	2:P:16:GLY:HA3	2.33	0.51
1:O:20:LEU:HD12	1:O:21:ALA:N	2.26	0.51
1:M:20:LEU:HD12	1:M:21:ALA:N	2.26	0.51
1:M:31:TYR:HB2	1:M:89:ALA:HB1	1.92	0.51
1:M:33:ILE:HG13	1:M:57:MET:HB2	1.93	0.51
2:F:126:ILE:HB	2:F:148:ILE:HG22	1.92	0.51
2:N:58:LEU:HD12	2:N:130:ILE:O	2.11	0.51
2:J:268:VAL:HG12	2:J:269:GLN:N	2.25	0.51
1:I:17:GLN:HA	1:I:67:ILE:O	2.11	0.51
1:K:110:ARG:HD3	2:L:277:VAL:HG13	1.93	0.51
2:B:57:THR:OG1	2:B:132:ARG:HB3	2.11	0.51
2:N:163:VAL:HG13	2:N:185:VAL:CG1	2.40	0.51
2:L:224:GLN:NE2	4:L:511:HOH:O	2.43	0.51
2:B:46:ASN:O	2:B:98:ARG:HA	2.11	0.51
2:J:84:PHE:HA	2:J:85:PRO:C	2.31	0.51
1:O:30:THR:OG1	1:O:58:LYS:HG2	2.11	0.51
1:I:95:LYS:O	1:I:96:SER:HB2	2.11	0.51
2:H:90:THR:HB	2:H:91:PRO:CD	2.40	0.51
2:H:23:ASN:HB3	4:H:620:HOH:O	2.09	0.51
1:A:44:LYS:HG3	4:A:212:HOH:O	2.11	0.51
1:M:13:ALA:HB3	1:M:118:ALA:CB	2.40	0.51
2:L:34:LEU:O	2:L:34:LEU:HG	2.11	0.51
1:A:188:ARG:HH11	1:A:188:ARG:HG2	1.76	0.50
1:E:188:ARG:CZ	1:E:197:THR:O	2.59	0.50
1:O:33:ILE:HG13	1:O:57:MET:HB2	1.94	0.50
2:H:135:ASN:ND2	2:H:138:ASN:H	2.09	0.50
2:D:57:THR:OG1	2:D:132:ARG:HB3	2.12	0.50
1:M:28:ASN:ND2	1:M:28:ASN:N	2.58	0.50
2:F:5:THR:HG22	2:F:9:THR:H	1.76	0.50
1:G:47:ARG:CB	1:G:83:PHE:HE2	2.24	0.50
1:M:95:LYS:O	1:M:96:SER:HB2	2.12	0.50
1:K:95:LYS:O	1:K:96:SER:HB2	2.11	0.50
2:H:90:THR:HB	2:H:91:PRO:HD2	1.93	0.50
1:M:128:ALA:HA	1:M:150:LEU:HD22	1.92	0.50
1:K:163:GLU:HB3	1:K:175:VAL:HG13	1.92	0.50
1:I:163:GLU:HB3	1:I:175:VAL:HG13	1.92	0.50
1:K:55:PHE:HE1	1:K:57:MET:HG3	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:17:GLN:HA	1:M:67:ILE:O	2.11	0.50
2:L:163:VAL:HG13	2:L:185:VAL:CG1	2.40	0.50
2:N:268:VAL:HG12	2:N:269:GLN:H	1.77	0.50
1:I:190:ILE:CD1	2:J:279:GLN:HG2	2.37	0.50
2:P:207:SER:O	2:P:224:GLN:HG3	2.10	0.50
1:K:80:GLU:HG3	1:K:147:PRO:O	2.12	0.50
2:L:193:LEU:HD12	2:L:243:VAL:HG21	1.93	0.50
2:H:46:ASN:O	2:H:98:ARG:HA	2.11	0.50
2:H:209:PHE:CD1	2:H:272:ILE:HD12	2.46	0.50
2:P:34:LEU:O	2:P:34:LEU:HG	2.12	0.50
2:B:174:ASP:O	2:B:176:PRO:N	2.44	0.50
1:K:33:ILE:HG13	1:K:57:MET:HB2	1.93	0.50
1:I:20:LEU:HD12	1:I:21:ALA:N	2.26	0.50
1:M:60:LYS:HD3	1:M:60:LYS:O	2.12	0.50
1:M:6:ALA:HB3	1:M:20:LEU:HD21	1.93	0.50
1:A:97:LYS:HD3	1:A:100:GLU:OE2	2.11	0.50
2:D:227:ARG:O	2:D:227:ARG:HG3	2.11	0.50
2:N:103:TRP:CE2	2:N:131:LEU:HD12	2.46	0.50
1:A:47:ARG:NH1	1:A:71:THR:HB	2.26	0.50
1:C:144:ASN:ND2	1:C:148:TYR:O	2.39	0.50
1:E:114:TYR:CE1	1:E:149:TYR:HB2	2.47	0.50
1:M:75:LEU:HB2	1:M:115:TYR:CE2	2.47	0.50
2:H:174:ASP:O	2:H:176:PRO:N	2.45	0.50
1:I:55:PHE:CE1	1:I:57:MET:HG3	2.47	0.50
1:I:33:ILE:HG13	1:I:57:MET:HB2	1.94	0.50
2:H:67:VAL:HG23	2:H:120:ILE:HD11	1.91	0.50
1:O:17:GLN:HA	1:O:67:ILE:O	2.11	0.50
2:L:96:ASN:HD22	2:L:96:ASN:H	1.60	0.50
2:J:201:THR:HA	2:J:209:PHE:HA	1.94	0.50
2:P:59:GLN:HE21	2:P:143:GLN:NE2	2.09	0.50
2:B:224:GLN:NE2	4:B:507:HOH:O	2.38	0.50
2:N:34:LEU:HG	2:N:34:LEU:O	2.11	0.50
2:N:210:THR:CG2	2:N:259:THR:HG21	2.30	0.50
1:C:131:LEU:HD23	1:C:187:TYR:CE2	2.46	0.50
1:K:20:LEU:HD12	1:K:21:ALA:N	2.26	0.50
1:K:31:TYR:O	1:K:33:ILE:N	2.44	0.50
1:K:55:PHE:CE1	1:K:57:MET:HG3	2.47	0.50
2:L:268:VAL:HG12	2:L:269:GLN:N	2.25	0.50
2:N:115:ALA:HB3	2:N:156:VAL:HG11	1.94	0.50
2:B:184:THR:HA	2:B:248:VAL:O	2.11	0.50
2:L:122:ALA:HB1	2:L:151:ASN:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:192:ASN:OD1	2:H:242:ALA:HB2	2.12	0.50
1:O:75:LEU:HB2	1:O:115:TYR:CE2	2.47	0.50
1:G:114:TYR:CE1	1:G:149:TYR:HB2	2.45	0.50
1:K:75:LEU:HB2	1:K:115:TYR:CE2	2.47	0.50
2:B:135:ASN:ND2	2:B:137:TYR:HB3	2.25	0.50
2:H:59:GLN:HE21	2:H:143:GLN:HE22	1.59	0.50
2:D:219:GLN:HA	4:D:625:HOH:O	2.11	0.50
2:L:224:GLN:CG	2:L:231:ILE:HD13	2.40	0.50
2:N:122:ALA:HB1	2:N:151:ASN:O	2.11	0.50
2:N:21:TYR:CB	2:N:151:ASN:HD21	2.24	0.50
1:C:188:ARG:HH12	1:C:198:PRO:HA	1.76	0.50
1:A:102:THR:O	2:B:269:GLN:HA	2.11	0.50
2:L:11:ILE:CG2	2:L:16:GLY:HA3	2.34	0.50
1:I:31:TYR:O	1:I:33:ILE:N	2.44	0.50
2:J:115:ALA:HB3	2:J:156:VAL:HG11	1.94	0.50
1:M:86:ASN:HA	1:M:109:SER:O	2.12	0.50
1:O:86:ASN:HA	1:O:109:SER:O	2.11	0.50
2:H:53:THR:HB	2:H:136:ASN:OD1	2.12	0.50
2:N:96:ASN:H	2:N:96:ASN:HD22	1.59	0.50
2:N:201:THR:HA	2:N:209:PHE:HA	1.94	0.50
2:J:131:LEU:HD22	2:J:144:PHE:HB2	1.92	0.50
1:E:47:ARG:NH1	1:E:71:THR:HB	2.27	0.50
2:N:55:TYR:HB3	2:N:92:ARG:HB2	1.93	0.50
2:J:268:VAL:HG12	2:J:269:GLN:H	1.77	0.50
2:H:181:ILE:HD11	2:H:254:ALA:HB2	1.94	0.50
2:P:5:THR:HG22	2:P:9:THR:N	2.27	0.50
2:P:201:THR:HA	2:P:209:PHE:HA	1.93	0.50
2:L:59:GLN:HE21	2:L:143:GLN:NE2	2.09	0.50
2:N:21:TYR:HB3	2:N:151:ASN:ND2	2.24	0.50
2:P:21:TYR:CB	2:P:151:ASN:HD21	2.24	0.50
2:L:48:TYR:CE1	3:L:504:MMA:H73	2.47	0.50
1:E:12:PRO:HB2	1:E:15:GLN:HG2	1.94	0.50
1:E:10:ILE:O	1:E:12:PRO:HD3	2.12	0.50
2:L:55:TYR:HB3	2:L:92:ARG:HB2	1.92	0.50
1:G:102:THR:O	2:H:269:GLN:HA	2.12	0.50
2:F:174:ASP:O	2:F:176:PRO:HD2	2.12	0.50
1:O:60:LYS:HD3	1:O:60:LYS:O	2.12	0.50
1:I:60:LYS:O	1:I:60:LYS:HD3	2.12	0.50
1:M:36:TRP:CH2	1:M:88:LYS:HE2	2.46	0.50
2:P:163:VAL:HG13	2:P:185:VAL:CG1	2.41	0.50
1:C:47:ARG:HH11	1:C:47:ARG:HG3	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:131:LEU:HD22	2:L:144:PHE:HB2	1.93	0.50
1:E:47:ARG:CB	1:E:83:PHE:HE2	2.24	0.50
1:G:77:GLN:HA	1:G:77:GLN:NE2	2.27	0.50
2:J:34:LEU:HG	2:J:34:LEU:O	2.12	0.50
1:I:143:ILE:HA	1:I:172:GLU:HB2	1.94	0.49
1:G:131:LEU:HD23	1:G:187:TYR:CE2	2.47	0.49
2:D:210:THR:HG22	2:D:211:ASN:N	2.26	0.49
2:B:126:ILE:HB	2:B:148:ILE:HG22	1.94	0.49
2:P:58:LEU:HD12	2:P:130:ILE:O	2.12	0.49
2:F:181:ILE:HD11	2:F:254:ALA:HB2	1.93	0.49
1:K:28:ASN:N	1:K:28:ASN:ND2	2.58	0.49
2:J:5:THR:HG22	2:J:9:THR:N	2.27	0.49
1:I:147:PRO:HA	1:I:169:PRO:HB3	1.93	0.49
2:D:5:THR:HG22	2:D:9:THR:H	1.77	0.49
1:A:9:VAL:HG12	1:A:113:LEU:HD13	1.94	0.49
2:B:192:ASN:OD1	2:B:242:ALA:HB2	2.11	0.49
1:C:121:ALA:HB3	4:C:216:HOH:O	2.12	0.49
2:D:174:ASP:O	2:D:176:PRO:HD2	2.11	0.49
1:O:55:PHE:HE1	1:O:57:MET:HG3	1.76	0.49
1:K:101:ASN:HB2	2:L:171:THR:O	2.12	0.49
1:K:86:ASN:HA	1:K:109:SER:O	2.11	0.49
1:C:88:LYS:CB	1:C:108:ILE:HG12	2.42	0.49
1:O:147:PRO:HA	1:O:169:PRO:HB3	1.93	0.49
2:H:227:ARG:HG3	2:H:227:ARG:O	2.12	0.49
2:F:227:ARG:HG3	2:F:227:ARG:O	2.12	0.49
2:F:192:ASN:OD1	2:F:242:ALA:HB2	2.12	0.49
1:I:104:GLN:HG3	2:J:168:VAL:HB	1.94	0.49
1:O:31:TYR:O	1:O:33:ILE:N	2.45	0.49
1:O:110:ARG:HD3	2:P:277:VAL:HG13	1.94	0.49
2:D:59:GLN:HG3	2:D:143:GLN:NE2	2.26	0.49
2:B:28:VAL:HG12	2:B:111:PRO:HG2	1.94	0.49
1:C:47:ARG:NH1	1:C:47:ARG:HG3	2.27	0.49
1:G:144:ASN:ND2	1:G:148:TYR:O	2.39	0.49
1:O:95:LYS:O	1:O:96:SER:HB2	2.12	0.49
2:L:271:ILE:O	2:L:271:ILE:HG13	2.13	0.49
2:D:174:ASP:O	2:D:176:PRO:N	2.45	0.49
1:M:104:GLN:HG3	2:N:168:VAL:HB	1.94	0.49
2:P:268:VAL:HG12	2:P:269:GLN:H	1.77	0.49
2:P:264:THR:HG22	2:P:265:ALA:N	2.20	0.49
2:N:126:ILE:N	2:N:148:ILE:O	2.45	0.49
2:F:46:ASN:O	2:F:98:ARG:HA	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:245:THR:HB	4:J:616:HOH:O	2.12	0.49
1:O:143:ILE:HA	1:O:172:GLU:HB2	1.94	0.49
1:C:188:ARG:HG2	1:C:188:ARG:HH11	1.78	0.49
2:H:173:PRO:HB2	2:H:177:GLY:HA3	1.93	0.49
1:G:156:ASN:HD22	1:G:186:THR:HB	1.78	0.49
2:D:126:ILE:HG13	2:D:150:ALA:HB2	1.94	0.49
1:I:75:LEU:HB2	1:I:115:TYR:CE2	2.47	0.49
2:L:268:VAL:HG12	2:L:269:GLN:H	1.77	0.49
1:A:88:LYS:CB	1:A:108:ILE:HG12	2.41	0.49
2:J:126:ILE:N	2:J:148:ILE:O	2.45	0.49
2:F:5:THR:HG23	2:F:7:ASN:N	2.26	0.49
2:F:131:LEU:HB3	2:F:144:PHE:HB2	1.94	0.49
1:G:80:GLU:HA	1:G:115:TYR:O	2.13	0.49
2:J:166:ARG:CG	2:J:182:PRO:HB2	2.43	0.49
1:I:20:LEU:HD12	1:I:21:ALA:H	1.78	0.49
1:M:31:TYR:O	1:M:33:ILE:N	2.45	0.49
1:M:55:PHE:HE1	1:M:57:MET:HG3	1.76	0.49
1:K:17:GLN:HA	1:K:67:ILE:O	2.11	0.49
2:B:92:ARG:NH1	4:B:558:HOH:O	2.45	0.49
2:B:135:ASN:ND2	2:B:138:ASN:H	2.11	0.49
2:L:103:TRP:CE2	2:L:131:LEU:HD12	2.48	0.49
1:G:47:ARG:HH11	1:G:47:ARG:HG3	1.77	0.49
1:O:189:THR:O	1:O:197:THR:HG23	2.13	0.49
1:A:156:ASN:OD1	1:A:161:VAL:HG23	2.12	0.49
2:N:271:ILE:HG13	2:N:271:ILE:O	2.13	0.49
1:O:55:PHE:CE1	1:O:57:MET:HG3	2.47	0.49
1:I:101:ASN:HB2	2:J:171:THR:O	2.13	0.49
1:K:153:THR:HG21	1:K:196:LEU:CD2	2.39	0.49
1:C:47:ARG:NH1	1:C:71:THR:HB	2.27	0.49
2:J:103:TRP:CE2	2:J:131:LEU:HD12	2.47	0.49
2:D:271:ILE:O	2:D:272:ILE:HD13	2.13	0.49
1:K:158:GLY:N	1:K:184:ASN:HD22	2.11	0.49
1:I:158:GLY:N	1:I:184:ASN:HD22	2.11	0.49
1:G:188:ARG:HG2	1:G:188:ARG:HH11	1.78	0.49
2:F:126:ILE:HG13	2:F:150:ALA:HB2	1.93	0.49
2:J:211:ASN:HD21	2:J:213:ALA:HB3	1.77	0.49
1:O:36:TRP:CH2	1:O:88:LYS:HE2	2.47	0.49
2:L:126:ILE:N	2:L:148:ILE:O	2.45	0.49
2:P:103:TRP:CE2	2:P:131:LEU:HD12	2.47	0.49
1:K:119:LYS:HE3	4:K:213:HOH:O	2.11	0.49
2:H:170:VAL:HG12	2:H:172:LEU:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:210:THR:HG22	2:H:211:ASN:N	2.27	0.49
2:L:166:ARG:CG	2:L:182:PRO:HB2	2.42	0.49
2:N:11:ILE:HG23	2:N:16:GLY:CA	2.32	0.49
2:B:126:ILE:HG13	2:B:150:ALA:HB2	1.93	0.49
2:D:135:ASN:ND2	2:D:137:TYR:HB3	2.26	0.49
2:F:185:VAL:O	2:F:243:VAL:HG11	2.13	0.49
1:G:97:LYS:HD3	1:G:100:GLU:OE2	2.13	0.49
2:N:131:LEU:HD22	2:N:144:PHE:HB2	1.94	0.49
1:G:47:ARG:NH1	1:G:71:THR:HB	2.28	0.49
1:G:39:ASN:ND2	1:G:43:VAL:HG22	2.28	0.49
2:B:75:VAL:O	2:B:75:VAL:HG13	2.12	0.49
1:A:188:ARG:HH12	1:A:198:PRO:HA	1.77	0.49
1:O:20:LEU:HD12	1:O:21:ALA:H	1.78	0.49
1:M:20:LEU:HD12	1:M:21:ALA:H	1.78	0.49
1:K:36:TRP:CH2	1:K:88:LYS:HE2	2.47	0.49
1:I:110:ARG:HD3	2:J:277:VAL:HG13	1.93	0.49
1:M:110:ARG:HD3	2:N:277:VAL:HG13	1.93	0.49
2:N:5:THR:HG22	2:N:9:THR:N	2.27	0.49
2:H:35:VAL:HA	2:H:107:LEU:O	2.12	0.49
1:A:77:GLN:HA	1:A:77:GLN:NE2	2.28	0.49
1:I:189:THR:O	1:I:197:THR:HG23	2.13	0.49
2:F:70:ASN:ND2	2:F:119:ALA:HA	2.28	0.49
1:G:188:ARG:HH12	1:G:198:PRO:HA	1.77	0.48
1:E:188:ARG:HH12	1:E:198:PRO:HA	1.77	0.48
2:H:174:ASP:O	2:H:176:PRO:HD2	2.13	0.48
1:O:104:GLN:HG3	2:P:168:VAL:HB	1.94	0.48
1:K:20:LEU:HD12	1:K:21:ALA:H	1.78	0.48
1:O:101:ASN:HB2	2:P:171:THR:O	2.14	0.48
1:E:27:GLU:HG3	1:E:60:LYS:HZ3	1.78	0.48
2:L:5:THR:HG22	2:L:9:THR:N	2.28	0.48
2:B:50:GLU:CD	2:B:98:ARG:HH12	2.16	0.48
2:D:46:ASN:O	2:D:98:ARG:HA	2.13	0.48
2:H:211:ASN:HD21	2:H:269:GLN:N	1.95	0.48
2:J:58:LEU:HD12	2:J:130:ILE:O	2.13	0.48
2:N:117:GLY:HA2	2:N:156:VAL:H	1.78	0.48
2:P:46:ASN:HD22	2:P:49:PRO:HA	1.78	0.48
2:J:46:ASN:HD22	2:J:49:PRO:HA	1.78	0.48
2:F:28:VAL:HG12	2:F:111:PRO:HG2	1.95	0.48
2:H:28:VAL:HG12	2:H:111:PRO:HG2	1.95	0.48
2:H:38:LEU:C	2:H:40:THR:N	2.66	0.48
2:H:50:GLU:CD	2:H:98:ARG:HH12	2.16	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:189:THR:O	1:K:197:THR:HG23	2.13	0.48
1:E:156:ASN:HD22	1:E:186:THR:HB	1.79	0.48
1:A:131:LEU:HD23	1:A:187:TYR:CE2	2.48	0.48
1:E:102:THR:OG1	2:F:269:GLN:HG2	2.13	0.48
2:B:173:PRO:O	2:B:174:ASP:C	2.52	0.48
2:P:271:ILE:O	2:P:271:ILE:HG13	2.13	0.48
2:J:271:ILE:HG13	2:J:271:ILE:O	2.13	0.48
1:M:55:PHE:CE1	1:M:57:MET:HG3	2.47	0.48
2:B:181:ILE:HD11	2:B:254:ALA:HB2	1.93	0.48
1:I:36:TRP:CH2	1:I:88:LYS:HE2	2.47	0.48
2:F:201:THR:HG23	2:F:202:ALA:N	2.29	0.48
2:L:264:THR:HG22	2:L:265:ALA:N	2.21	0.48
2:D:50:GLU:CD	2:D:98:ARG:HH12	2.17	0.48
2:L:84:PHE:HA	2:L:85:PRO:C	2.32	0.48
1:C:114:TYR:CE1	1:C:149:TYR:HB2	2.48	0.48
2:H:239:SER:HB3	4:H:640:HOH:O	2.13	0.48
1:M:132:ARG:HB2	1:M:143:ILE:HG23	1.95	0.48
2:P:115:ALA:HB3	2:P:156:VAL:HG11	1.94	0.48
2:D:28:VAL:HG12	2:D:111:PRO:HG2	1.95	0.48
2:P:201:THR:HG21	2:P:206:ASN:ND2	2.29	0.48
2:L:21:TYR:CB	2:L:151:ASN:HD21	2.24	0.48
2:J:21:TYR:CB	2:J:151:ASN:HD21	2.25	0.48
1:K:133:PHE:CE1	1:K:202:GLY:HA3	2.48	0.48
1:A:11:TYR:HB2	1:A:113:LEU:HD11	1.96	0.48
1:E:47:ARG:HG3	1:E:47:ARG:NH1	2.27	0.48
1:E:124:PRO:HD3	1:E:148:TYR:OH	2.13	0.48
1:G:114:TYR:CE1	1:G:149:TYR:CB	2.96	0.48
1:E:9:VAL:HA	4:E:209:HOH:O	2.13	0.48
2:N:57:THR:HG22	2:N:91:PRO:O	2.13	0.48
1:E:102:THR:O	2:F:269:GLN:HA	2.12	0.48
2:F:174:ASP:O	2:F:176:PRO:N	2.47	0.48
1:C:102:THR:O	2:D:269:GLN:HA	2.12	0.48
2:J:211:ASN:HD21	2:J:213:ALA:CB	2.27	0.48
2:H:57:THR:OG1	2:H:132:ARG:HB3	2.13	0.48
2:F:57:THR:OG1	2:F:132:ARG:HB3	2.14	0.48
2:F:218:ALA:HA	2:F:265:ALA:O	2.14	0.48
2:P:224:GLN:CG	2:P:231:ILE:HD13	2.41	0.48
2:P:193:LEU:HD12	2:P:243:VAL:HG21	1.94	0.48
2:P:122:ALA:HB2	2:P:152:ASN:O	2.13	0.48
2:L:21:TYR:HB3	2:L:151:ASN:ND2	2.25	0.48
2:P:84:PHE:HA	2:P:85:PRO:C	2.33	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:ASN:ND2	1:A:43:VAL:HG22	2.29	0.48
1:K:143:ILE:HA	1:K:172:GLU:HB2	1.94	0.48
2:F:173:PRO:O	2:F:174:ASP:C	2.51	0.48
1:A:102:THR:OG1	2:B:269:GLN:HG2	2.14	0.48
2:F:175:TYR:O	2:F:256:TYR:CD1	2.67	0.48
2:D:67:VAL:HG23	2:D:120:ILE:HD11	1.94	0.48
1:A:135:ARG:NH1	1:A:135:ARG:HB2	2.29	0.48
2:H:185:VAL:O	2:H:243:VAL:HG11	2.14	0.48
1:I:153:THR:HG21	1:I:196:LEU:CD2	2.39	0.48
1:E:107:ILE:HD12	1:E:107:ILE:N	2.28	0.48
2:J:193:LEU:HD12	2:J:243:VAL:HG21	1.95	0.48
2:H:5:THR:HG23	2:H:7:ASN:N	2.27	0.48
2:D:82:TYR:OH	2:D:91:PRO:HD2	2.14	0.48
1:M:189:THR:O	1:M:197:THR:HG23	2.13	0.48
1:G:204:MET:N	1:G:204:MET:SD	2.87	0.48
1:M:158:GLY:N	1:M:184:ASN:HD22	2.12	0.48
1:M:101:ASN:HB2	2:N:171:THR:O	2.13	0.48
1:C:135:ARG:HB2	1:C:135:ARG:NH1	2.28	0.48
2:B:185:VAL:O	2:B:243:VAL:HG11	2.13	0.48
1:O:79:ARG:HB2	1:O:169:PRO:CB	2.44	0.48
2:N:38:LEU:HD12	2:N:38:LEU:N	2.29	0.48
1:E:11:TYR:HB2	1:E:113:LEU:HD11	1.95	0.48
1:C:77:GLN:NE2	1:C:77:GLN:HA	2.29	0.48
1:A:31:TYR:O	1:A:56:ALA:HA	2.14	0.48
2:D:173:PRO:O	2:D:174:ASP:C	2.52	0.48
2:P:211:ASN:HD21	2:P:213:ALA:HB3	1.78	0.48
2:B:262:GLN:HG3	2:B:262:GLN:O	2.14	0.48
2:N:264:THR:HG22	2:N:265:ALA:N	2.21	0.48
2:F:92:ARG:HG3	2:F:92:ARG:NH1	2.27	0.48
1:E:135:ARG:HB2	1:E:135:ARG:NH1	2.28	0.48
1:I:188:ARG:NH2	1:I:196:LEU:HB2	2.29	0.48
2:N:46:ASN:HD22	2:N:49:PRO:HA	1.79	0.48
2:J:19:ASN:OD1	2:L:262:GLN:NE2	2.47	0.48
1:M:79:ARG:HB2	1:M:169:PRO:CB	2.44	0.48
1:K:79:ARG:HB2	1:K:169:PRO:CB	2.44	0.48
1:K:191:ASN:HD21	1:K:195:ALA:HB3	1.79	0.48
1:E:39:ASN:ND2	1:E:43:VAL:HG22	2.29	0.48
1:E:77:GLN:HA	1:E:77:GLN:NE2	2.29	0.48
2:P:48:TYR:CE1	3:P:607:MMA:H73	2.49	0.48
1:M:143:ILE:HA	1:M:172:GLU:HB2	1.95	0.48
2:B:170:VAL:HG12	2:B:172:LEU:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:91:PRO:HB2	1:M:104:GLN:HE21	1.78	0.48
1:C:156:ASN:HD22	1:C:186:THR:HB	1.79	0.48
1:I:103:LEU:H	2:J:168:VAL:HG22	1.79	0.48
2:D:175:TYR:O	2:D:256:TYR:CD2	2.66	0.48
2:L:262:GLN:O	2:L:262:GLN:HG3	2.14	0.48
1:C:11:TYR:HB2	1:C:113:LEU:HD11	1.96	0.48
2:N:201:THR:HG21	2:N:206:ASN:ND2	2.29	0.48
2:F:116:GLY:HA2	2:F:189:LYS:CE	2.42	0.48
1:M:133:PHE:CE1	1:M:202:GLY:HA3	2.49	0.48
2:B:82:TYR:OH	2:B:91:PRO:HD2	2.14	0.48
2:D:192:ASN:OD1	2:D:242:ALA:HB2	2.13	0.48
2:P:57:THR:HG22	2:P:91:PRO:O	2.13	0.48
1:M:141:THR:C	1:M:174:THR:HG22	2.33	0.47
2:H:173:PRO:O	2:H:174:ASP:C	2.52	0.47
2:F:170:VAL:HG12	2:F:172:LEU:HB2	1.94	0.47
1:K:102:THR:HB	2:L:168:VAL:HG21	1.95	0.47
2:N:226:THR:CG2	2:N:253:THR:HB	2.42	0.47
2:D:185:VAL:O	2:D:243:VAL:HG11	2.14	0.47
1:O:133:PHE:CE1	1:O:202:GLY:HA3	2.48	0.47
2:J:48:TYR:CE1	3:J:605:MMA:H73	2.49	0.47
1:E:31:TYR:O	1:E:56:ALA:HA	2.14	0.47
1:C:80:GLU:HA	1:C:115:TYR:O	2.14	0.47
1:O:132:ARG:HB2	1:O:143:ILE:HG23	1.96	0.47
1:O:158:GLY:N	1:O:184:ASN:HD22	2.11	0.47
2:L:11:ILE:HG23	2:L:16:GLY:CA	2.32	0.47
2:L:211:ASN:HD21	2:L:213:ALA:HB3	1.79	0.47
2:L:115:ALA:HB3	2:L:156:VAL:HG11	1.94	0.47
2:H:218:ALA:HA	2:H:265:ALA:O	2.14	0.47
2:P:262:GLN:O	2:P:262:GLN:HG3	2.14	0.47
2:J:201:THR:HG21	2:J:206:ASN:ND2	2.29	0.47
1:A:142:LEU:CD2	1:A:142:LEU:N	2.77	0.47
1:G:31:TYR:O	1:G:56:ALA:HA	2.13	0.47
1:O:103:LEU:H	2:P:168:VAL:HG22	1.79	0.47
1:K:103:LEU:H	2:L:168:VAL:HG22	1.80	0.47
2:F:135:ASN:ND2	2:F:138:ASN:H	2.12	0.47
2:P:41:GLN:NE2	2:P:41:GLN:HA	2.29	0.47
2:J:38:LEU:N	2:J:38:LEU:HD12	2.28	0.47
1:E:47:ARG:HG3	1:E:47:ARG:HH11	1.78	0.47
2:B:70:ASN:ND2	2:B:119:ALA:HA	2.29	0.47
2:J:216:SER:N	2:J:217:PRO:CD	2.77	0.47
1:C:31:TYR:O	1:C:56:ALA:HA	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:188:ARG:NE	1:E:196:LEU:HD22	2.28	0.47
2:D:170:VAL:HG12	2:D:172:LEU:HB2	1.96	0.47
1:I:52:PRO:HG2	1:I:55:PHE:CE2	2.50	0.47
2:P:211:ASN:HD21	2:P:213:ALA:CB	2.28	0.47
2:D:181:ILE:HD11	2:D:254:ALA:HB2	1.95	0.47
2:P:117:GLY:HA2	2:P:156:VAL:H	1.79	0.47
2:N:211:ASN:HD21	2:N:213:ALA:HB3	1.79	0.47
2:J:224:GLN:CG	2:J:231:ILE:HD13	2.41	0.47
2:N:206:ASN:C	2:N:206:ASN:HD22	2.16	0.47
2:L:206:ASN:C	2:L:206:ASN:HD22	2.17	0.47
1:I:79:ARG:HB2	1:I:169:PRO:CB	2.44	0.47
1:K:46:GLY:C	1:K:48:PHE:H	2.18	0.47
1:C:39:ASN:ND2	1:C:43:VAL:HG22	2.30	0.47
2:D:75:VAL:O	2:D:75:VAL:HG13	2.15	0.47
2:H:70:ASN:ND2	2:H:119:ALA:HA	2.29	0.47
2:L:58:LEU:HD12	2:L:130:ILE:O	2.14	0.47
1:G:135:ARG:HB2	1:G:135:ARG:NH1	2.29	0.47
1:A:86:ASN:HD21	1:A:110:ARG:NE	2.09	0.47
2:P:206:ASN:C	2:P:206:ASN:HD22	2.16	0.47
2:P:126:ILE:N	2:P:148:ILE:O	2.45	0.47
2:N:122:ALA:HB2	2:N:152:ASN:O	2.13	0.47
2:B:227:ARG:O	2:B:227:ARG:HG3	2.14	0.47
1:G:39:ASN:CG	1:G:43:VAL:HG22	2.34	0.47
2:J:208:ILE:HA	2:J:223:VAL:O	2.15	0.47
2:P:216:SER:N	2:P:217:PRO:CD	2.78	0.47
1:K:132:ARG:HB2	1:K:143:ILE:HG23	1.96	0.47
1:O:141:THR:C	1:O:174:THR:HG22	2.34	0.47
1:O:91:PRO:HB2	1:O:104:GLN:HE21	1.79	0.47
1:I:193:TYR:CD2	2:J:155:VAL:HG21	2.50	0.47
2:N:202:ALA:N	2:N:208:ILE:O	2.48	0.47
2:L:117:GLY:HA2	2:L:156:VAL:H	1.79	0.47
1:C:133:PHE:HD2	1:C:140:LEU:HD21	1.80	0.47
2:D:218:ALA:HA	2:D:265:ALA:O	2.14	0.47
2:P:234:ALA:O	2:P:235:ASN:HB2	2.15	0.47
2:J:206:ASN:HD22	2:J:206:ASN:C	2.17	0.47
2:D:5:THR:HG23	2:D:7:ASN:N	2.28	0.47
2:D:38:LEU:C	2:D:40:THR:N	2.66	0.47
2:D:116:GLY:HA2	2:D:189:LYS:CE	2.44	0.47
2:B:38:LEU:C	2:B:40:THR:N	2.68	0.47
2:D:131:LEU:HB3	2:D:144:PHE:HB2	1.95	0.47
1:A:112:LYS:HE3	2:B:279:GLN:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:TYR:CE1	1:A:149:TYR:CB	2.98	0.47
1:O:160:ARG:CD	1:O:180:ASP:HB2	2.41	0.47
1:I:132:ARG:HB2	1:I:143:ILE:HG23	1.95	0.47
1:A:188:ARG:NE	1:A:196:LEU:HD22	2.29	0.47
1:G:102:THR:OG1	2:H:269:GLN:HG2	2.14	0.47
2:N:166:ARG:CG	2:N:182:PRO:HB2	2.43	0.47
1:M:102:THR:HB	2:N:168:VAL:HG21	1.95	0.47
1:M:103:LEU:H	2:N:168:VAL:CG2	2.28	0.47
1:I:91:PRO:HB2	1:I:104:GLN:HE21	1.79	0.47
2:B:120:ILE:HG23	2:B:126:ILE:HD11	1.97	0.47
2:L:61:GLY:HA2	2:L:128:VAL:O	2.15	0.47
2:L:225:LEU:HA	2:L:253:THR:O	2.15	0.47
1:I:149:TYR:CB	1:I:166:LEU:HD11	2.39	0.47
2:P:208:ILE:HA	2:P:223:VAL:O	2.14	0.47
2:N:208:ILE:HA	2:N:223:VAL:O	2.15	0.47
1:I:86:ASN:HD21	1:I:110:ARG:HG3	1.80	0.47
1:A:132:ARG:HD2	1:A:205:GLU:HB3	1.96	0.47
1:O:188:ARG:NH2	1:O:196:LEU:HB2	2.29	0.47
2:N:50:GLU:OE1	2:N:98:ARG:NH2	2.48	0.47
1:E:86:ASN:HD21	1:E:110:ARG:NE	2.10	0.47
1:G:11:TYR:HB2	1:G:113:LEU:HD11	1.95	0.47
2:J:138:ASN:HD21	2:J:140:ASP:HB2	1.80	0.47
2:L:201:THR:HG21	2:L:206:ASN:ND2	2.29	0.47
2:P:26:PRO:HA	2:P:154:VAL:HA	1.97	0.47
2:J:122:ALA:HB2	2:J:152:ASN:O	2.14	0.47
2:F:38:LEU:C	2:F:40:THR:N	2.67	0.47
1:A:9:VAL:HG12	1:A:113:LEU:CD1	2.45	0.47
1:G:112:LYS:HE3	2:H:279:GLN:O	2.14	0.47
1:E:82:LEU:HD12	1:E:83:PHE:N	2.29	0.47
1:O:46:GLY:C	1:O:48:PHE:H	2.17	0.47
2:B:271:ILE:O	2:B:272:ILE:HD13	2.15	0.47
1:E:114:TYR:CE1	1:E:149:TYR:CB	2.98	0.47
2:N:34:LEU:CG	2:N:34:LEU:O	2.62	0.47
2:J:34:LEU:O	2:J:34:LEU:CG	2.63	0.47
2:N:90:THR:HB	2:N:91:PRO:HD2	1.96	0.47
1:E:39:ASN:CG	1:E:43:VAL:HG22	2.35	0.47
1:M:191:ASN:HD21	1:M:195:ALA:HB3	1.78	0.47
2:J:26:PRO:HA	2:J:154:VAL:HA	1.97	0.47
1:E:80:GLU:HA	1:E:115:TYR:O	2.15	0.47
2:L:202:ALA:N	2:L:208:ILE:O	2.47	0.47
1:I:54:LEU:C	1:I:54:LEU:HD23	2.35	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:GLU:HA	1:A:115:TYR:O	2.15	0.47
2:P:202:ALA:N	2:P:208:ILE:O	2.48	0.47
2:P:225:LEU:HA	2:P:253:THR:O	2.14	0.47
2:L:213:ALA:C	2:L:215:PHE:H	2.18	0.47
2:L:116:GLY:HA2	2:L:189:LYS:CG	2.41	0.47
2:D:135:ASN:ND2	2:D:138:ASN:H	2.12	0.47
1:A:133:PHE:HD2	1:A:140:LEU:HD21	1.80	0.47
2:P:50:GLU:OE1	2:P:98:ARG:NH2	2.48	0.47
1:A:38:GLU:CD	1:A:110:ARG:NH2	2.68	0.47
2:J:262:GLN:HG3	2:J:262:GLN:O	2.15	0.47
2:N:26:PRO:HA	2:N:154:VAL:HA	1.97	0.47
2:L:208:ILE:HA	2:L:223:VAL:O	2.15	0.47
2:D:106:ALA:HB3	4:D:626:HOH:O	2.15	0.47
1:C:142:LEU:CD2	1:C:142:LEU:N	2.78	0.47
1:M:160:ARG:CD	1:M:180:ASP:HB2	2.40	0.47
1:M:105:LEU:HA	2:N:272:ILE:O	2.15	0.47
2:J:117:GLY:HA2	2:J:156:VAL:H	1.80	0.47
2:D:92:ARG:NH1	2:D:92:ARG:HG3	2.30	0.47
1:E:132:ARG:HD2	1:E:205:GLU:HB3	1.97	0.47
2:L:46:ASN:HD22	2:L:49:PRO:HA	1.80	0.47
1:M:188:ARG:NH2	1:M:196:LEU:HB2	2.29	0.47
1:I:133:PHE:CE1	1:I:202:GLY:HA3	2.49	0.47
2:B:131:LEU:HB3	2:B:144:PHE:HB2	1.96	0.47
2:B:175:TYR:O	2:B:256:TYR:CD1	2.68	0.47
1:M:46:GLY:C	1:M:48:PHE:H	2.18	0.47
1:K:54:LEU:HD23	1:K:54:LEU:C	2.34	0.47
2:N:216:SER:N	2:N:217:PRO:CD	2.78	0.47
2:N:258:ARG:HE	2:N:263:VAL:CG2	2.28	0.47
1:O:103:LEU:H	2:P:168:VAL:CG2	2.28	0.47
1:O:193:TYR:CD2	2:P:155:VAL:HG21	2.49	0.47
1:K:188:ARG:NH2	1:K:196:LEU:HB2	2.29	0.47
1:E:107:ILE:HG12	2:F:163:VAL:HG11	1.97	0.47
2:B:209:PHE:CG	2:B:272:ILE:HD11	2.50	0.47
1:A:39:ASN:CG	1:A:43:VAL:HG22	2.35	0.47
1:I:191:ASN:HD21	1:I:195:ALA:HB3	1.80	0.47
1:I:46:GLY:C	1:I:48:PHE:H	2.18	0.47
1:M:103:LEU:H	2:N:168:VAL:HG22	1.79	0.46
2:N:213:ALA:C	2:N:215:PHE:H	2.18	0.46
1:C:132:ARG:HD2	1:C:205:GLU:HB3	1.96	0.46
2:L:50:GLU:OE1	2:L:98:ARG:NH2	2.48	0.46
2:L:148:ILE:CD1	2:L:148:ILE:N	2.78	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:26:PRO:HA	2:L:154:VAL:HA	1.97	0.46
2:F:209:PHE:CG	2:F:272:ILE:HD11	2.50	0.46
2:L:216:SER:N	2:L:217:PRO:CD	2.78	0.46
2:F:211:ASN:HD21	2:F:269:GLN:N	1.97	0.46
1:O:105:LEU:HA	2:P:272:ILE:O	2.16	0.46
2:F:120:ILE:HG23	2:F:126:ILE:HD11	1.96	0.46
1:M:193:TYR:CD2	2:N:155:VAL:HG21	2.50	0.46
1:G:86:ASN:HD21	1:G:110:ARG:HH21	1.62	0.46
2:B:116:GLY:HA2	2:B:189:LYS:CE	2.44	0.46
1:C:39:ASN:CG	1:C:43:VAL:HG22	2.35	0.46
2:D:70:ASN:ND2	2:D:119:ALA:HA	2.30	0.46
1:O:54:LEU:C	1:O:54:LEU:HD23	2.35	0.46
1:A:129:GLU:HA	1:A:200:MET:HE2	1.97	0.46
2:J:225:LEU:HA	2:J:253:THR:O	2.15	0.46
2:D:201:THR:HG23	2:D:203:ASP:H	1.81	0.46
2:N:262:GLN:O	2:N:262:GLN:HG3	2.15	0.46
2:L:138:ASN:HD21	2:L:140:ASP:HB2	1.80	0.46
2:L:234:ALA:O	2:L:235:ASN:HB2	2.15	0.46
2:L:122:ALA:HB2	2:L:152:ASN:O	2.15	0.46
2:L:38:LEU:N	2:L:38:LEU:HD12	2.30	0.46
2:F:50:GLU:CD	2:F:98:ARG:HH12	2.17	0.46
2:P:136:ASN:H	2:P:136:ASN:HD22	1.64	0.46
2:H:175:TYR:O	2:H:256:TYR:CD2	2.69	0.46
1:C:204:MET:SD	1:C:204:MET:N	2.89	0.46
2:P:258:ARG:HE	2:P:263:VAL:CG2	2.28	0.46
2:F:221:VAL:CG1	2:F:222:GLY:H	2.20	0.46
2:P:226:THR:CG2	2:P:253:THR:HB	2.43	0.46
2:L:211:ASN:HD21	2:L:213:ALA:CB	2.29	0.46
2:H:59:GLN:NE2	2:H:143:GLN:HE22	2.12	0.46
2:H:57:THR:HG22	2:H:92:ARG:HA	1.98	0.46
1:G:185:ILE:O	1:G:201:THR:HA	2.16	0.46
1:E:9:VAL:HG12	1:E:113:LEU:HD13	1.97	0.46
2:L:57:THR:HG22	2:L:91:PRO:O	2.16	0.46
1:C:154:GLU:OE1	1:C:188:ARG:CD	2.63	0.46
2:N:225:LEU:HA	2:N:253:THR:O	2.15	0.46
1:K:86:ASN:HD21	1:K:110:ARG:HG3	1.81	0.46
2:D:59:GLN:HE21	2:D:143:GLN:HE22	1.63	0.46
1:M:28:ASN:N	1:M:28:ASN:HD22	1.99	0.46
1:A:107:ILE:HG12	2:B:163:VAL:HG11	1.96	0.46
2:B:218:ALA:HA	2:B:265:ALA:O	2.15	0.46
2:P:138:ASN:HD21	2:P:140:ASP:HB2	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:9:VAL:HG12	1:G:113:LEU:HD13	1.96	0.46
2:F:262:GLN:O	2:F:262:GLN:HG3	2.15	0.46
1:A:78:ASP:OD2	1:A:79:ARG:NH2	2.46	0.46
2:D:25:ALA:HA	2:D:26:PRO:HD3	1.82	0.46
2:F:78:SER:N	4:F:547:HOH:O	2.49	0.46
1:M:54:LEU:C	1:M:54:LEU:HD23	2.36	0.46
1:O:162:LEU:HB3	1:O:175:VAL:CG1	2.44	0.46
2:J:258:ARG:HE	2:J:263:VAL:CG2	2.29	0.46
1:K:52:PRO:HG2	1:K:55:PHE:CE2	2.50	0.46
1:O:52:PRO:HG2	1:O:55:PHE:CE2	2.50	0.46
2:J:213:ALA:C	2:J:215:PHE:H	2.18	0.46
2:N:211:ASN:HD21	2:N:213:ALA:CB	2.29	0.46
2:D:59:GLN:NE2	2:D:143:GLN:HE22	2.14	0.46
2:N:138:ASN:HD21	2:N:140:ASP:HB2	1.79	0.46
2:F:48:TYR:H	3:F:502:MMA:H62	1.80	0.46
1:C:78:ASP:OD2	1:C:79:ARG:NH2	2.47	0.46
2:J:90:THR:HB	2:J:91:PRO:HD2	1.97	0.46
2:L:158:THR:HG23	2:L:158:THR:O	2.15	0.46
2:P:166:ARG:CG	2:P:182:PRO:HB2	2.42	0.46
1:K:91:PRO:HB2	1:K:104:GLN:HE21	1.80	0.46
1:I:105:LEU:HA	2:J:272:ILE:O	2.16	0.46
1:I:52:PRO:HG2	1:I:55:PHE:HE2	1.81	0.46
1:M:52:PRO:HG2	1:M:55:PHE:CE2	2.50	0.46
1:K:193:TYR:CD2	2:L:155:VAL:HG11	2.51	0.46
2:N:116:GLY:HA2	2:N:189:LYS:CG	2.41	0.46
1:M:110:ARG:N	2:N:276:PHE:O	2.49	0.46
1:G:132:ARG:HD2	1:G:205:GLU:HB3	1.98	0.46
2:J:50:GLU:OE1	2:J:98:ARG:NH2	2.48	0.46
2:H:185:VAL:O	2:H:247:ALA:HA	2.16	0.46
2:N:19:ASN:OD1	2:P:262:GLN:NE2	2.49	0.46
1:C:9:VAL:HG12	1:C:113:LEU:HD13	1.98	0.46
1:C:185:ILE:O	1:C:201:THR:HA	2.16	0.46
2:N:60:ARG:HG2	2:N:61:GLY:N	2.21	0.46
1:C:112:LYS:HE3	2:D:279:GLN:O	2.14	0.46
1:K:39:ASN:O	1:K:84:TRP:HD1	1.99	0.46
1:M:108:ILE:HD12	2:N:275:THR:OG1	2.16	0.46
1:K:28:ASN:N	1:K:28:ASN:HD22	1.99	0.46
1:G:88:LYS:CB	1:G:108:ILE:HG12	2.43	0.46
2:P:206:ASN:HD21	2:P:234:ALA:CB	2.28	0.46
1:E:185:ILE:O	1:E:201:THR:HA	2.16	0.46
2:L:41:GLN:NE2	2:L:41:GLN:HA	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:162:LEU:HB3	1:I:175:VAL:CG1	2.45	0.46
1:C:129:GLU:HA	1:C:200:MET:HE2	1.97	0.46
2:H:211:ASN:ND2	2:H:269:GLN:N	2.59	0.46
1:I:102:THR:HB	2:J:168:VAL:HG21	1.95	0.46
2:J:226:THR:CG2	2:J:253:THR:HB	2.42	0.46
1:K:100:GLU:CG	2:L:172:LEU:HD12	2.46	0.46
1:K:193:TYR:CD2	2:L:155:VAL:HG21	2.50	0.46
2:D:57:THR:HG22	2:D:92:ARG:HA	1.98	0.46
2:N:41:GLN:NE2	2:N:41:GLN:HA	2.30	0.46
2:D:262:GLN:O	2:D:262:GLN:HG3	2.16	0.46
2:D:209:PHE:CG	2:D:272:ILE:HD11	2.50	0.46
1:A:204:MET:N	1:A:204:MET:SD	2.89	0.46
1:M:132:ARG:CG	1:M:203:VAL:O	2.63	0.46
1:O:52:PRO:HG2	1:O:55:PHE:HE2	1.81	0.46
1:M:100:GLU:CG	2:N:172:LEU:HD12	2.46	0.46
1:E:135:ARG:HB2	1:E:135:ARG:HH11	1.81	0.46
1:E:112:LYS:HE3	2:F:279:GLN:O	2.16	0.46
2:L:34:LEU:O	2:L:34:LEU:CG	2.62	0.46
2:J:202:ALA:N	2:J:208:ILE:O	2.48	0.46
1:G:142:LEU:CD2	1:G:142:LEU:N	2.79	0.46
2:N:158:THR:HG23	2:N:158:THR:O	2.16	0.46
2:P:158:THR:HG23	2:P:158:THR:O	2.16	0.46
2:L:258:ARG:HE	2:L:263:VAL:CG2	2.28	0.45
2:D:211:ASN:HD22	2:D:212:THR:N	2.14	0.45
2:D:120:ILE:HG23	2:D:126:ILE:HD11	1.98	0.45
2:D:201:THR:HG23	2:D:202:ALA:N	2.31	0.45
1:I:88:LYS:CG	1:I:108:ILE:HG12	2.42	0.45
1:G:135:ARG:HB2	1:G:135:ARG:HH11	1.82	0.45
1:C:135:ARG:HB2	1:C:135:ARG:HH11	1.81	0.45
2:N:234:ALA:O	2:N:235:ASN:HB2	2.15	0.45
2:P:41:GLN:HE21	2:P:41:GLN:HA	1.81	0.45
2:H:49:PRO:HG3	2:H:98:ARG:HG3	1.98	0.45
2:P:90:THR:HB	2:P:91:PRO:HD2	1.98	0.45
1:C:153:THR:HA	1:C:164:ASN:OD1	2.16	0.45
1:O:191:ASN:HD21	1:O:195:ALA:HB3	1.79	0.45
1:K:103:LEU:H	2:L:168:VAL:CG2	2.28	0.45
2:D:211:ASN:ND2	2:D:269:GLN:N	2.60	0.45
1:C:102:THR:OG1	2:D:269:GLN:HG2	2.16	0.45
1:I:103:LEU:H	2:J:168:VAL:CG2	2.28	0.45
2:L:226:THR:CG2	2:L:253:THR:HB	2.42	0.45
1:O:110:ARG:N	2:P:276:PHE:O	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:185:VAL:O	2:B:247:ALA:HA	2.16	0.45
1:I:169:PRO:O	1:I:171:GLY:N	2.48	0.45
2:B:5:THR:HG23	2:B:7:ASN:N	2.27	0.45
2:P:38:LEU:HD12	2:P:38:LEU:N	2.30	0.45
2:J:41:GLN:HA	2:J:41:GLN:NE2	2.31	0.45
1:O:13:ALA:CB	1:O:118:ALA:H	2.29	0.45
1:C:114:TYR:CE1	1:C:149:TYR:CB	2.99	0.45
2:N:90:THR:HB	2:N:91:PRO:CD	2.47	0.45
2:B:195:TYR:CE1	2:B:238:VAL:HB	2.51	0.45
2:L:106:ALA:CB	2:L:108:TYR:HE1	2.29	0.45
1:K:132:ARG:CG	1:K:203:VAL:O	2.62	0.45
1:O:102:THR:HB	2:P:168:VAL:HG21	1.95	0.45
1:G:160:ARG:HH11	1:G:160:ARG:HG3	1.81	0.45
1:K:105:LEU:HA	2:L:272:ILE:O	2.16	0.45
1:M:52:PRO:HG2	1:M:55:PHE:HE2	1.81	0.45
2:P:213:ALA:C	2:P:215:PHE:H	2.19	0.45
2:N:113:SER:O	2:N:115:ALA:N	2.48	0.45
2:F:201:THR:HG23	2:F:203:ASP:H	1.80	0.45
1:O:39:ASN:O	1:O:84:TRP:HD1	1.99	0.45
2:F:57:THR:HG22	2:F:92:ARG:HA	1.98	0.45
2:J:148:ILE:N	2:J:148:ILE:CD1	2.79	0.45
2:N:71:PHE:CA	2:N:110:THR:O	2.64	0.45
1:C:46:GLY:O	1:C:48:PHE:N	2.50	0.45
2:F:82:TYR:OH	2:F:91:PRO:HD2	2.17	0.45
2:H:82:TYR:OH	2:H:91:PRO:HD2	2.16	0.45
1:G:77:GLN:HE21	1:G:117:PRO:HB3	1.80	0.45
1:M:162:LEU:HB3	1:M:175:VAL:CG1	2.45	0.45
1:M:177:LEU:C	1:M:179:SER:H	2.20	0.45
1:E:129:GLU:HA	1:E:200:MET:HE2	1.99	0.45
1:C:154:GLU:CD	1:C:188:ARG:HD3	2.37	0.45
1:C:159:THR:HB	1:C:180:ASP:C	2.37	0.45
2:J:211:ASN:CG	2:J:268:VAL:HG13	2.37	0.45
1:K:37:VAL:HG22	1:K:85:MET:HG2	1.99	0.45
1:O:193:TYR:CD2	2:P:155:VAL:HG11	2.51	0.45
1:I:110:ARG:N	2:J:276:PHE:O	2.50	0.45
1:A:135:ARG:HB2	1:A:135:ARG:HH11	1.82	0.45
1:E:133:PHE:HD2	1:E:140:LEU:HD21	1.80	0.45
1:I:188:ARG:NH2	1:I:196:LEU:CB	2.80	0.45
2:D:185:VAL:O	2:D:247:ALA:HA	2.16	0.45
2:P:71:PHE:CA	2:P:110:THR:O	2.63	0.45
1:O:144:ASN:HB3	1:O:167:VAL:CG1	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:144:ASN:HB3	1:I:167:VAL:CG1	2.47	0.45
1:I:24:ASN:HB2	1:I:57:MET:HE1	1.99	0.45
1:I:193:TYR:CD2	2:J:155:VAL:HG11	2.51	0.45
2:P:211:ASN:CG	2:P:268:VAL:HG13	2.37	0.45
1:K:110:ARG:N	2:L:276:PHE:O	2.49	0.45
1:M:86:ASN:HD21	1:M:110:ARG:HG3	1.81	0.45
1:E:38:GLU:CD	1:E:110:ARG:NH2	2.68	0.45
2:L:23:ASN:O	2:L:24:LEU:HD23	2.16	0.45
2:L:136:ASN:HD22	2:L:136:ASN:H	1.64	0.45
2:J:57:THR:HG22	2:J:91:PRO:O	2.16	0.45
2:J:90:THR:HB	2:J:91:PRO:CD	2.47	0.45
1:E:204:MET:N	1:E:204:MET:SD	2.89	0.45
1:M:140:LEU:O	1:M:142:LEU:HG	2.17	0.45
1:A:154:GLU:OE1	1:A:188:ARG:CD	2.65	0.45
1:A:159:THR:HB	1:A:180:ASP:C	2.37	0.45
1:K:24:ASN:HB2	1:K:57:MET:HE1	1.98	0.45
2:N:61:GLY:HA2	2:N:128:VAL:O	2.16	0.45
2:J:61:GLY:HA2	2:J:128:VAL:O	2.16	0.45
2:L:211:ASN:CG	2:L:268:VAL:HG13	2.37	0.45
1:M:193:TYR:CD2	2:N:155:VAL:HG11	2.51	0.45
2:B:57:THR:HG22	2:B:92:ARG:HA	1.99	0.45
2:B:92:ARG:NH1	2:B:92:ARG:HG3	2.31	0.45
1:C:135:ARG:HH12	1:C:177:LEU:HD21	1.81	0.45
1:M:188:ARG:NH2	1:M:196:LEU:CB	2.79	0.45
2:N:190:SER:CB	2:N:244:GLY:HA2	2.45	0.45
2:F:71:PHE:CE2	2:F:111:PRO:HG3	2.52	0.45
2:N:144:PHE:H	2:N:144:PHE:HD1	1.64	0.45
1:A:124:PRO:HD3	1:A:148:TYR:OH	2.16	0.45
1:G:46:GLY:O	1:G:48:PHE:N	2.50	0.45
2:P:34:LEU:O	2:P:34:LEU:CG	2.63	0.45
2:F:25:ALA:HA	2:F:26:PRO:HD3	1.82	0.45
2:N:66:GLY:O	2:N:70:ASN:HB2	2.17	0.45
2:J:158:THR:HG23	2:J:158:THR:O	2.17	0.45
1:E:142:LEU:CD2	1:E:142:LEU:N	2.79	0.45
2:F:75:VAL:HG13	2:F:75:VAL:O	2.15	0.45
1:K:135:ARG:CB	1:K:140:LEU:HD23	2.47	0.45
2:F:211:ASN:HD22	2:F:212:THR:N	2.15	0.45
2:N:11:ILE:CG2	2:N:16:GLY:HA3	2.33	0.45
2:L:196:TYR:HB3	2:L:237:THR:CA	2.47	0.45
2:P:196:TYR:HB3	2:P:237:THR:CA	2.46	0.45
1:M:11:TYR:CD1	1:M:18:VAL:HG21	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:39:ASN:O	1:I:84:TRP:HD1	2.00	0.45
1:O:86:ASN:HD21	1:O:110:ARG:HG3	1.81	0.45
2:D:185:VAL:HG23	2:D:243:VAL:HG11	1.99	0.45
2:J:209:PHE:HE2	2:J:234:ALA:HB2	1.78	0.45
2:J:234:ALA:O	2:J:235:ASN:HB2	2.16	0.45
2:L:39:SER:HB2	4:L:508:HOH:O	2.15	0.45
2:J:136:ASN:H	2:J:136:ASN:HD22	1.65	0.45
1:M:13:ALA:CB	1:M:118:ALA:H	2.30	0.45
1:C:167:VAL:HA	1:C:168:PRO:HD2	1.79	0.45
2:N:106:ALA:CB	2:N:108:TYR:HE1	2.29	0.45
1:E:159:THR:HB	1:E:180:ASP:C	2.37	0.45
1:A:160:ARG:HH11	1:A:160:ARG:HG3	1.82	0.45
1:M:10:ILE:HD13	1:M:114:TYR:HB2	1.99	0.45
1:O:11:TYR:CD1	1:O:18:VAL:HG21	2.52	0.45
1:M:49:ILE:HD12	1:M:49:ILE:N	2.32	0.45
2:F:59:GLN:NE2	2:F:143:GLN:HE22	2.14	0.45
1:G:38:GLU:CD	1:G:110:ARG:NH2	2.70	0.45
2:J:233:PRO:HG2	2:J:236:ASN:HB2	1.99	0.45
1:O:116:ARG:HD3	1:O:148:TYR:HE2	1.82	0.45
2:P:209:PHE:HE2	2:P:234:ALA:HB2	1.79	0.45
2:B:263:VAL:N	4:B:550:HOH:O	2.49	0.45
1:I:13:ALA:CB	1:I:118:ALA:H	2.30	0.45
2:J:23:ASN:O	2:J:24:LEU:HD23	2.15	0.45
2:L:90:THR:HB	2:L:91:PRO:HD2	1.97	0.45
2:D:164:SER:HA	4:D:611:HOH:O	2.17	0.45
1:K:141:THR:C	1:K:174:THR:HG22	2.34	0.45
1:K:160:ARG:CD	1:K:180:ASP:HB2	2.40	0.45
1:M:39:ASN:O	1:M:84:TRP:HD1	1.99	0.45
1:C:205:GLU:OXT	1:C:205:GLU:HG3	2.16	0.45
2:F:59:GLN:HE21	2:F:143:GLN:HE22	1.63	0.45
1:O:80:GLU:CD	1:O:148:TYR:HA	2.37	0.45
2:N:209:PHE:HE2	2:N:234:ALA:HB2	1.77	0.45
1:I:116:ARG:HD3	1:I:148:TYR:HE2	1.82	0.45
2:L:41:GLN:HA	2:L:41:GLN:HE21	1.82	0.45
2:P:144:PHE:H	2:P:144:PHE:HD1	1.64	0.45
2:J:106:ALA:CB	2:J:108:TYR:HE1	2.29	0.45
2:J:66:GLY:O	2:J:70:ASN:HB2	2.17	0.45
1:K:152:VAL:O	1:K:164:ASN:HB3	2.17	0.45
1:K:140:LEU:O	1:K:142:LEU:HG	2.17	0.45
1:K:177:LEU:O	1:K:179:SER:N	2.50	0.45
1:I:177:LEU:C	1:I:179:SER:H	2.20	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:160:ARG:CD	1:I:180:ASP:HB2	2.40	0.45
1:E:160:ARG:HG3	1:E:160:ARG:HH11	1.82	0.45
2:F:172:LEU:C	2:F:172:LEU:HD23	2.38	0.45
2:N:196:TYR:HB3	2:N:237:THR:CA	2.46	0.45
2:F:201:THR:CB	2:F:206:ASN:HD22	2.30	0.45
1:O:108:ILE:HD12	2:P:275:THR:OG1	2.17	0.45
2:B:5:THR:CG2	2:B:7:ASN:HB2	2.47	0.45
2:L:90:THR:HB	2:L:91:PRO:CD	2.47	0.45
2:L:66:GLY:O	2:L:70:ASN:HB2	2.17	0.45
1:E:129:GLU:HA	1:E:200:MET:HE1	1.98	0.44
2:B:211:ASN:HD22	2:B:212:THR:N	2.15	0.44
2:P:184:THR:HG22	2:P:249:SER:CA	2.47	0.44
2:H:201:THR:HG23	2:H:203:ASP:H	1.82	0.44
2:J:196:TYR:HB3	2:J:237:THR:CA	2.46	0.44
2:F:201:THR:CG2	2:F:202:ALA:N	2.80	0.44
1:G:133:PHE:HD2	1:G:140:LEU:HD21	1.81	0.44
2:B:185:VAL:HG23	2:B:243:VAL:HG11	1.99	0.44
2:H:267:ASN:N	2:H:267:ASN:ND2	2.63	0.44
2:J:144:PHE:H	2:J:144:PHE:HD1	1.64	0.44
1:K:81:SER:O	1:K:83:PHE:CD1	2.70	0.44
2:B:6:ALA:HB3	4:B:553:HOH:O	2.16	0.44
1:M:152:VAL:O	1:M:164:ASN:HB3	2.17	0.44
2:P:118:VAL:HG12	2:P:121:LYS:HE2	1.99	0.44
1:E:153:THR:HA	1:E:164:ASN:OD1	2.17	0.44
2:H:105:VAL:HG11	2:H:129:LEU:HD13	1.99	0.44
1:K:52:PRO:HG2	1:K:55:PHE:HE2	1.81	0.44
2:H:120:ILE:HG23	2:H:126:ILE:HD11	1.98	0.44
1:G:205:GLU:OXT	1:G:205:GLU:HG3	2.17	0.44
2:H:92:ARG:NH1	2:H:92:ARG:HG3	2.31	0.44
1:E:205:GLU:HG3	1:E:205:GLU:OXT	2.17	0.44
2:D:71:PHE:CE2	2:D:111:PRO:HG3	2.52	0.44
1:C:38:GLU:CD	1:C:110:ARG:NH2	2.70	0.44
2:J:41:GLN:HA	2:J:41:GLN:HE21	1.83	0.44
1:C:66:ARG:HG2	1:C:66:ARG:NH1	2.32	0.44
2:L:144:PHE:H	2:L:144:PHE:HD1	1.64	0.44
1:G:66:ARG:HG2	1:G:66:ARG:NH1	2.32	0.44
1:K:13:ALA:CB	1:K:118:ALA:H	2.30	0.44
1:A:30:THR:HG22	1:A:31:TYR:N	2.32	0.44
1:A:167:VAL:HA	1:A:168:PRO:HD2	1.79	0.44
1:K:162:LEU:HB3	1:K:175:VAL:CG1	2.45	0.44
1:K:177:LEU:C	1:K:179:SER:H	2.20	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:177:LEU:O	1:M:179:SER:N	2.50	0.44
1:O:177:LEU:C	1:O:179:SER:H	2.20	0.44
1:C:129:GLU:HG3	1:C:130:LYS:N	2.33	0.44
2:H:211:ASN:HD22	2:H:212:THR:N	2.16	0.44
2:B:174:ASP:C	2:B:176:PRO:HD2	2.38	0.44
2:P:61:GLY:HA2	2:P:128:VAL:O	2.17	0.44
2:N:211:ASN:CG	2:N:268:VAL:HG13	2.37	0.44
2:B:201:THR:HG23	2:B:203:ASP:H	1.82	0.44
1:M:110:ARG:HB3	2:N:277:VAL:HA	1.98	0.44
1:O:88:LYS:CG	1:O:108:ILE:HG12	2.42	0.44
1:K:116:ARG:HD3	1:K:148:TYR:HE2	1.83	0.44
1:C:46:GLY:O	1:C:47:ARG:C	2.56	0.44
1:A:9:VAL:CG1	1:A:113:LEU:HD13	2.47	0.44
2:H:116:GLY:HA2	2:H:189:LYS:CE	2.45	0.44
2:J:15:GLY:HA2	2:J:144:PHE:CG	2.53	0.44
1:C:142:LEU:HD12	1:C:152:VAL:HG21	1.99	0.44
1:E:58:LYS:HG3	4:E:222:HOH:O	2.17	0.44
2:D:1:PHE:CG	2:D:133:ASN:ND2	2.86	0.44
1:G:159:THR:HB	1:G:180:ASP:C	2.37	0.44
2:N:184:THR:HG22	2:N:249:SER:CA	2.47	0.44
2:J:181:ILE:HA	2:J:182:PRO:HD3	1.81	0.44
2:J:184:THR:HG22	2:J:249:SER:CA	2.47	0.44
1:K:4:LEU:HD11	1:K:87:VAL:HG23	2.00	0.44
1:M:51:THR:O	1:M:66:ARG:N	2.50	0.44
1:M:52:PRO:HG2	1:M:65:LEU:HD23	2.00	0.44
2:H:201:THR:CB	2:H:206:ASN:HD22	2.31	0.44
1:O:10:ILE:HD13	1:O:114:TYR:HB2	1.99	0.44
1:O:100:GLU:CG	2:P:172:LEU:HD12	2.45	0.44
1:I:108:ILE:HD12	2:J:275:THR:OG1	2.17	0.44
2:F:218:ALA:HB2	2:F:266:GLY:HA3	1.99	0.44
2:P:23:ASN:O	2:P:24:LEU:HD23	2.17	0.44
2:H:209:PHE:CG	2:H:272:ILE:HD11	2.52	0.44
2:N:136:ASN:HD22	2:N:136:ASN:H	1.65	0.44
1:A:39:ASN:OD1	1:A:43:VAL:HG22	2.18	0.44
2:H:87:THR:HG21	2:L:68:LEU:CD1	2.48	0.44
1:G:75:LEU:HD22	1:G:76:PRO:HD2	1.99	0.44
1:I:135:ARG:CB	1:I:140:LEU:HD23	2.47	0.44
1:I:177:LEU:O	1:I:179:SER:N	2.50	0.44
1:K:52:PRO:HG2	1:K:65:LEU:HD23	2.00	0.44
2:H:221:VAL:CG1	2:H:222:GLY:H	2.19	0.44
1:M:149:TYR:CD2	1:M:168:PRO:HA	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:110:ARG:HB3	2:L:277:VAL:HA	1.99	0.44
2:J:190:SER:CB	2:J:244:GLY:HA2	2.45	0.44
2:P:233:PRO:HG2	2:P:236:ASN:HB2	1.99	0.44
1:M:116:ARG:HD3	1:M:148:TYR:HE2	1.81	0.44
2:L:209:PHE:HE2	2:L:234:ALA:HB2	1.78	0.44
2:N:41:GLN:HE21	2:N:41:GLN:HA	1.82	0.44
2:D:5:THR:CG2	2:D:7:ASN:HB2	2.48	0.44
2:D:49:PRO:HG3	2:D:98:ARG:HG3	2.00	0.44
2:F:167:ASP:O	2:F:168:VAL:C	2.56	0.44
1:K:49:ILE:N	1:K:49:ILE:HD12	2.33	0.44
1:O:135:ARG:CB	1:O:140:LEU:HD23	2.47	0.44
2:L:184:THR:HG22	2:L:249:SER:CA	2.48	0.44
1:O:31:TYR:HB3	1:O:89:ALA:HB1	1.98	0.44
2:B:33:ASN:ND2	2:B:110:THR:OG1	2.51	0.44
1:A:205:GLU:HG3	1:A:205:GLU:OXT	2.17	0.44
2:H:185:VAL:HG23	2:H:243:VAL:HG11	1.99	0.44
1:K:80:GLU:CD	1:K:148:TYR:HA	2.38	0.44
1:K:80:GLU:OE2	1:K:116:ARG:NE	2.47	0.44
2:N:148:ILE:N	2:N:148:ILE:CD1	2.80	0.44
1:I:78:ASP:OD1	1:I:79:ARG:N	2.51	0.44
2:F:5:THR:CG2	2:F:7:ASN:HB2	2.48	0.44
2:N:59:GLN:HG3	2:N:143:GLN:NE2	2.31	0.44
2:F:49:PRO:HG3	2:F:98:ARG:HG3	2.00	0.44
1:E:28:ASN:ND2	1:E:28:ASN:N	2.66	0.44
1:O:81:SER:O	1:O:83:PHE:CD1	2.70	0.44
2:P:55:TYR:OH	2:P:136:ASN:HB3	2.18	0.44
2:H:82:TYR:N	2:H:82:TYR:CD1	2.86	0.44
2:B:148:ILE:N	2:B:148:ILE:HD12	2.32	0.44
1:O:49:ILE:N	1:O:49:ILE:HD12	2.33	0.44
1:K:11:TYR:CD1	1:K:18:VAL:HG21	2.52	0.44
1:A:27:GLU:HG3	1:A:60:LYS:HZ3	1.79	0.44
1:E:140:LEU:HB2	1:E:177:LEU:HD13	2.00	0.44
2:L:233:PRO:HG2	2:L:236:ASN:HB2	1.99	0.44
2:B:71:PHE:CE2	2:B:111:PRO:HG3	2.53	0.44
1:I:80:GLU:CD	1:I:148:TYR:HA	2.38	0.44
2:P:148:ILE:N	2:P:148:ILE:CD1	2.81	0.44
1:A:185:ILE:O	1:A:201:THR:HA	2.17	0.44
2:H:5:THR:CG2	2:H:7:ASN:HB2	2.48	0.44
2:H:262:GLN:O	2:H:262:GLN:HG3	2.18	0.44
1:G:77:GLN:HA	1:G:77:GLN:HE21	1.82	0.44
2:J:118:VAL:HG12	2:J:121:LYS:HE2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:THR:HA	1:A:164:ASN:OD1	2.18	0.44
2:N:118:VAL:HG12	2:N:121:LYS:HE2	2.00	0.44
1:I:49:ILE:N	1:I:49:ILE:HD12	2.33	0.44
1:O:177:LEU:O	1:O:179:SER:N	2.50	0.44
1:I:140:LEU:O	1:I:142:LEU:HG	2.17	0.44
2:L:168:VAL:O	2:L:168:VAL:HG13	2.18	0.44
2:N:168:VAL:O	2:N:168:VAL:HG13	2.18	0.44
1:O:24:ASN:HB2	1:O:57:MET:HE1	2.00	0.44
1:M:67:ILE:HD11	1:M:85:MET:SD	2.58	0.44
1:I:110:ARG:HB3	2:J:277:VAL:HA	1.99	0.44
2:H:135:ASN:HD21	2:H:138:ASN:H	1.65	0.44
1:K:188:ARG:NH2	1:K:196:LEU:CB	2.80	0.44
1:M:176:LYS:HB2	1:M:176:LYS:HZ3	1.82	0.44
2:P:106:ALA:CB	2:P:108:TYR:HE1	2.30	0.44
2:D:167:ASP:O	2:D:168:VAL:C	2.55	0.44
1:A:77:GLN:HE21	1:A:117:PRO:HB3	1.83	0.44
1:E:16:LYS:HB3	4:E:223:HOH:O	2.18	0.44
1:C:160:ARG:HH11	1:C:160:ARG:HG3	1.82	0.44
1:I:51:THR:O	1:I:66:ARG:N	2.50	0.44
1:I:52:PRO:HG2	1:I:65:LEU:HD23	2.00	0.44
1:I:4:LEU:HD11	1:I:87:VAL:HG23	2.00	0.44
1:K:149:TYR:CB	1:K:166:LEU:HD11	2.39	0.44
2:J:112:VAL:O	2:J:113:SER:C	2.57	0.44
1:I:11:TYR:CD1	1:I:18:VAL:HG21	2.52	0.44
1:I:17:GLN:HB3	1:I:68:LEU:CD2	2.41	0.44
2:F:201:THR:HB	4:F:529:HOH:O	2.17	0.44
2:F:185:VAL:HG23	2:F:243:VAL:HG11	2.00	0.44
2:F:185:VAL:O	2:F:247:ALA:HA	2.18	0.44
2:B:218:ALA:HB2	2:B:266:GLY:HA3	1.99	0.44
1:M:80:GLU:OE2	1:M:116:ARG:NE	2.47	0.44
2:H:71:PHE:CE2	2:H:111:PRO:HG3	2.53	0.44
2:P:75:VAL:HB	2:P:84:PHE:HB2	2.00	0.44
1:M:127:ALA:HA	1:M:146:THR:HG21	2.00	0.44
1:I:81:SER:O	1:I:83:PHE:CD1	2.70	0.44
1:E:142:LEU:HD12	1:E:152:VAL:HG21	2.00	0.44
2:P:66:GLY:O	2:P:70:ASN:HB2	2.17	0.44
1:A:129:GLU:HA	1:A:200:MET:HE1	2.00	0.43
1:G:154:GLU:CD	1:G:188:ARG:HD3	2.38	0.43
2:F:174:ASP:C	2:F:176:PRO:HD2	2.39	0.43
2:J:184:THR:HG22	2:J:249:SER:HA	1.99	0.43
2:J:172:LEU:C	2:J:172:LEU:HD23	2.38	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:201:THR:HB	4:D:633:HOH:O	2.18	0.43
2:D:201:THR:CG2	2:D:202:ALA:N	2.81	0.43
1:I:85:MET:HB2	1:I:111:ILE:HG13	2.00	0.43
2:L:172:LEU:C	2:L:172:LEU:HD23	2.38	0.43
2:J:116:GLY:HA2	2:J:189:LYS:CG	2.40	0.43
1:O:28:ASN:N	1:O:28:ASN:ND2	2.57	0.43
1:K:127:ALA:HA	1:K:146:THR:HG21	2.00	0.43
2:N:233:PRO:HG2	2:N:236:ASN:HB2	1.98	0.43
1:M:80:GLU:CD	1:M:148:TYR:HA	2.38	0.43
2:J:206:ASN:HD21	2:J:234:ALA:CB	2.28	0.43
2:B:49:PRO:HG3	2:B:98:ARG:HG3	2.00	0.43
1:G:46:GLY:O	1:G:47:ARG:C	2.56	0.43
1:G:5:GLY:O	2:H:159:GLY:HA2	2.18	0.43
1:O:152:VAL:O	1:O:164:ASN:HB3	2.18	0.43
2:L:118:VAL:HG12	2:L:121:LYS:HE2	2.00	0.43
1:O:163:GLU:N	1:O:175:VAL:HG11	2.14	0.43
1:M:24:ASN:HB2	1:M:57:MET:HE1	2.01	0.43
1:I:149:TYR:CD2	1:I:168:PRO:HA	2.53	0.43
2:B:89:GLU:N	4:B:528:HOH:O	2.35	0.43
2:N:192:ASN:HB2	2:N:279:GLN:NE2	2.34	0.43
1:O:188:ARG:NH2	1:O:196:LEU:CB	2.80	0.43
2:P:190:SER:CB	2:P:244:GLY:HA2	2.45	0.43
1:A:77:GLN:HA	1:A:77:GLN:HE21	1.82	0.43
1:A:142:LEU:HD12	1:A:152:VAL:HG21	2.00	0.43
2:B:87:THR:HG21	2:P:68:LEU:CD1	2.47	0.43
1:E:75:LEU:HD22	1:E:76:PRO:HD2	2.00	0.43
1:M:135:ARG:CB	1:M:140:LEU:HD23	2.48	0.43
2:J:258:ARG:HG2	2:J:263:VAL:HG23	2.01	0.43
2:H:174:ASP:C	2:H:176:PRO:HD2	2.39	0.43
2:P:184:THR:HG22	2:P:249:SER:HA	1.99	0.43
1:O:51:THR:O	1:O:66:ARG:N	2.50	0.43
2:H:201:THR:HG23	2:H:202:ALA:N	2.32	0.43
1:M:85:MET:HE3	4:M:206:HOH:O	2.17	0.43
1:K:108:ILE:HD12	2:L:275:THR:OG1	2.18	0.43
1:C:185:ILE:CB	1:C:202:GLY:HA3	2.47	0.43
1:C:82:LEU:HD12	1:C:83:PHE:N	2.33	0.43
1:K:128:ALA:CA	1:K:150:LEU:HD22	2.48	0.43
2:N:55:TYR:OH	2:N:136:ASN:HB3	2.18	0.43
2:H:25:ALA:HA	2:H:26:PRO:HD3	1.83	0.43
2:F:105:VAL:HG11	2:F:129:LEU:HD13	2.00	0.43
2:P:258:ARG:HG2	2:P:263:VAL:HG23	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:258:ARG:HG2	2:N:263:VAL:HG23	2.01	0.43
1:K:51:THR:O	1:K:66:ARG:N	2.50	0.43
1:O:52:PRO:HG2	1:O:65:LEU:HD23	2.01	0.43
1:I:24:ASN:HD22	1:I:60:LYS:HA	1.83	0.43
1:I:20:LEU:O	1:I:65:LEU:N	2.51	0.43
1:I:10:ILE:HD13	1:I:114:TYR:HB2	1.99	0.43
1:I:100:GLU:CG	2:J:172:LEU:HD12	2.46	0.43
1:M:85:MET:HB2	1:M:111:ILE:HG13	2.00	0.43
1:O:110:ARG:HB3	2:P:277:VAL:HA	1.99	0.43
1:E:135:ARG:HH12	1:E:177:LEU:HD21	1.83	0.43
1:M:8:ARG:NH1	1:M:8:ARG:CB	2.81	0.43
1:C:185:ILE:HB	1:C:202:GLY:CA	2.44	0.43
2:N:206:ASN:HD21	2:N:234:ALA:CB	2.29	0.43
1:G:185:ILE:HB	1:G:202:GLY:CA	2.46	0.43
1:E:185:ILE:HB	1:E:202:GLY:CA	2.47	0.43
2:B:167:ASP:O	2:B:168:VAL:C	2.56	0.43
1:M:128:ALA:CA	1:M:150:LEU:HD22	2.48	0.43
1:E:77:GLN:HE21	1:E:117:PRO:HB3	1.83	0.43
2:L:258:ARG:HG2	2:L:263:VAL:HG23	2.00	0.43
2:D:226:THR:HG23	2:D:253:THR:HB	2.01	0.43
2:N:184:THR:HG22	2:N:249:SER:HA	1.99	0.43
1:M:20:LEU:O	1:M:65:LEU:N	2.51	0.43
2:P:60:ARG:HG2	2:P:61:GLY:N	2.21	0.43
1:K:149:TYR:HD2	1:K:166:LEU:HG	1.83	0.43
2:N:112:VAL:O	2:N:113:SER:C	2.57	0.43
1:K:28:ASN:O	1:K:28:ASN:ND2	2.51	0.43
2:L:103:TRP:CH2	2:L:131:LEU:HB2	2.54	0.43
1:A:46:GLY:O	1:A:47:ARG:C	2.57	0.43
1:A:82:LEU:HD12	1:A:83:PHE:N	2.34	0.43
1:E:46:GLY:O	1:E:48:PHE:N	2.51	0.43
1:A:28:ASN:N	1:A:28:ASN:ND2	2.65	0.43
1:A:75:LEU:HD22	1:A:76:PRO:HD2	1.99	0.43
2:F:82:TYR:N	2:F:82:TYR:CD1	2.86	0.43
1:M:81:SER:O	1:M:83:PHE:CD1	2.71	0.43
1:I:128:ALA:CA	1:I:150:LEU:HD22	2.48	0.43
1:E:30:THR:HG22	1:E:31:TYR:N	2.33	0.43
1:C:30:THR:HG22	1:C:31:TYR:N	2.33	0.43
2:F:1:PHE:CG	2:F:133:ASN:ND2	2.87	0.43
1:A:154:GLU:CD	1:A:188:ARG:HD3	2.38	0.43
1:G:154:GLU:OE1	1:G:188:ARG:CD	2.65	0.43
1:C:127:ALA:C	1:C:129:GLU:H	2.22	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:226:THR:HG23	2:H:253:THR:HB	2.01	0.43
1:O:149:TYR:CD2	1:O:168:PRO:HA	2.54	0.43
2:F:221:VAL:HG11	2:F:256:TYR:HD2	1.83	0.43
2:J:211:ASN:ND2	2:J:269:GLN:H	2.17	0.43
1:K:88:LYS:CG	1:K:108:ILE:HG12	2.42	0.43
2:N:172:LEU:C	2:N:172:LEU:HD23	2.39	0.43
2:B:135:ASN:HD21	2:B:138:ASN:H	1.67	0.43
1:M:28:ASN:ND2	1:M:28:ASN:O	2.52	0.43
1:E:88:LYS:CB	1:E:108:ILE:HG12	2.44	0.43
2:L:206:ASN:HD21	2:L:234:ALA:CB	2.28	0.43
2:L:59:GLN:HG3	2:L:143:GLN:NE2	2.29	0.43
2:L:15:GLY:HA2	2:L:144:PHE:CG	2.53	0.43
1:G:82:LEU:HD12	1:G:83:PHE:N	2.33	0.43
2:B:82:TYR:N	2:B:82:TYR:CD1	2.87	0.43
2:D:82:TYR:CD1	2:D:82:TYR:N	2.86	0.43
2:P:90:THR:HB	2:P:91:PRO:CD	2.48	0.43
2:F:195:TYR:CE1	2:F:238:VAL:HB	2.53	0.43
2:B:1:PHE:CG	2:B:133:ASN:ND2	2.87	0.43
1:K:135:ARG:HB3	1:K:140:LEU:HD23	2.00	0.43
1:M:135:ARG:HD3	1:M:136:SER:O	2.18	0.43
1:O:140:LEU:O	1:O:142:LEU:HG	2.18	0.43
1:O:132:ARG:CG	1:O:203:VAL:O	2.63	0.43
1:G:129:GLU:HG3	1:G:130:LYS:N	2.32	0.43
2:D:174:ASP:C	2:D:176:PRO:HD2	2.39	0.43
1:I:31:TYR:HB3	1:I:89:ALA:HB1	1.99	0.43
1:I:37:VAL:HG22	1:I:85:MET:HG2	2.00	0.43
2:P:112:VAL:O	2:P:113:SER:C	2.57	0.43
2:N:211:ASN:ND2	2:N:269:GLN:H	2.17	0.43
1:G:86:ASN:HD21	1:G:110:ARG:NE	2.10	0.43
1:O:169:PRO:O	1:O:171:GLY:N	2.48	0.43
2:N:23:ASN:O	2:N:24:LEU:HD23	2.18	0.43
2:F:267:ASN:ND2	2:F:267:ASN:N	2.65	0.43
2:F:116:GLY:HA2	2:F:189:LYS:NZ	2.33	0.43
1:E:66:ARG:HG2	1:E:66:ARG:NH1	2.33	0.43
1:M:126:GLN:HE21	1:M:126:GLN:HB2	1.53	0.43
1:E:46:GLY:O	1:E:47:ARG:C	2.56	0.43
2:D:105:VAL:HG11	2:D:129:LEU:HD13	2.00	0.43
1:G:153:THR:HA	1:G:164:ASN:OD1	2.18	0.43
1:M:135:ARG:HB3	1:M:140:LEU:HD23	2.00	0.43
1:I:135:ARG:HD3	1:I:136:SER:O	2.18	0.43
1:A:127:ALA:C	1:A:129:GLU:H	2.22	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:GLU:HG3	1:A:130:LYS:N	2.33	0.43
1:E:129:GLU:HG3	1:E:130:LYS:N	2.32	0.43
2:F:226:THR:HG23	2:F:253:THR:HB	2.01	0.43
2:P:168:VAL:HG13	2:P:168:VAL:O	2.18	0.43
1:O:24:ASN:HB3	1:O:60:LYS:HA	2.00	0.43
1:K:10:ILE:O	1:K:12:PRO:HD3	2.19	0.43
2:D:126:ILE:HD11	2:D:150:ALA:HB2	2.01	0.43
1:I:108:ILE:HG22	1:I:109:SER:N	2.34	0.43
2:H:218:ALA:HB2	2:H:266:GLY:HA3	1.99	0.43
2:B:34:LEU:HD12	2:B:34:LEU:HA	1.90	0.43
1:K:78:ASP:OD1	1:K:79:ARG:N	2.52	0.43
1:K:185:ILE:CG2	1:K:202:GLY:HA3	2.48	0.43
1:E:28:ASN:N	1:E:28:ASN:HD22	2.16	0.43
2:B:60:ARG:HD3	4:B:545:HOH:O	2.18	0.43
1:M:134:ARG:CZ	1:M:141:THR:HG21	2.49	0.43
1:O:135:ARG:HB3	1:O:140:LEU:HD23	2.00	0.43
1:I:135:ARG:HB3	1:I:140:LEU:HD23	2.00	0.43
1:C:188:ARG:NE	1:C:196:LEU:HD22	2.31	0.43
2:B:172:LEU:HD23	2:B:172:LEU:C	2.39	0.43
2:D:172:LEU:HD23	2:D:172:LEU:C	2.38	0.43
2:J:168:VAL:HG13	2:J:168:VAL:O	2.18	0.43
1:M:4:LEU:HD11	1:M:87:VAL:HG23	2.00	0.43
1:O:37:VAL:HG22	1:O:85:MET:HG2	2.00	0.43
1:K:85:MET:HB2	1:K:111:ILE:HG13	2.01	0.43
1:A:140:LEU:HB2	1:A:177:LEU:HD13	2.01	0.43
2:L:43:PHE:HE2	2:L:102:PRO:HG3	1.82	0.43
2:J:75:VAL:HB	2:J:84:PHE:HB2	2.00	0.43
2:J:55:TYR:OH	2:J:136:ASN:HB3	2.19	0.43
2:B:48:TYR:HE2	3:B:500:MMA:H73	1.83	0.43
2:L:55:TYR:OH	2:L:136:ASN:HB3	2.19	0.43
2:D:195:TYR:CE1	2:D:238:VAL:HB	2.53	0.43
1:I:152:VAL:O	1:I:164:ASN:HB3	2.18	0.43
1:G:67:ILE:N	1:G:67:ILE:HD12	2.34	0.43
2:H:78:SER:N	4:H:636:HOH:O	2.52	0.43
1:M:24:ASN:HB3	1:M:60:LYS:HA	2.01	0.43
2:F:148:ILE:HD12	2:F:148:ILE:N	2.33	0.43
1:O:149:TYR:HD2	1:O:166:LEU:HG	1.83	0.43
2:P:116:GLY:HA2	2:P:189:LYS:CG	2.40	0.43
2:J:49:PRO:HD2	2:J:98:ARG:CZ	2.49	0.43
1:E:38:GLU:CD	1:E:110:ARG:HH22	2.22	0.43
1:M:116:ARG:HA	1:M:117:PRO:HD3	1.87	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:24:LEU:O	2:L:152:ASN:ND2	2.52	0.43
2:N:15:GLY:HA2	2:N:144:PHE:CG	2.53	0.43
2:P:15:GLY:HA2	2:P:144:PHE:CG	2.53	0.43
2:J:43:PHE:HE2	2:J:102:PRO:HG3	1.83	0.43
2:L:35:VAL:HA	2:L:107:LEU:O	2.19	0.43
3:H:603:MMA:H2	4:H:645:HOH:O	2.19	0.43
1:M:48:PHE:HA	1:M:48:PHE:HD1	1.72	0.43
1:K:135:ARG:HD3	1:K:136:SER:O	2.18	0.42
1:O:135:ARG:HA	1:O:140:LEU:HA	2.01	0.42
1:I:163:GLU:HB3	1:I:175:VAL:CG1	2.49	0.42
1:G:188:ARG:NE	1:G:196:LEU:HD22	2.31	0.42
1:E:127:ALA:C	1:E:129:GLU:H	2.23	0.42
2:H:172:LEU:C	2:H:172:LEU:HD23	2.39	0.42
1:K:31:TYR:HB3	1:K:89:ALA:HB1	1.99	0.42
2:H:201:THR:CG2	2:H:202:ALA:N	2.82	0.42
1:O:149:TYR:CD2	1:O:166:LEU:HG	2.54	0.42
2:P:172:LEU:C	2:P:172:LEU:HD23	2.38	0.42
2:B:201:THR:CB	2:B:206:ASN:HD22	2.32	0.42
1:M:108:ILE:HG22	1:M:109:SER:N	2.34	0.42
1:A:38:GLU:CD	1:A:110:ARG:HH22	2.21	0.42
2:J:71:PHE:CA	2:J:110:THR:O	2.64	0.42
1:O:126:GLN:HB2	1:O:126:GLN:HE21	1.53	0.42
1:G:103:LEU:HD11	2:H:272:ILE:HG12	2.01	0.42
1:E:9:VAL:HG22	4:E:209:HOH:O	2.19	0.42
2:H:1:PHE:CG	2:H:133:ASN:ND2	2.87	0.42
2:H:75:VAL:O	2:H:75:VAL:HG13	2.19	0.42
1:O:135:ARG:HD3	1:O:136:SER:O	2.19	0.42
1:O:134:ARG:CZ	1:O:141:THR:HG21	2.49	0.42
2:D:170:VAL:C	2:D:172:LEU:N	2.72	0.42
1:K:4:LEU:O	2:L:160:GLY:N	2.47	0.42
1:O:24:ASN:HD22	1:O:60:LYS:HA	1.83	0.42
1:O:4:LEU:HD11	1:O:87:VAL:HG23	2.00	0.42
1:K:149:TYR:CD2	1:K:168:PRO:HA	2.54	0.42
1:I:149:TYR:HD2	1:I:166:LEU:HG	1.84	0.42
2:P:211:ASN:ND2	2:P:269:GLN:H	2.17	0.42
2:P:268:VAL:C	2:P:269:GLN:HG3	2.38	0.42
1:K:67:ILE:HD11	1:K:85:MET:SD	2.60	0.42
2:B:59:GLN:NE2	2:B:143:GLN:HE22	2.17	0.42
1:O:127:ALA:HA	1:O:146:THR:HG21	2.01	0.42
1:G:9:VAL:HG12	1:G:113:LEU:CD1	2.48	0.42
1:C:86:ASN:HD21	1:C:110:ARG:HH21	1.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:116:GLY:HA2	2:B:189:LYS:NZ	2.34	0.42
1:A:28:ASN:N	1:A:28:ASN:HD22	2.16	0.42
1:O:128:ALA:CA	1:O:150:LEU:HD22	2.48	0.42
1:E:77:GLN:HA	1:E:77:GLN:HE21	1.84	0.42
1:C:75:LEU:HD22	1:C:76:PRO:HD2	2.01	0.42
2:N:200:THR:O	2:N:200:THR:HG22	2.19	0.42
2:P:36:VAL:O	2:P:36:VAL:HG12	2.19	0.42
2:J:200:THR:O	2:J:200:THR:HG22	2.19	0.42
1:K:135:ARG:NH2	1:K:177:LEU:CD2	2.82	0.42
2:P:181:ILE:HA	2:P:182:PRO:HD3	1.81	0.42
2:L:166:ARG:HG2	2:L:182:PRO:CB	2.47	0.42
1:K:20:LEU:O	1:K:65:LEU:N	2.52	0.42
1:K:33:ILE:HG13	1:K:55:PHE:CE1	2.54	0.42
2:J:173:PRO:O	2:J:174:ASP:O	2.38	0.42
1:K:108:ILE:HG22	1:K:109:SER:N	2.34	0.42
1:I:28:ASN:O	1:I:28:ASN:ND2	2.52	0.42
1:A:86:ASN:HD21	1:A:110:ARG:HH21	1.68	0.42
1:E:9:VAL:HG12	1:E:113:LEU:CD1	2.48	0.42
1:G:30:THR:HG22	1:G:31:TYR:N	2.32	0.42
1:I:194:GLY:HA3	2:J:158:THR:CG2	2.49	0.42
2:J:134:THR:HG22	2:J:141:ASP:HA	2.01	0.42
2:J:36:VAL:O	2:J:36:VAL:HG12	2.20	0.42
2:N:258:ARG:NE	2:N:263:VAL:HG23	2.35	0.42
1:A:188:ARG:NH1	1:A:188:ARG:HG2	2.33	0.42
2:B:211:ASN:HD21	2:B:269:GLN:N	1.96	0.42
2:L:184:THR:HG22	2:L:249:SER:HA	2.00	0.42
1:O:20:LEU:O	1:O:65:LEU:N	2.53	0.42
1:I:24:ASN:HB3	1:I:60:LYS:HA	2.00	0.42
1:K:10:ILE:HD13	1:K:114:TYR:HB2	1.99	0.42
2:L:113:SER:O	2:L:115:ALA:N	2.47	0.42
1:O:108:ILE:HG22	1:O:109:SER:N	2.35	0.42
2:J:192:ASN:HB2	2:J:279:GLN:NE2	2.34	0.42
2:N:192:ASN:HB2	2:N:279:GLN:HE21	1.84	0.42
1:A:135:ARG:HH12	1:A:177:LEU:HD21	1.83	0.42
2:P:49:PRO:HD2	2:P:98:ARG:CZ	2.50	0.42
1:O:8:ARG:CB	1:O:8:ARG:NH1	2.81	0.42
1:C:107:ILE:HG12	2:D:163:VAL:HG11	1.99	0.42
1:M:78:ASP:OD1	1:M:79:ARG:N	2.53	0.42
1:O:78:ASP:OD1	1:O:79:ARG:N	2.51	0.42
2:L:71:PHE:CA	2:L:110:THR:O	2.63	0.42
2:J:15:GLY:HA2	2:J:144:PHE:CE1	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:28:ASN:ND2	1:C:28:ASN:N	2.66	0.42
2:N:75:VAL:HB	2:N:84:PHE:HB2	2.00	0.42
1:E:39:ASN:OD1	1:E:43:VAL:HG22	2.20	0.42
1:G:167:VAL:HA	1:G:168:PRO:HD2	1.79	0.42
1:A:5:GLY:O	2:B:159:GLY:HA2	2.19	0.42
1:K:134:ARG:CZ	1:K:141:THR:HG21	2.49	0.42
1:O:23:THR:CG2	1:O:24:ASN:N	2.82	0.42
2:L:196:TYR:HD1	2:L:197:LEU:O	2.02	0.42
2:J:268:VAL:C	2:J:269:GLN:HG3	2.39	0.42
1:K:17:GLN:HB3	1:K:68:LEU:CD2	2.41	0.42
2:F:201:THR:CB	2:F:206:ASN:ND2	2.82	0.42
2:F:240:LEU:HA	2:F:240:LEU:HD23	1.86	0.42
1:G:107:ILE:HG12	2:H:163:VAL:HG11	2.01	0.42
1:A:185:ILE:HB	1:A:202:GLY:CA	2.46	0.42
2:L:13:ILE:HG22	2:L:14:GLY:N	2.34	0.42
1:C:28:ASN:HD22	1:C:28:ASN:N	2.17	0.42
1:M:118:ALA:O	1:M:119:LYS:HB2	2.20	0.42
2:B:117:GLY:O	2:B:155:VAL:HG22	2.19	0.42
1:O:143:ILE:HA	1:O:172:GLU:HB3	2.00	0.42
1:G:127:ALA:C	1:G:129:GLU:H	2.23	0.42
1:I:149:TYR:CD2	1:I:166:LEU:HG	2.55	0.42
2:H:183:LEU:HD22	2:H:250:LEU:CD1	2.49	0.42
2:D:33:ASN:ND2	2:D:110:THR:OG1	2.52	0.42
1:O:28:ASN:O	1:O:28:ASN:ND2	2.53	0.42
2:F:185:VAL:O	2:F:243:VAL:CG1	2.68	0.42
2:J:138:ASN:C	2:J:138:ASN:HD22	2.23	0.42
2:F:34:LEU:HA	2:F:34:LEU:HD12	1.91	0.42
2:D:267:ASN:N	2:D:267:ASN:ND2	2.64	0.42
2:P:24:LEU:O	2:P:152:ASN:ND2	2.53	0.42
2:P:41:GLN:HE21	2:P:41:GLN:CA	2.33	0.42
2:L:52:ILE:HG23	2:L:137:TYR:CB	2.49	0.42
2:P:35:VAL:HA	2:P:107:LEU:O	2.19	0.42
1:A:46:GLY:O	1:A:48:PHE:N	2.53	0.42
2:H:167:ASP:O	2:H:168:VAL:C	2.57	0.42
1:C:39:ASN:OD1	1:C:43:VAL:HG22	2.19	0.42
2:L:134:THR:HG22	2:L:141:ASP:HA	2.02	0.42
2:P:175:TYR:N	2:P:176:PRO:HD2	2.35	0.42
1:M:103:LEU:HD22	2:N:254:ALA:HB2	2.02	0.42
1:K:23:THR:HB	4:K:212:HOH:O	2.19	0.42
1:K:24:ASN:HD22	1:K:60:LYS:HA	1.84	0.42
1:I:23:THR:CG2	1:I:24:ASN:N	2.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:201:THR:CB	2:H:206:ASN:ND2	2.83	0.42
1:K:114:TYR:OH	1:K:149:TYR:HB2	2.20	0.42
1:O:85:MET:HB2	1:O:111:ILE:HG13	2.01	0.42
2:D:201:THR:CB	2:D:206:ASN:HD22	2.31	0.42
1:O:84:TRP:CE3	1:O:110:ARG:HG2	2.55	0.42
2:N:45:HIS:CD2	2:N:98:ARG:O	2.73	0.42
2:B:185:VAL:O	2:B:243:VAL:CG1	2.68	0.42
1:C:107:ILE:N	1:C:107:ILE:CD1	2.83	0.42
1:G:38:GLU:CD	1:G:110:ARG:HH22	2.22	0.42
1:I:127:ALA:HA	1:I:146:THR:HG21	2.00	0.42
1:G:39:ASN:OD1	1:G:43:VAL:HG22	2.19	0.42
1:C:77:GLN:HE21	1:C:117:PRO:HB3	1.84	0.42
1:K:194:GLY:HA3	2:L:158:THR:CG2	2.50	0.42
1:M:194:GLY:HA3	2:N:158:THR:CG2	2.49	0.42
2:D:55:TYR:CD1	2:D:94:VAL:HG12	2.55	0.42
1:O:98:LEU:O	1:O:98:LEU:HD22	2.19	0.42
2:N:36:VAL:O	2:N:36:VAL:HG12	2.20	0.42
1:G:65:LEU:HD23	1:G:65:LEU:HA	1.75	0.42
1:M:135:ARG:HA	1:M:140:LEU:HA	2.02	0.42
1:I:132:ARG:CG	1:I:203:VAL:O	2.63	0.42
2:L:258:ARG:NE	2:L:263:VAL:HG23	2.35	0.42
2:F:173:PRO:CG	2:F:179:VAL:HG13	2.34	0.42
1:K:24:ASN:HB3	1:K:60:LYS:HA	2.01	0.42
2:H:148:ILE:N	2:H:148:ILE:HD12	2.35	0.42
2:N:211:ASN:ND2	2:N:213:ALA:H	2.18	0.42
2:N:268:VAL:C	2:N:269:GLN:HG3	2.39	0.42
2:B:201:THR:HG23	2:B:202:ALA:N	2.35	0.42
2:N:185:VAL:HG11	2:N:276:PHE:CZ	2.55	0.42
2:L:192:ASN:HB2	2:L:279:GLN:NE2	2.35	0.42
1:C:140:LEU:HB2	1:C:177:LEU:HD13	2.02	0.42
2:J:98:ARG:CG	2:J:98:ARG:HH11	2.32	0.42
2:N:49:PRO:HD2	2:N:98:ARG:CZ	2.50	0.42
1:M:169:PRO:O	1:M:171:GLY:N	2.49	0.42
2:J:59:GLN:HG3	2:J:143:GLN:NE2	2.31	0.42
2:D:116:GLY:HA2	2:D:189:LYS:NZ	2.35	0.42
2:J:75:VAL:O	2:J:75:VAL:HG13	2.20	0.42
2:F:209:PHE:CG	2:F:272:ILE:CD1	3.03	0.42
2:J:136:ASN:N	2:J:136:ASN:HD22	2.18	0.42
1:I:48:PHE:HA	1:I:48:PHE:HD1	1.72	0.42
2:H:96:ASN:H	2:H:96:ASN:HD22	1.68	0.42
1:I:134:ARG:CZ	1:I:141:THR:HG21	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:188:ARG:HG2	1:E:188:ARG:NH1	2.34	0.42
2:B:226:THR:HG23	2:B:253:THR:HB	2.02	0.42
1:C:161:VAL:O	1:C:162:LEU:CG	2.68	0.42
1:O:4:LEU:O	2:P:160:GLY:N	2.50	0.42
1:M:24:ASN:HD22	1:M:60:LYS:HA	1.83	0.42
1:K:149:TYR:CD2	1:K:166:LEU:HG	2.54	0.42
1:M:149:TYR:CB	1:M:166:LEU:HD11	2.39	0.42
1:O:67:ILE:HD11	1:O:85:MET:SD	2.59	0.42
2:P:192:ASN:HB2	2:P:279:GLN:NE2	2.35	0.42
1:G:148:TYR:N	1:G:148:TYR:CD1	2.87	0.42
2:J:35:VAL:HA	2:J:107:LEU:O	2.20	0.42
2:N:35:VAL:HA	2:N:107:LEU:O	2.20	0.42
2:N:75:VAL:O	2:N:75:VAL:HG13	2.19	0.42
1:C:124:PRO:HD3	1:C:148:TYR:OH	2.19	0.42
1:C:148:TYR:CD1	1:C:148:TYR:N	2.88	0.42
2:L:75:VAL:O	2:L:75:VAL:HG13	2.18	0.42
1:G:28:ASN:N	1:G:28:ASN:ND2	2.66	0.42
2:H:48:TYR:HE2	3:H:603:MMA:H73	1.85	0.42
2:P:55:TYR:CG	2:P:92:ARG:HD2	2.55	0.42
1:A:142:LEU:N	1:A:142:LEU:HD23	2.34	0.42
1:E:182:GLY:O	1:E:183:SER:HB2	2.20	0.42
2:P:258:ARG:NE	2:P:263:VAL:HG23	2.35	0.42
1:E:154:GLU:CD	1:E:188:ARG:HD3	2.40	0.42
1:O:103:LEU:HD22	2:P:254:ALA:HB2	2.01	0.42
1:K:103:LEU:HD22	2:L:254:ALA:HB2	2.02	0.42
1:M:31:TYR:HB3	1:M:89:ALA:HB1	1.99	0.42
2:D:201:THR:CB	2:D:206:ASN:ND2	2.83	0.42
1:I:84:TRP:CE3	1:I:110:ARG:HG2	2.55	0.42
2:B:201:THR:CB	2:B:206:ASN:ND2	2.83	0.42
1:M:84:TRP:CE3	1:M:110:ARG:HG2	2.55	0.42
2:D:218:ALA:HB1	2:D:264:THR:O	2.20	0.42
2:F:218:ALA:HB1	2:F:264:THR:O	2.19	0.42
1:C:9:VAL:HG12	1:C:113:LEU:CD1	2.49	0.42
2:B:5:THR:HG22	2:B:9:THR:N	2.35	0.42
1:A:148:TYR:N	1:A:148:TYR:CD1	2.87	0.42
2:L:75:VAL:HB	2:L:84:PHE:HB2	2.01	0.42
1:G:28:ASN:N	1:G:28:ASN:HD22	2.17	0.42
1:E:103:LEU:HD11	2:F:272:ILE:HG12	2.01	0.42
1:C:103:LEU:HD11	2:D:272:ILE:HG12	2.02	0.42
2:N:121:LYS:HD2	2:N:121:LYS:N	2.35	0.42
2:F:96:ASN:HD22	2:F:96:ASN:H	1.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:104:GLN:O	2:P:271:ILE:HA	2.20	0.41
1:I:103:LEU:HD22	2:J:254:ALA:HB2	2.02	0.41
1:M:149:TYR:HD2	1:M:166:LEU:HG	1.85	0.41
2:N:196:TYR:HD1	2:N:197:LEU:O	2.03	0.41
2:L:211:ASN:ND2	2:L:269:GLN:H	2.18	0.41
2:P:185:VAL:HG11	2:P:276:PHE:CZ	2.55	0.41
2:N:24:LEU:O	2:N:152:ASN:ND2	2.53	0.41
2:N:24:LEU:O	2:N:26:PRO:HD3	2.20	0.41
1:O:185:ILE:CG2	1:O:202:GLY:HA3	2.48	0.41
2:L:77:TYR:HD1	2:L:105:VAL:HG22	1.84	0.41
1:A:103:LEU:HD11	2:B:272:ILE:HG12	2.02	0.41
2:L:36:VAL:O	2:L:36:VAL:HG12	2.19	0.41
1:K:163:GLU:HB3	1:K:175:VAL:CG1	2.50	0.41
1:K:143:ILE:HA	1:K:172:GLU:HB3	2.01	0.41
1:K:163:GLU:N	1:K:175:VAL:HG11	2.15	0.41
1:O:163:GLU:HB3	1:O:175:VAL:CG1	2.50	0.41
2:F:126:ILE:HD11	2:F:150:ALA:HB2	2.02	0.41
2:B:221:VAL:CG1	2:B:222:GLY:H	2.22	0.41
2:J:196:TYR:HD1	2:J:197:LEU:O	2.03	0.41
2:P:211:ASN:ND2	2:P:213:ALA:H	2.18	0.41
2:J:269:GLN:NE2	4:J:610:HOH:O	2.51	0.41
2:L:268:VAL:C	2:L:269:GLN:HG3	2.39	0.41
1:M:37:VAL:HG22	1:M:85:MET:HG2	2.00	0.41
2:B:59:GLN:HE21	2:B:143:GLN:HE22	1.67	0.41
2:L:192:ASN:HB2	2:L:279:GLN:HE21	1.85	0.41
1:G:140:LEU:HB2	1:G:177:LEU:HD13	2.02	0.41
2:N:41:GLN:CA	2:N:41:GLN:HE21	2.34	0.41
2:L:15:GLY:HA2	2:L:144:PHE:CE1	2.56	0.41
1:G:124:PRO:HD3	1:G:148:TYR:OH	2.20	0.41
2:B:209:PHE:CG	2:B:272:ILE:CD1	3.02	0.41
2:J:55:TYR:CG	2:J:92:ARG:HD2	2.55	0.41
1:C:142:LEU:HD23	1:C:142:LEU:H	1.85	0.41
2:H:195:TYR:CE1	2:H:238:VAL:HB	2.55	0.41
2:F:73:GLY:HA2	4:F:513:HOH:O	2.20	0.41
1:E:168:PRO:HA	1:E:169:PRO:HD3	1.96	0.41
1:C:67:ILE:HD12	1:C:67:ILE:N	2.35	0.41
1:E:67:ILE:HD12	1:E:67:ILE:N	2.35	0.41
1:C:5:GLY:O	2:D:159:GLY:HA2	2.20	0.41
1:E:162:LEU:HD21	1:E:178:PRO:HD2	2.02	0.41
2:P:166:ARG:HG2	2:P:182:PRO:CB	2.47	0.41
1:I:4:LEU:HB3	1:I:6:ALA:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:113:SER:O	2:J:115:ALA:N	2.47	0.41
2:P:196:TYR:HD1	2:P:197:LEU:O	2.02	0.41
2:L:185:VAL:HG11	2:L:276:PHE:CZ	2.54	0.41
2:J:192:ASN:HB2	2:J:279:GLN:HE21	1.85	0.41
2:P:45:HIS:CD2	2:P:98:ARG:O	2.73	0.41
2:J:96:ASN:HD22	2:J:96:ASN:H	1.59	0.41
2:D:5:THR:N	2:D:9:THR:O	2.48	0.41
2:P:13:ILE:HG22	2:P:14:GLY:N	2.34	0.41
2:N:15:GLY:HA2	2:N:144:PHE:CE1	2.56	0.41
2:P:136:ASN:HD22	2:P:136:ASN:N	2.17	0.41
1:G:77:GLN:HE21	1:G:77:GLN:CA	2.34	0.41
2:P:121:LYS:HD2	2:P:121:LYS:N	2.35	0.41
2:L:121:LYS:HD2	2:L:121:LYS:N	2.35	0.41
2:H:14:GLY:HA2	2:H:142:PHE:CD1	2.55	0.41
1:A:182:GLY:O	1:A:183:SER:HB2	2.20	0.41
2:F:55:TYR:CD1	2:F:94:VAL:HG12	2.55	0.41
2:D:14:GLY:HA2	2:D:142:PHE:CD1	2.56	0.41
2:B:55:TYR:CD1	2:B:94:VAL:HG12	2.56	0.41
1:I:135:ARG:HA	1:I:140:LEU:HA	2.02	0.41
1:E:156:ASN:C	1:E:158:GLY:N	2.73	0.41
1:A:159:THR:HB	1:A:160:ARG:H	1.63	0.41
1:G:156:ASN:C	1:G:158:GLY:N	2.73	0.41
1:C:162:LEU:HD21	1:C:178:PRO:HD2	2.02	0.41
1:O:24:ASN:HD21	1:O:26:ASP:HB2	1.86	0.41
1:M:4:LEU:HB3	1:M:6:ALA:O	2.21	0.41
1:I:10:ILE:O	1:I:12:PRO:HD3	2.20	0.41
2:P:227:ARG:O	2:P:229:GLY:N	2.53	0.41
2:L:211:ASN:ND2	2:L:213:ALA:H	2.19	0.41
2:J:185:VAL:HG11	2:J:276:PHE:CZ	2.56	0.41
1:C:193:TYR:CG	2:D:155:VAL:HG11	2.56	0.41
1:G:9:VAL:CG1	1:G:113:LEU:HD13	2.50	0.41
1:C:38:GLU:CD	1:C:110:ARG:HH22	2.23	0.41
2:N:13:ILE:HG22	2:N:14:GLY:N	2.35	0.41
2:P:52:ILE:HG23	2:P:137:TYR:CB	2.49	0.41
2:J:52:ILE:HG23	2:J:137:TYR:CB	2.50	0.41
1:C:142:LEU:N	1:C:142:LEU:HD23	2.35	0.41
2:B:105:VAL:HG11	2:B:129:LEU:HD13	2.02	0.41
1:G:182:GLY:O	1:G:183:SER:HB2	2.20	0.41
1:C:65:LEU:HD23	1:C:65:LEU:HA	1.76	0.41
2:J:258:ARG:NE	2:J:263:VAL:HG23	2.35	0.41
2:F:226:THR:CG2	2:F:253:THR:HB	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:104:GLN:O	2:L:271:ILE:HA	2.20	0.41
1:K:23:THR:CG2	1:K:24:ASN:N	2.83	0.41
1:M:33:ILE:HG13	1:M:55:PHE:CE1	2.55	0.41
1:I:67:ILE:HD11	1:I:85:MET:SD	2.60	0.41
1:M:49:ILE:HB	1:M:68:LEU:HB2	2.02	0.41
2:L:112:VAL:O	2:L:113:SER:C	2.58	0.41
2:H:218:ALA:HB1	2:H:264:THR:O	2.20	0.41
1:K:8:ARG:NH1	1:K:8:ARG:CB	2.81	0.41
2:P:162:ASP:N	2:P:186:TYR:O	2.54	0.41
1:I:116:ARG:HA	1:I:117:PRO:HD3	1.87	0.41
2:P:123:GLY:N	2:P:150:ALA:O	2.53	0.41
1:O:48:PHE:HA	1:O:48:PHE:HD1	1.72	0.41
2:J:228:ASN:ND2	2:J:228:ASN:O	2.54	0.41
2:D:96:ASN:HD22	2:D:96:ASN:H	1.69	0.41
2:L:200:THR:HG22	2:L:200:THR:O	2.19	0.41
2:H:170:VAL:C	2:H:172:LEU:N	2.72	0.41
1:I:33:ILE:HG13	1:I:55:PHE:CE1	2.55	0.41
1:M:149:TYR:CD2	1:M:166:LEU:HG	2.55	0.41
2:P:173:PRO:O	2:P:174:ASP:O	2.38	0.41
2:H:185:VAL:O	2:H:243:VAL:CG1	2.69	0.41
2:N:162:ASP:N	2:N:186:TYR:O	2.54	0.41
2:P:15:GLY:HA2	2:P:144:PHE:CE1	2.55	0.41
2:P:43:PHE:HE2	2:P:102:PRO:HG3	1.82	0.41
2:B:3:CYS:HA	2:B:43:PHE:O	2.20	0.41
2:J:75:VAL:HG23	2:J:107:LEU:CD1	2.50	0.41
2:D:209:PHE:CG	2:D:272:ILE:CD1	3.04	0.41
1:K:118:ALA:O	1:K:119:LYS:HB2	2.20	0.41
1:A:142:LEU:HD23	1:A:142:LEU:H	1.84	0.41
1:G:142:LEU:HD12	1:G:152:VAL:HG21	2.02	0.41
1:M:143:ILE:HA	1:M:172:GLU:HB3	2.02	0.41
1:M:163:GLU:HB3	1:M:175:VAL:CG1	2.49	0.41
2:J:175:TYR:N	2:J:176:PRO:HD2	2.35	0.41
1:O:33:ILE:HG13	1:O:55:PHE:CE1	2.55	0.41
1:M:23:THR:CG2	1:M:24:ASN:N	2.82	0.41
1:O:10:ILE:O	1:O:12:PRO:HD3	2.21	0.41
2:B:255:ASN:HB3	4:B:511:HOH:O	2.20	0.41
2:J:211:ASN:ND2	2:J:213:ALA:H	2.19	0.41
2:P:227:ARG:C	2:P:229:GLY:N	2.73	0.41
2:D:221:VAL:HG11	2:D:256:TYR:HD1	1.85	0.41
1:M:101:ASN:O	2:N:171:THR:N	2.54	0.41
2:B:201:THR:HG21	2:B:206:ASN:ND2	2.25	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:107:ILE:CD1	1:G:107:ILE:N	2.84	0.41
2:J:162:ASP:N	2:J:186:TYR:O	2.54	0.41
1:M:144:ASN:HB3	1:M:167:VAL:CG1	2.46	0.41
2:N:77:TYR:HD1	2:N:105:VAL:HG22	1.85	0.41
1:C:8:ARG:CZ	1:C:8:ARG:HB3	2.50	0.41
1:K:135:ARG:HA	1:K:140:LEU:HA	2.02	0.41
2:L:175:TYR:N	2:L:176:PRO:HD2	2.35	0.41
2:J:258:ARG:CD	2:J:261:GLY:HA2	2.20	0.41
1:G:161:VAL:O	1:G:162:LEU:CG	2.66	0.41
1:M:104:GLN:O	2:N:271:ILE:HA	2.21	0.41
2:N:166:ARG:HG2	2:N:182:PRO:CB	2.48	0.41
1:I:24:ASN:HD21	1:I:26:ASP:HB2	1.85	0.41
1:I:114:TYR:OH	1:I:149:TYR:HB2	2.20	0.41
2:D:148:ILE:HD12	2:D:148:ILE:N	2.36	0.41
1:M:10:ILE:O	1:M:12:PRO:HD3	2.20	0.41
2:N:173:PRO:O	2:N:174:ASP:O	2.38	0.41
1:O:153:THR:OG1	1:O:154:GLU:HG3	2.21	0.41
2:H:5:THR:N	2:H:9:THR:O	2.48	0.41
2:L:21:TYR:O	2:L:151:ASN:ND2	2.54	0.41
2:J:13:ILE:HG22	2:J:14:GLY:N	2.35	0.41
2:N:43:PHE:HE2	2:N:102:PRO:HG3	1.82	0.41
1:E:148:TYR:CD1	1:E:148:TYR:N	2.89	0.41
2:N:55:TYR:CG	2:N:92:ARG:HD2	2.56	0.41
1:A:168:PRO:HA	1:A:169:PRO:HD3	1.96	0.41
2:N:134:THR:HG22	2:N:141:ASP:HA	2.02	0.41
2:P:228:ASN:ND2	2:P:228:ASN:O	2.54	0.41
1:I:143:ILE:HA	1:I:172:GLU:HB3	2.01	0.41
1:I:141:THR:C	1:I:174:THR:HG22	2.34	0.41
1:I:135:ARG:NH2	1:I:177:LEU:CD2	2.83	0.41
1:E:159:THR:HB	1:E:160:ARG:H	1.63	0.41
1:E:158:GLY:CA	1:E:184:ASN:O	2.69	0.41
1:C:188:ARG:HG2	1:C:188:ARG:NH1	2.36	0.41
1:A:162:LEU:HD21	1:A:178:PRO:HD2	2.03	0.41
2:F:179:VAL:O	2:F:253:THR:CG2	2.69	0.41
2:B:226:THR:CG2	2:B:253:THR:HB	2.51	0.41
2:P:248:VAL:HG13	4:P:614:HOH:O	2.21	0.41
1:I:105:LEU:HD11	2:J:183:LEU:HD11	2.03	0.41
1:K:4:LEU:C	1:K:6:ALA:N	2.74	0.41
1:O:4:LEU:HB3	1:O:6:ALA:O	2.21	0.41
2:N:60:ARG:HB3	2:N:130:ILE:HD13	2.02	0.41
2:J:29:ASN:OD1	2:J:157:PRO:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:84:TRP:CE3	1:K:110:ARG:HG2	2.55	0.41
2:B:33:ASN:HD22	2:B:33:ASN:HA	1.55	0.41
1:G:138:ASN:OD1	1:G:139:SER:N	2.51	0.41
2:P:192:ASN:HB2	2:P:279:GLN:HE21	1.85	0.41
1:I:8:ARG:NH1	1:I:8:ARG:CB	2.80	0.41
1:K:169:PRO:O	1:K:171:GLY:N	2.48	0.41
2:P:209:PHE:CZ	2:P:234:ALA:HB2	2.55	0.41
2:L:162:ASP:N	2:L:186:TYR:O	2.54	0.41
2:L:110:THR:HA	2:L:111:PRO:HD3	1.95	0.41
2:J:67:VAL:HA	2:J:71:PHE:HD1	1.86	0.41
2:N:123:GLY:N	2:N:150:ALA:O	2.52	0.41
2:N:21:TYR:O	2:N:151:ASN:ND2	2.54	0.41
2:H:5:THR:HG22	2:H:9:THR:N	2.35	0.41
2:J:21:TYR:O	2:J:151:ASN:ND2	2.54	0.41
1:I:185:ILE:CG2	1:I:202:GLY:HA3	2.49	0.41
2:J:103:TRP:CH2	2:J:131:LEU:HB2	2.56	0.41
2:P:144:PHE:N	2:P:144:PHE:CD1	2.89	0.41
1:G:8:ARG:CZ	1:G:8:ARG:HB3	2.50	0.41
2:D:3:CYS:HA	2:D:43:PHE:O	2.20	0.41
1:E:9:VAL:CG1	1:E:113:LEU:HD13	2.50	0.41
1:E:11:TYR:HA	1:E:12:PRO:HD3	1.83	0.41
1:C:43:VAL:HG23	1:C:43:VAL:O	2.21	0.41
1:K:48:PHE:HA	1:K:48:PHE:HD1	1.73	0.41
1:E:125:ASP:N	1:E:125:ASP:OD1	2.53	0.41
2:B:77:TYR:N	2:B:80:SER:O	2.54	0.41
1:C:182:GLY:O	1:C:183:SER:HB2	2.21	0.41
1:G:125:ASP:OD1	1:G:125:ASP:N	2.54	0.41
1:I:98:LEU:O	1:I:98:LEU:HD22	2.20	0.41
1:M:123:PRO:C	1:M:125:ASP:H	2.24	0.41
1:O:135:ARG:NH2	1:O:177:LEU:CD2	2.82	0.41
2:N:175:TYR:N	2:N:176:PRO:HD2	2.36	0.41
1:C:129:GLU:HA	1:C:200:MET:HE1	2.02	0.41
1:A:156:ASN:C	1:A:158:GLY:N	2.74	0.41
1:O:105:LEU:HD11	2:P:183:LEU:HD11	2.03	0.41
1:G:162:LEU:HD21	1:G:178:PRO:HD2	2.03	0.41
1:I:104:GLN:O	2:J:271:ILE:HA	2.21	0.41
1:K:24:ASN:HD21	1:K:26:ASP:HB2	1.86	0.41
1:I:4:LEU:C	1:I:6:ALA:N	2.72	0.41
2:P:60:ARG:HB3	2:P:130:ILE:HD13	2.02	0.41
1:O:17:GLN:HB3	1:O:68:LEU:CD2	2.41	0.41
2:P:223:VAL:HA	2:P:255:ASN:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:107:ILE:CD1	1:M:107:ILE:N	2.81	0.41
2:J:45:HIS:CD2	2:J:98:ARG:O	2.73	0.41
2:N:138:ASN:ND2	2:N:140:ASP:HB2	2.36	0.41
2:L:138:ASN:HD22	2:L:138:ASN:C	2.24	0.41
2:N:209:PHE:CZ	2:N:234:ALA:HB2	2.55	0.41
1:E:185:ILE:CB	1:E:202:GLY:HA3	2.48	0.41
2:N:144:PHE:CD1	2:N:144:PHE:N	2.89	0.41
2:P:75:VAL:O	2:P:75:VAL:HG13	2.21	0.41
2:P:134:THR:HG22	2:P:141:ASP:HA	2.02	0.41
2:F:77:TYR:N	2:F:80:SER:O	2.54	0.41
1:E:65:LEU:HD23	1:E:65:LEU:HA	1.72	0.41
1:E:5:GLY:O	2:F:159:GLY:HA2	2.21	0.41
2:D:211:ASN:HD21	2:D:269:GLN:N	1.96	0.40
1:K:4:LEU:HB3	1:K:6:ALA:O	2.21	0.40
1:M:4:LEU:C	1:M:6:ALA:N	2.73	0.40
2:L:60:ARG:HG2	2:L:61:GLY:N	2.22	0.40
1:I:101:ASN:O	2:J:171:THR:N	2.54	0.40
1:K:11:TYR:HB3	1:K:115:TYR:HA	2.03	0.40
1:K:101:ASN:O	2:L:171:THR:N	2.54	0.40
2:H:183:LEU:HD22	2:H:250:LEU:HD11	2.03	0.40
2:H:33:ASN:ND2	2:H:110:THR:OG1	2.53	0.40
2:L:45:HIS:CD2	2:L:98:ARG:O	2.74	0.40
2:L:67:VAL:HA	2:L:71:PHE:HD1	1.85	0.40
2:P:67:VAL:HA	2:P:71:PHE:HD1	1.87	0.40
2:P:77:TYR:HD1	2:P:105:VAL:HG22	1.86	0.40
2:N:136:ASN:HD22	2:N:136:ASN:N	2.18	0.40
2:B:96:ASN:H	2:B:96:ASN:HD22	1.70	0.40
2:L:228:ASN:ND2	2:L:228:ASN:O	2.54	0.40
1:G:188:ARG:NH1	1:G:188:ARG:HG2	2.35	0.40
2:F:170:VAL:C	2:F:172:LEU:N	2.72	0.40
2:N:181:ILE:HA	2:N:182:PRO:HD3	1.81	0.40
1:M:21:ALA:HA	1:M:64:THR:CA	2.40	0.40
1:K:114:TYR:CE2	1:K:149:TYR:HB2	2.56	0.40
1:I:11:TYR:HB3	1:I:115:TYR:HA	2.03	0.40
2:H:135:ASN:OD1	2:H:138:ASN:ND2	2.55	0.40
2:L:49:PRO:HD2	2:L:98:ARG:CZ	2.50	0.40
1:K:145:PRO:HG2	1:K:146:THR:H	1.86	0.40
1:O:145:PRO:HG2	1:O:146:THR:H	1.85	0.40
1:C:9:VAL:CG1	1:C:113:LEU:HD13	2.51	0.40
1:O:116:ARG:HA	1:O:117:PRO:HD3	1.88	0.40
2:J:209:PHE:CZ	2:J:234:ALA:HB2	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:ILE:CB	1:A:202:GLY:HA3	2.49	0.40
1:M:77:GLN:CA	1:M:77:GLN:HE21	2.26	0.40
2:J:63:ALA:C	2:J:64:TYR:CD1	2.95	0.40
1:C:71:THR:OG1	1:C:74:GLN:HB2	2.22	0.40
2:P:35:VAL:HG22	2:P:108:TYR:CD2	2.56	0.40
2:L:136:ASN:N	2:L:136:ASN:HD22	2.18	0.40
1:I:123:PRO:C	1:I:125:ASP:H	2.23	0.40
2:F:39:SER:HB3	4:F:512:HOH:O	2.21	0.40
1:A:125:ASP:N	1:A:125:ASP:OD1	2.53	0.40
1:K:98:LEU:O	1:K:98:LEU:HD22	2.20	0.40
1:M:24:ASN:HD21	1:M:26:ASP:HB2	1.85	0.40
2:D:135:ASN:OD1	2:D:138:ASN:ND2	2.54	0.40
2:P:98:ARG:HH11	2:P:98:ARG:CG	2.33	0.40
1:E:86:ASN:HD21	1:E:110:ARG:HH21	1.70	0.40
2:P:138:ASN:HD22	2:P:138:ASN:C	2.23	0.40
2:J:138:ASN:ND2	2:J:140:ASP:HB2	2.37	0.40
1:I:169:PRO:C	1:I:171:GLY:N	2.75	0.40
2:L:24:LEU:O	2:L:26:PRO:HD3	2.21	0.40
2:H:116:GLY:HA2	2:H:189:LYS:NZ	2.36	0.40
2:N:103:TRP:CH2	2:N:131:LEU:HB2	2.56	0.40
2:N:75:VAL:HG23	2:N:107:LEU:CD1	2.51	0.40
2:F:3:CYS:HA	2:F:43:PHE:O	2.21	0.40
1:I:118:ALA:O	1:I:119:LYS:HB2	2.21	0.40
1:O:118:ALA:O	1:O:119:LYS:HB2	2.21	0.40
2:H:209:PHE:CG	2:H:272:ILE:CD1	3.04	0.40
1:K:189:THR:O	1:K:197:THR:N	2.54	0.40
2:J:24:LEU:O	2:J:26:PRO:HD3	2.21	0.40
1:O:123:PRO:C	1:O:125:ASP:H	2.25	0.40
2:D:77:TYR:N	2:D:80:SER:O	2.54	0.40
1:M:135:ARG:NH2	1:M:177:LEU:CD2	2.82	0.40
1:E:161:VAL:O	1:E:162:LEU:CG	2.68	0.40
2:J:227:ARG:O	2:J:229:GLY:N	2.53	0.40
2:J:60:ARG:HB3	2:J:130:ILE:HD13	2.03	0.40
1:O:49:ILE:HB	1:O:68:LEU:HB2	2.03	0.40
2:P:113:SER:O	2:P:115:ALA:N	2.47	0.40
1:O:8:ARG:HG3	1:O:192:ASP:O	2.22	0.40
1:C:86:ASN:HD21	1:C:110:ARG:NE	2.12	0.40
2:P:24:LEU:O	2:P:26:PRO:HD3	2.21	0.40
2:P:42:ILE:HG21	2:P:146:TRP:CZ2	2.57	0.40
2:L:123:GLY:N	2:L:150:ALA:O	2.54	0.40
1:K:144:ASN:HB3	1:K:167:VAL:CG1	2.47	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:77:TYR:HD1	2:J:105:VAL:HG22	1.86	0.40
2:L:144:PHE:N	2:L:144:PHE:CD1	2.89	0.40
2:P:103:TRP:CH2	2:P:131:LEU:HB2	2.56	0.40
2:L:75:VAL:HG23	2:L:107:LEU:CD1	2.51	0.40
1:I:13:ALA:HB3	1:I:118:ALA:HB3	2.04	0.40
2:L:55:TYR:CG	2:L:92:ARG:HD2	2.57	0.40
1:E:43:VAL:HG23	1:E:43:VAL:O	2.21	0.40
2:F:14:GLY:HA2	2:F:142:PHE:CD1	2.56	0.40
2:H:172:LEU:N	2:H:173:PRO:CD	2.83	0.40
2:J:166:ARG:HG2	2:J:182:PRO:CB	2.47	0.40
2:L:60:ARG:HB3	2:L:130:ILE:HD13	2.04	0.40
2:J:227:ARG:C	2:J:229:GLY:N	2.74	0.40
2:N:223:VAL:HA	2:N:255:ASN:O	2.21	0.40
2:N:29:ASN:OD1	2:N:157:PRO:HB2	2.20	0.40
1:K:193:TYR:HB3	2:L:155:VAL:HG11	2.03	0.40
2:L:29:ASN:OD1	2:L:157:PRO:HB2	2.21	0.40
1:A:133:PHE:HD2	1:A:140:LEU:CD2	2.35	0.40
1:O:169:PRO:C	1:O:171:GLY:N	2.75	0.40
2:L:41:GLN:CA	2:L:41:GLN:HE21	2.34	0.40
1:M:35:SER:CB	1:M:50:VAL:HG11	2.52	0.40
1:K:13:ALA:HB3	1:K:118:ALA:HB3	2.04	0.40
2:N:68:LEU:HG	2:N:68:LEU:O	2.22	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	203/205 (99%)	164 (81%)	27 (13%)	12 (6%)	2 11
1	C	203/205 (99%)	163 (80%)	28 (14%)	12 (6%)	2 11
1	E	203/205 (99%)	163 (80%)	29 (14%)	11 (5%)	2 14

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	G	203/205 (99%)	164 (81%)	28 (14%)	11 (5%)	2 14
1	I	203/205 (99%)	138 (68%)	47 (23%)	18 (9%)	1 4
1	K	203/205 (99%)	138 (68%)	47 (23%)	18 (9%)	1 4
1	M	203/205 (99%)	138 (68%)	47 (23%)	18 (9%)	1 4
1	O	203/205 (99%)	138 (68%)	47 (23%)	18 (9%)	1 4
2	B	277/279 (99%)	248 (90%)	18 (6%)	11 (4%)	4 21
2	D	277/279 (99%)	248 (90%)	18 (6%)	11 (4%)	4 21
2	F	277/279 (99%)	248 (90%)	18 (6%)	11 (4%)	4 21
2	H	277/279 (99%)	249 (90%)	18 (6%)	10 (4%)	4 24
2	J	277/279 (99%)	203 (73%)	57 (21%)	17 (6%)	2 11
2	L	277/279 (99%)	204 (74%)	56 (20%)	17 (6%)	2 11
2	N	277/279 (99%)	204 (74%)	56 (20%)	17 (6%)	2 11
2	P	277/279 (99%)	203 (73%)	57 (21%)	17 (6%)	2 11
All	All	3840/3872 (99%)	3013 (78%)	598 (16%)	229 (6%)	2 11

All (229) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	29	SER
1	A	72	ASN
1	A	159	THR
1	A	179	SER
1	A	180	ASP
1	A	183	SER
2	B	168	VAL
2	B	175	TYR
2	B	218	ALA
1	C	29	SER
1	C	72	ASN
1	C	159	THR
1	C	179	SER
1	C	180	ASP
1	C	183	SER
2	D	168	VAL
2	D	173	PRO
2	D	175	TYR
2	D	218	ALA

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Mol	Chain	Res	Type
1	E	29	SER
1	E	72	ASN
1	E	159	THR
1	E	179	SER
1	E	180	ASP
1	E	183	SER
2	F	168	VAL
2	F	173	PRO
2	F	175	TYR
2	F	218	ALA
1	G	29	SER
1	G	72	ASN
1	G	159	THR
1	G	179	SER
1	G	180	ASP
1	G	183	SER
2	H	168	VAL
2	H	173	PRO
2	H	175	TYR
2	H	218	ALA
1	I	45	ASP
1	I	96	SER
1	I	119	LYS
2	J	174	ASP
2	J	210	THR
1	K	45	ASP
1	K	96	SER
1	K	119	LYS
2	L	174	ASP
2	L	210	THR
1	M	96	SER
1	M	119	LYS
2	N	174	ASP
2	N	210	THR
2	N	225	LEU
1	O	96	SER
1	O	119	LYS
2	P	174	ASP
2	P	210	THR
2	P	225	LEU
2	B	116	GLY
2	B	167	ASP

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Mol	Chain	Res	Type
2	B	173	PRO
2	B	177	GLY
2	B	262	GLN
1	C	47	ARG
2	D	116	GLY
2	D	167	ASP
2	D	177	GLY
2	D	262	GLN
1	E	192	ASP
2	F	116	GLY
2	F	167	ASP
2	F	177	GLY
2	F	262	GLN
1	G	47	ARG
2	H	116	GLY
2	H	167	ASP
2	H	177	GLY
2	H	262	GLN
1	I	64	THR
1	I	94	ASP
1	I	137	ALA
1	I	203	VAL
2	J	40	THR
2	J	91	PRO
2	J	167	ASP
2	J	198	SER
2	J	217	PRO
2	J	225	LEU
2	J	247	ALA
2	J	251	GLY
1	K	64	THR
1	K	94	ASP
1	K	137	ALA
1	K	203	VAL
2	L	40	THR
2	L	91	PRO
2	L	167	ASP
2	L	217	PRO
2	L	225	LEU
2	L	247	ALA
2	L	251	GLY
1	M	45	ASP

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Mol	Chain	Res	Type
1	M	64	THR
1	M	94	ASP
1	M	137	ALA
1	M	203	VAL
2	N	40	THR
2	N	91	PRO
2	N	167	ASP
2	N	198	SER
2	N	217	PRO
2	N	247	ALA
2	N	251	GLY
1	O	45	ASP
1	O	64	THR
1	O	94	ASP
1	O	137	ALA
1	O	203	VAL
2	P	40	THR
2	P	91	PRO
2	P	167	ASP
2	P	217	PRO
2	P	247	ALA
2	P	251	GLY
1	A	27	GLU
1	A	47	ARG
1	A	192	ASP
2	B	174	ASP
1	C	27	GLU
1	C	192	ASP
2	D	174	ASP
1	E	27	GLU
1	E	47	ARG
2	F	174	ASP
1	G	27	GLU
1	G	192	ASP
2	H	174	ASP
1	I	71	THR
1	I	155	LEU
1	I	183	SER
1	I	184	ASN
1	I	204	MET
2	J	104	PRO
2	J	117	GLY

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Mol	Chain	Res	Type
2	J	229	GLY
2	J	260	GLY
1	K	71	THR
1	K	155	LEU
1	K	183	SER
1	K	184	ASN
1	K	204	MET
2	L	104	PRO
2	L	117	GLY
2	L	198	SER
2	L	229	GLY
2	L	260	GLY
1	M	71	THR
1	M	155	LEU
1	M	183	SER
1	M	184	ASN
1	M	204	MET
2	N	104	PRO
2	N	117	GLY
2	N	229	GLY
2	N	260	GLY
1	O	71	THR
1	O	155	LEU
1	O	183	SER
1	O	184	ASN
1	O	204	MET
2	P	104	PRO
2	P	117	GLY
2	P	198	SER
2	P	229	GLY
2	P	260	GLY
1	A	121	ALA
1	A	164	ASN
1	C	121	ALA
1	E	121	ALA
1	G	121	ALA
1	I	32	LEU
1	I	46	GLY
1	I	178	PRO
1	I	200	MET
2	J	65	GLY
1	K	32	LEU

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Mol	Chain	Res	Type
1	K	46	GLY
1	K	178	PRO
1	K	200	MET
2	L	65	GLY
1	M	32	LEU
1	M	46	GLY
1	M	178	PRO
1	M	200	MET
2	N	65	GLY
1	O	46	GLY
1	O	178	PRO
1	O	200	MET
2	P	65	GLY
2	B	265	ALA
1	C	164	ASN
2	D	265	ALA
1	E	164	ASN
2	F	265	ALA
1	G	164	ASN
1	I	29	SER
1	I	145	PRO
1	K	29	SER
1	K	145	PRO
1	M	29	SER
1	M	145	PRO
1	O	29	SER
1	O	32	LEU
1	O	145	PRO
2	F	104	PRO
2	J	35	VAL
2	L	35	VAL
2	N	35	VAL
2	P	35	VAL
2	B	104	PRO
2	D	104	PRO
2	H	104	PRO
2	J	157	PRO
2	L	157	PRO
2	N	157	PRO
2	P	157	PRO
1	C	143	ILE
1	A	143	ILE

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	176/176 (100%)	160 (91%)	16 (9%)	12	41
1	C	176/176 (100%)	160 (91%)	16 (9%)	12	41
1	E	176/176 (100%)	160 (91%)	16 (9%)	12	41
1	G	176/176 (100%)	160 (91%)	16 (9%)	12	41
1	I	176/176 (100%)	163 (93%)	13 (7%)	17	52
1	K	176/176 (100%)	163 (93%)	13 (7%)	17	52
1	M	176/176 (100%)	163 (93%)	13 (7%)	17	52
1	O	176/176 (100%)	163 (93%)	13 (7%)	17	52
2	B	226/226 (100%)	206 (91%)	20 (9%)	12	42
2	D	226/226 (100%)	207 (92%)	19 (8%)	14	45
2	F	226/226 (100%)	208 (92%)	18 (8%)	15	47
2	H	226/226 (100%)	207 (92%)	19 (8%)	14	45
2	J	226/226 (100%)	211 (93%)	15 (7%)	21	57
2	L	226/226 (100%)	211 (93%)	15 (7%)	21	57
2	N	226/226 (100%)	211 (93%)	15 (7%)	21	57
2	P	226/226 (100%)	211 (93%)	15 (7%)	21	57
All	All	3216/3216 (100%)	2964 (92%)	252 (8%)	16	49

All (252) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ARG
1	A	23	THR
1	A	28	ASN
1	A	35	SER
1	A	47	ARG
1	A	62	GLU
1	A	66	ARG
1	A	93	MET

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Mol	Chain	Res	Type
1	A	98	LEU
1	A	104	GLN
1	A	122	LEU
1	A	135	ARG
1	A	142	LEU
1	A	176	LYS
1	A	180	ASP
1	A	186	THR
2	B	4	LYS
2	B	5	THR
2	B	13	ILE
2	B	33	ASN
2	B	59	GLN
2	B	85	PRO
2	B	87	THR
2	B	96	ASN
2	B	104	PRO
2	B	107	LEU
2	B	121	LYS
2	B	133	ASN
2	B	136	ASN
2	B	138	ASN
2	B	158	THR
2	B	201	THR
2	B	206	ASN
2	B	211	ASN
2	B	255	ASN
2	B	267	ASN
1	C	8	ARG
1	C	23	THR
1	C	28	ASN
1	C	35	SER
1	C	47	ARG
1	C	62	GLU
1	C	66	ARG
1	C	93	MET
1	C	98	LEU
1	C	104	GLN
1	C	122	LEU
1	C	135	ARG
1	C	142	LEU
1	C	176	LYS

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Mol	Chain	Res	Type
1	C	180	ASP
1	C	186	THR
2	D	4	LYS
2	D	5	THR
2	D	13	ILE
2	D	33	ASN
2	D	59	GLN
2	D	85	PRO
2	D	87	THR
2	D	96	ASN
2	D	107	LEU
2	D	121	LYS
2	D	133	ASN
2	D	136	ASN
2	D	138	ASN
2	D	158	THR
2	D	201	THR
2	D	206	ASN
2	D	211	ASN
2	D	255	ASN
2	D	267	ASN
1	E	8	ARG
1	E	23	THR
1	E	28	ASN
1	E	35	SER
1	E	47	ARG
1	E	62	GLU
1	E	66	ARG
1	E	93	MET
1	E	98	LEU
1	E	104	GLN
1	E	122	LEU
1	E	135	ARG
1	E	142	LEU
1	E	176	LYS
1	E	180	ASP
1	E	186	THR
2	F	4	LYS
2	F	5	THR
2	F	13	ILE
2	F	33	ASN
2	F	59	GLN

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Mol	Chain	Res	Type
2	F	85	PRO
2	F	87	THR
2	F	96	ASN
2	F	107	LEU
2	F	121	LYS
2	F	133	ASN
2	F	136	ASN
2	F	138	ASN
2	F	158	THR
2	F	201	THR
2	F	211	ASN
2	F	255	ASN
2	F	267	ASN
1	G	8	ARG
1	G	23	THR
1	G	28	ASN
1	G	35	SER
1	G	47	ARG
1	G	62	GLU
1	G	66	ARG
1	G	93	MET
1	G	98	LEU
1	G	104	GLN
1	G	122	LEU
1	G	135	ARG
1	G	142	LEU
1	G	176	LYS
1	G	180	ASP
1	G	186	THR
2	H	4	LYS
2	H	5	THR
2	H	13	ILE
2	H	33	ASN
2	H	59	GLN
2	H	85	PRO
2	H	87	THR
2	H	96	ASN
2	H	107	LEU
2	H	121	LYS
2	H	133	ASN
2	H	136	ASN
2	H	138	ASN

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Mol	Chain	Res	Type
2	H	158	THR
2	H	201	THR
2	H	206	ASN
2	H	211	ASN
2	H	255	ASN
2	H	267	ASN
1	I	8	ARG
1	I	28	ASN
1	I	39	ASN
1	I	45	ASP
1	I	47	ARG
1	I	48	PHE
1	I	58	LYS
1	I	60	LYS
1	I	62	GLU
1	I	125	ASP
1	I	126	GLN
1	I	135	ARG
1	I	176	LYS
2	J	54	ASP
2	J	59	GLN
2	J	96	ASN
2	J	107	LEU
2	J	121	LYS
2	J	133	ASN
2	J	136	ASN
2	J	138	ASN
2	J	153	ASP
2	J	157	PRO
2	J	187	CYS
2	J	206	ASN
2	J	210	THR
2	J	211	ASN
2	J	228	ASN
1	K	8	ARG
1	K	28	ASN
1	K	39	ASN
1	K	45	ASP
1	K	47	ARG
1	K	48	PHE
1	K	58	LYS
1	K	60	LYS

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Mol	Chain	Res	Type
1	K	62	GLU
1	K	125	ASP
1	K	126	GLN
1	K	135	ARG
1	K	176	LYS
2	L	54	ASP
2	L	59	GLN
2	L	96	ASN
2	L	107	LEU
2	L	121	LYS
2	L	133	ASN
2	L	136	ASN
2	L	138	ASN
2	L	153	ASP
2	L	157	PRO
2	L	187	CYS
2	L	206	ASN
2	L	210	THR
2	L	211	ASN
2	L	228	ASN
1	M	8	ARG
1	M	28	ASN
1	M	39	ASN
1	M	45	ASP
1	M	47	ARG
1	M	48	PHE
1	M	58	LYS
1	M	60	LYS
1	M	62	GLU
1	M	125	ASP
1	M	126	GLN
1	M	135	ARG
1	M	176	LYS
2	N	54	ASP
2	N	59	GLN
2	N	96	ASN
2	N	107	LEU
2	N	121	LYS
2	N	133	ASN
2	N	136	ASN
2	N	138	ASN
2	N	153	ASP

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Mol	Chain	Res	Type
2	N	157	PRO
2	N	187	CYS
2	N	206	ASN
2	N	210	THR
2	N	211	ASN
2	N	228	ASN
1	O	8	ARG
1	O	28	ASN
1	O	39	ASN
1	O	45	ASP
1	O	47	ARG
1	O	48	PHE
1	O	58	LYS
1	O	60	LYS
1	O	62	GLU
1	O	125	ASP
1	O	126	GLN
1	O	135	ARG
1	O	176	LYS
2	P	54	ASP
2	P	59	GLN
2	P	96	ASN
2	P	107	LEU
2	P	121	LYS
2	P	133	ASN
2	P	136	ASN
2	P	138	ASN
2	P	153	ASP
2	P	157	PRO
2	P	187	CYS
2	P	206	ASN
2	P	210	THR
2	P	211	ASN
2	P	228	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (215) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	GLN
1	A	19	GLN
1	A	28	ASN
1	A	72	ASN

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Mol	Chain	Res	Type
1	A	73	ASN
1	A	74	GLN
1	A	77	GLN
1	A	86	ASN
1	A	104	GLN
2	B	7	ASN
2	B	33	ASN
2	B	41	GLN
2	B	70	ASN
2	B	96	ASN
2	B	133	ASN
2	B	135	ASN
2	B	136	ASN
2	B	138	ASN
2	B	143	GLN
2	B	206	ASN
2	B	211	ASN
2	B	219	GLN
2	B	255	ASN
2	B	262	GLN
2	B	267	ASN
2	B	279	GLN
1	C	17	GLN
1	C	19	GLN
1	C	28	ASN
1	C	72	ASN
1	C	73	ASN
1	C	74	GLN
1	C	77	GLN
1	C	86	ASN
1	C	104	GLN
2	D	7	ASN
2	D	33	ASN
2	D	41	GLN
2	D	70	ASN
2	D	96	ASN
2	D	133	ASN
2	D	135	ASN
2	D	136	ASN
2	D	138	ASN
2	D	143	GLN
2	D	206	ASN

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Mol	Chain	Res	Type
2	D	211	ASN
2	D	219	GLN
2	D	255	ASN
2	D	262	GLN
2	D	267	ASN
2	D	279	GLN
1	E	17	GLN
1	E	19	GLN
1	E	28	ASN
1	E	72	ASN
1	E	73	ASN
1	E	74	GLN
1	E	77	GLN
1	E	86	ASN
1	E	104	GLN
2	F	33	ASN
2	F	41	GLN
2	F	70	ASN
2	F	96	ASN
2	F	133	ASN
2	F	135	ASN
2	F	136	ASN
2	F	138	ASN
2	F	143	GLN
2	F	206	ASN
2	F	211	ASN
2	F	219	GLN
2	F	255	ASN
2	F	262	GLN
2	F	267	ASN
2	F	279	GLN
1	G	17	GLN
1	G	19	GLN
1	G	28	ASN
1	G	72	ASN
1	G	73	ASN
1	G	74	GLN
1	G	77	GLN
1	G	86	ASN
1	G	104	GLN
2	H	33	ASN
2	H	41	GLN

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Mol	Chain	Res	Type
2	H	70	ASN
2	H	96	ASN
2	H	133	ASN
2	H	135	ASN
2	H	136	ASN
2	H	138	ASN
2	H	143	GLN
2	H	206	ASN
2	H	211	ASN
2	H	219	GLN
2	H	255	ASN
2	H	262	GLN
2	H	267	ASN
2	H	279	GLN
1	I	19	GLN
1	I	24	ASN
1	I	28	ASN
1	I	72	ASN
1	I	74	GLN
1	I	77	GLN
1	I	86	ASN
1	I	104	GLN
1	I	126	GLN
1	I	138	ASN
1	I	184	ASN
2	J	7	ASN
2	J	41	GLN
2	J	45	HIS
2	J	136	ASN
2	J	138	ASN
2	J	143	GLN
2	J	151	ASN
2	J	192	ASN
2	J	206	ASN
2	J	211	ASN
2	J	219	GLN
2	J	224	GLN
2	J	228	ASN
2	J	235	ASN
2	J	255	ASN
2	J	269	GLN
2	J	279	GLN

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Mol	Chain	Res	Type
1	K	19	GLN
1	K	24	ASN
1	K	28	ASN
1	K	72	ASN
1	K	74	GLN
1	K	77	GLN
1	K	86	ASN
1	K	104	GLN
1	K	126	GLN
1	K	138	ASN
1	K	184	ASN
2	L	7	ASN
2	L	19	ASN
2	L	41	GLN
2	L	136	ASN
2	L	138	ASN
2	L	143	GLN
2	L	151	ASN
2	L	192	ASN
2	L	206	ASN
2	L	211	ASN
2	L	219	GLN
2	L	224	GLN
2	L	228	ASN
2	L	235	ASN
2	L	255	ASN
2	L	269	GLN
2	L	279	GLN
1	M	19	GLN
1	M	24	ASN
1	M	28	ASN
1	M	72	ASN
1	M	74	GLN
1	M	77	GLN
1	M	86	ASN
1	M	104	GLN
1	M	126	GLN
1	M	138	ASN
1	M	184	ASN
2	N	7	ASN
2	N	41	GLN
2	N	45	HIS

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Mol	Chain	Res	Type
2	N	136	ASN
2	N	138	ASN
2	N	143	GLN
2	N	151	ASN
2	N	192	ASN
2	N	206	ASN
2	N	211	ASN
2	N	219	GLN
2	N	224	GLN
2	N	228	ASN
2	N	235	ASN
2	N	255	ASN
2	N	269	GLN
2	N	279	GLN
1	O	19	GLN
1	O	24	ASN
1	O	28	ASN
1	O	72	ASN
1	O	74	GLN
1	O	77	GLN
1	O	86	ASN
1	O	104	GLN
1	O	126	GLN
1	O	138	ASN
1	O	184	ASN
2	P	7	ASN
2	P	19	ASN
2	P	41	GLN
2	P	45	HIS
2	P	136	ASN
2	P	138	ASN
2	P	143	GLN
2	P	151	ASN
2	P	192	ASN
2	P	206	ASN
2	P	211	ASN
2	P	219	GLN
2	P	224	GLN
2	P	228	ASN
2	P	235	ASN
2	P	255	ASN
2	P	269	GLN

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Mol	Chain	Res	Type
2	P	279	GLN

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

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	MMA	B	500	-	13,13,13	1.55	3 (23%)	18,18,18	0.94	0
3	MMA	D	601	-	13,13,13	1.50	3 (23%)	18,18,18	0.91	0
3	MMA	F	502	-	13,13,13	1.49	3 (23%)	18,18,18	0.91	0
3	MMA	H	603	-	13,13,13	1.60	3 (23%)	18,18,18	0.90	0
3	MMA	J	605	-	13,13,13	1.34	2 (15%)	18,18,18	0.94	0
3	MMA	L	504	-	13,13,13	1.46	2 (15%)	18,18,18	0.85	0
3	MMA	N	506	-	13,13,13	1.42	2 (15%)	18,18,18	0.86	0
3	MMA	P	607	-	13,13,13	1.46	2 (15%)	18,18,18	0.87	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical

component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MMA	B	500	-	-	0/4/24/24	0/1/1/1
3	MMA	D	601	-	-	0/4/24/24	0/1/1/1
3	MMA	F	502	-	-	0/4/24/24	0/1/1/1
3	MMA	H	603	-	-	0/4/24/24	0/1/1/1
3	MMA	J	605	-	-	0/4/24/24	0/1/1/1
3	MMA	L	504	-	-	0/4/24/24	0/1/1/1
3	MMA	N	506	-	-	0/4/24/24	0/1/1/1
3	MMA	P	607	-	-	0/4/24/24	0/1/1/1

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	502	MMA	C1-C2	2.24	1.59	1.52
3	B	500	MMA	C1-C2	2.29	1.59	1.52
3	D	601	MMA	C1-C2	2.34	1.59	1.52
3	H	603	MMA	C1-C2	2.37	1.59	1.52
3	J	605	MMA	O5-C1	2.38	1.47	1.41
3	L	504	MMA	O5-C1	2.60	1.48	1.41
3	N	506	MMA	O5-C1	2.68	1.48	1.41
3	P	607	MMA	O5-C1	2.79	1.49	1.41
3	B	500	MMA	O5-C1	2.80	1.49	1.41
3	D	601	MMA	O5-C1	2.87	1.49	1.41
3	F	502	MMA	O5-C1	2.94	1.49	1.41
3	H	603	MMA	O5-C1	3.11	1.49	1.41
3	J	605	MMA	O1-C1	3.17	1.45	1.40
3	P	607	MMA	O1-C1	3.34	1.45	1.40
3	N	506	MMA	O1-C1	3.39	1.46	1.40
3	F	502	MMA	O1-C1	3.46	1.46	1.40
3	L	504	MMA	O1-C1	3.57	1.46	1.40
3	D	601	MMA	O1-C1	3.63	1.46	1.40
3	H	603	MMA	O1-C1	3.90	1.46	1.40
3	B	500	MMA	O1-C1	3.93	1.47	1.40

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	500	MMA	2	0
3	F	502	MMA	2	0
3	H	603	MMA	3	0
3	J	605	MMA	1	0
3	L	504	MMA	1	0
3	N	506	MMA	1	0
3	P	607	MMA	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	205/205 (100%)	-0.18	2 (0%) 84 60	15, 44, 85, 105	0
1	C	205/205 (100%)	-0.19	1 (0%) 91 76	12, 44, 86, 105	0
1	E	205/205 (100%)	-0.19	0 100 100	16, 43, 87, 103	0
1	G	205/205 (100%)	-0.24	1 (0%) 91 76	12, 44, 85, 102	0
1	I	205/205 (100%)	1.83	67 (32%) 1 0	20, 133, 152, 161	0
1	K	205/205 (100%)	2.02	92 (44%) 0 0	20, 133, 149, 161	0
1	M	205/205 (100%)	1.92	77 (37%) 0 0	20, 133, 149, 159	0
1	O	205/205 (100%)	1.93	76 (37%) 0 0	20, 133, 149, 162	0
2	B	279/279 (100%)	-0.28	1 (0%) 93 80	11, 35, 66, 97	0
2	D	279/279 (100%)	-0.34	0 100 100	11, 35, 70, 97	0
2	F	279/279 (100%)	-0.27	0 100 100	11, 35, 66, 96	0
2	H	279/279 (100%)	-0.26	1 (0%) 93 80	12, 33, 68, 97	0
2	J	279/279 (100%)	1.03	55 (19%) 1 1	52, 98, 154, 164	0
2	L	279/279 (100%)	1.16	59 (21%) 1 1	51, 97, 156, 163	0
2	N	279/279 (100%)	1.03	54 (19%) 1 1	53, 98, 154, 163	0
2	P	279/279 (100%)	1.08	59 (21%) 1 1	52, 100, 154, 160	0
All	All	3872/3872 (100%)	0.59	545 (14%) 4 1	11, 71, 148, 164	0

All (545) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	104	GLN	15.9
1	I	103	LEU	14.1
1	O	104	GLN	13.9
1	I	104	GLN	13.5
1	M	104	GLN	9.8

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Mol	Chain	Res	Type	RSRZ
1	K	102	THR	9.0
2	L	168	VAL	8.8
1	M	51	THR	8.8
1	K	103	LEU	8.7
1	I	128	ALA	8.7
2	L	222	GLY	8.5
1	M	102	THR	8.2
1	I	102	THR	8.0
2	L	201	THR	7.7
2	L	169	THR	7.5
1	O	127	ALA	7.2
1	K	100	GLU	7.1
1	O	52	PRO	7.1
1	O	103	LEU	7.0
1	K	173	SER	7.0
1	M	101	ASN	6.9
1	I	165	ALA	6.9
1	O	176	LYS	6.8
2	P	175	TYR	6.7
1	M	127	ALA	6.7
1	O	102	THR	6.7
1	K	177	LEU	6.7
2	P	119	ALA	6.6
2	L	271	ILE	6.6
1	O	128	ALA	6.6
1	M	103	LEU	6.5
2	P	160	GLY	6.4
1	M	5	GLY	6.4
2	L	167	ASP	6.3
2	N	175	TYR	6.2
2	J	178	SER	6.2
2	N	178	SER	6.1
2	N	201	THR	6.1
1	O	50	VAL	6.0
1	I	176	LYS	6.0
2	P	270	SER	6.0
2	L	178	SER	5.9
1	I	173	SER	5.9
2	L	254	ALA	5.9
1	M	54	LEU	5.9
1	K	52	PRO	5.9
1	K	67	ILE	5.9

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Mol	Chain	Res	Type	RSRZ
2	J	175	TYR	5.9
2	J	256	TYR	5.8
1	M	50	VAL	5.7
1	K	174	THR	5.7
1	O	173	SER	5.7
1	I	205	GLU	5.7
1	O	69	ASP	5.7
1	M	174	THR	5.7
1	I	101	ASN	5.7
1	I	105	LEU	5.6
1	O	177	LEU	5.6
2	N	172	LEU	5.5
2	P	218	ALA	5.5
2	J	259	THR	5.5
2	P	269	GLN	5.5
2	J	268	VAL	5.4
1	K	107	ILE	5.3
1	I	67	ILE	5.3
1	I	127	ALA	5.3
1	M	176	LYS	5.3
1	O	54	LEU	5.2
1	O	106	ALA	5.2
2	N	182	PRO	5.1
1	I	177	LEU	5.1
1	K	201	THR	5.0
2	L	172	LEU	5.0
2	P	254	ALA	5.0
1	I	95	LYS	5.0
2	N	256	TYR	4.9
2	N	171	THR	4.9
1	M	48	PHE	4.9
1	I	174	THR	4.9
1	O	181	ALA	4.9
1	K	66	ARG	4.8
1	M	201	THR	4.8
1	O	55	PHE	4.8
2	P	179	VAL	4.8
2	L	165	ALA	4.8
2	J	269	GLN	4.8
2	P	261	GLY	4.8
2	B	165	ALA	4.8
2	N	271	ILE	4.7

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Mol	Chain	Res	Type	RSRZ
1	O	105	LEU	4.7
2	L	160	GLY	4.7
2	L	223	VAL	4.7
1	O	101	ASN	4.7
1	K	92	SER	4.7
2	P	172	LEU	4.7
2	P	201	THR	4.6
1	O	99	THR	4.6
2	N	169	THR	4.6
1	K	127	ALA	4.6
1	K	101	ASN	4.6
1	I	64	THR	4.6
1	M	95	LYS	4.6
2	J	165	ALA	4.6
1	K	181	ALA	4.5
1	M	126	GLN	4.5
2	L	270	SER	4.5
1	O	150	LEU	4.5
1	O	139	SER	4.4
2	P	178	SER	4.4
1	O	4	LEU	4.4
1	K	5	GLY	4.4
1	M	68	LEU	4.4
2	L	232	ILE	4.4
2	N	232	ILE	4.4
1	I	202	GLY	4.4
2	N	161	CYS	4.4
1	K	65	LEU	4.4
2	P	256	TYR	4.4
1	M	97	LYS	4.4
1	M	66	ARG	4.4
1	M	180	ASP	4.4
1	K	55	PHE	4.4
2	N	181	ILE	4.4
1	M	55	PHE	4.3
1	I	167	VAL	4.3
2	P	267	ASN	4.3
1	O	30	THR	4.3
1	O	100	GLU	4.3
2	N	179	VAL	4.3
2	N	252	LEU	4.3
2	J	232	ILE	4.3

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Mol	Chain	Res	Type	RSRZ
2	J	260	GLY	4.3
2	L	269	GLN	4.2
1	K	205	GLU	4.2
2	N	167	ASP	4.2
2	P	268	VAL	4.2
1	M	202	GLY	4.2
2	N	199	GLY	4.2
1	I	32	LEU	4.2
1	K	75	LEU	4.2
1	M	165	ALA	4.1
2	J	250	LEU	4.1
2	P	181	ILE	4.1
2	P	182	PRO	4.1
1	M	197	THR	4.1
1	O	95	LYS	4.1
1	I	51	THR	4.1
1	I	55	PHE	4.1
2	L	252	LEU	4.1
1	I	170	MET	4.1
2	P	253	THR	4.1
2	P	257	ALA	4.1
1	O	72	ASN	4.0
1	O	201	THR	4.0
1	K	18	VAL	4.0
1	I	68	LEU	4.0
1	I	66	ARG	4.0
1	I	153	THR	4.0
1	K	10	ILE	4.0
2	L	164	SER	4.0
1	M	4	LEU	4.0
1	M	181	ALA	4.0
2	L	202	ALA	4.0
2	J	267	ASN	4.0
2	L	208	ILE	3.9
1	I	201	THR	3.9
2	P	252	LEU	3.9
1	K	79	ARG	3.9
2	L	199	GLY	3.9
1	K	175	VAL	3.9
2	J	254	ALA	3.9
2	L	218	ALA	3.9
2	N	165	ALA	3.9

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Mol	Chain	Res	Type	RSRZ
2	L	177	GLY	3.9
2	N	260	GLY	3.9
1	K	143	ILE	3.8
2	N	168	VAL	3.8
1	O	49	ILE	3.8
2	N	217	PRO	3.8
1	M	143	ILE	3.8
2	P	271	ILE	3.8
2	L	267	ASN	3.8
1	K	196	LEU	3.8
1	K	105	LEU	3.7
2	J	199	GLY	3.7
1	K	140	LEU	3.7
1	M	100	GLU	3.7
1	O	51	THR	3.7
1	I	147	PRO	3.7
1	M	74	GLN	3.7
1	K	106	ALA	3.7
1	K	176	LYS	3.6
2	P	167	ASP	3.6
2	N	269	GLN	3.6
1	M	49	ILE	3.6
2	N	216	SER	3.6
1	I	100	GLU	3.6
2	J	168	VAL	3.6
2	P	255	ASN	3.6
2	N	193	LEU	3.6
1	M	132	ARG	3.6
1	O	3	ALA	3.6
1	O	98	LEU	3.6
1	M	173	SER	3.6
1	I	94	ASP	3.5
2	L	179	VAL	3.5
2	P	20	VAL	3.5
1	O	179	SER	3.5
2	N	270	SER	3.5
1	K	51	THR	3.5
1	M	139	SER	3.5
1	O	48	PHE	3.5
2	P	232	ILE	3.4
2	P	272	ILE	3.4
2	L	266	GLY	3.4

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Mol	Chain	Res	Type	RSRZ
2	P	202	ALA	3.4
2	L	181	ILE	3.4
2	N	160	GLY	3.4
1	I	60	LYS	3.4
2	P	262	GLN	3.4
2	L	209	PHE	3.4
1	O	174	THR	3.4
1	I	90	ILE	3.4
1	O	187	TYR	3.4
2	P	177	GLY	3.4
2	N	124	SER	3.4
1	O	67	ILE	3.4
1	I	72	ASN	3.4
1	O	113	LEU	3.3
1	K	141	THR	3.3
1	I	132	ARG	3.3
1	K	165	ALA	3.3
2	L	257	ALA	3.3
2	N	257	ALA	3.3
1	O	26	ASP	3.3
1	O	138	ASN	3.3
1	I	197	THR	3.3
2	J	223	VAL	3.3
1	I	187	TYR	3.3
1	M	96	SER	3.3
1	M	21	ALA	3.3
2	P	251	GLY	3.3
2	J	200	THR	3.2
2	J	252	LEU	3.2
1	O	32	LEU	3.2
1	O	56	ALA	3.2
1	M	133	PHE	3.2
2	L	104	PRO	3.2
1	M	198	PRO	3.2
2	J	167	ASP	3.2
1	M	138	ASN	3.2
2	P	184	THR	3.2
1	O	147	PRO	3.2
1	K	56	ALA	3.2
1	M	53	PRO	3.2
1	M	18	VAL	3.1
1	O	68	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	O	132	ARG	3.1
1	K	6	ALA	3.1
1	M	177	LEU	3.1
2	J	179	VAL	3.1
1	I	150	LEU	3.1
1	O	75	LEU	3.1
1	O	200	MET	3.1
1	O	205	GLU	3.1
2	L	256	TYR	3.1
1	M	179	SER	3.1
1	M	99	THR	3.1
1	O	66	ARG	3.1
2	P	126	ILE	3.1
1	O	204	MET	3.1
2	N	166	ARG	3.1
1	K	170	MET	3.0
1	O	197	THR	3.0
1	K	128	ALA	3.0
1	M	160	ARG	3.0
1	O	5	GLY	3.0
2	J	201	THR	3.0
1	K	90	ILE	3.0
1	K	19	GLN	3.0
1	O	94	ASP	3.0
1	O	133	PHE	3.0
2	N	273	GLY	3.0
1	K	26	ASP	3.0
1	M	87	VAL	3.0
2	P	22	VAL	3.0
2	P	168	VAL	3.0
1	M	52	PRO	2.9
2	J	119	ALA	2.9
1	M	141	THR	2.9
2	J	183	LEU	2.9
1	I	50	VAL	2.9
1	I	65	LEU	2.9
1	K	142	LEU	2.9
2	N	229	GLY	2.9
1	I	6	ALA	2.9
1	O	140	LEU	2.9
2	P	217	PRO	2.9
2	L	175	TYR	2.9

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Mol	Chain	Res	Type	RSRZ
2	L	268	VAL	2.9
1	M	142	LEU	2.9
1	M	72	ASN	2.9
2	L	255	ASN	2.9
2	J	160	GLY	2.9
2	P	233	PRO	2.9
2	P	129	LEU	2.9
1	M	64	THR	2.9
1	K	187	TYR	2.9
1	K	138	ASN	2.8
2	N	250	LEU	2.8
2	L	226	THR	2.8
2	P	169	THR	2.8
1	M	147	PRO	2.8
1	I	30	THR	2.8
2	P	250	LEU	2.8
1	K	147	PRO	2.8
1	I	5	GLY	2.8
1	K	20	LEU	2.8
2	N	170	VAL	2.8
2	L	183	LEU	2.8
1	I	9	VAL	2.8
2	J	164	SER	2.8
2	L	116	GLY	2.8
1	M	196	LEU	2.8
2	L	115	ALA	2.8
2	P	234	ALA	2.8
1	K	126	GLN	2.8
1	M	119	LYS	2.7
2	N	163	VAL	2.7
1	I	138	ASN	2.7
2	L	216	SER	2.7
1	M	67	ILE	2.7
1	O	90	ILE	2.7
2	L	170	VAL	2.7
2	P	214	SER	2.7
1	M	204	MET	2.7
2	L	203	ASP	2.7
2	N	219	GLN	2.7
1	O	158	GLY	2.7
2	J	253	THR	2.7
2	L	166	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
1	M	65	LEU	2.7
2	J	124	SER	2.7
2	L	258	ARG	2.7
1	I	33	ILE	2.7
1	K	139	SER	2.7
1	M	129	GLU	2.7
2	J	169	THR	2.7
2	P	120	ILE	2.7
2	J	217	PRO	2.7
2	P	104	PRO	2.7
2	L	200	THR	2.7
2	J	172	LEU	2.7
1	K	74	GLN	2.7
1	O	180	ASP	2.7
2	J	202	ALA	2.6
2	J	222	GLY	2.6
1	O	148	TYR	2.6
2	N	239	SER	2.6
1	K	84	TRP	2.6
2	L	193	LEU	2.6
2	L	217	PRO	2.6
1	K	95	LYS	2.6
1	M	203	VAL	2.6
1	A	178	PRO	2.6
1	I	164	ASN	2.6
1	K	200	MET	2.6
1	M	30	THR	2.6
2	J	163	VAL	2.6
1	I	89	ALA	2.6
1	M	98	LEU	2.6
2	J	173	PRO	2.6
1	K	85	MET	2.6
1	M	6	ALA	2.6
2	P	115	ALA	2.6
1	M	63	ASN	2.6
2	N	231	ILE	2.6
2	P	226	THR	2.6
1	M	26	ASP	2.6
1	K	197	THR	2.6
1	K	87	VAL	2.6
2	P	203	ASP	2.5
2	N	253	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	K	158	GLY	2.5
2	J	135	ASN	2.5
1	I	31	TYR	2.5
1	M	32	LEU	2.5
1	I	139	SER	2.5
2	J	208	ILE	2.5
1	I	203	VAL	2.5
2	N	173	PRO	2.5
1	O	53	PRO	2.5
1	O	202	GLY	2.5
1	K	96	SER	2.5
2	P	200	THR	2.5
2	P	148	ILE	2.5
1	O	125	ASP	2.5
1	K	117	PRO	2.5
1	I	133	PHE	2.5
2	J	126	ILE	2.5
2	J	257	ALA	2.5
2	N	222	GLY	2.5
1	O	169	PRO	2.5
1	K	179	SER	2.5
1	O	167	VAL	2.5
2	J	102	PRO	2.5
1	K	159	THR	2.5
1	I	175	VAL	2.5
1	I	52	PRO	2.4
1	I	56	ALA	2.4
1	O	129	GLU	2.4
2	N	254	ALA	2.4
2	J	104	PRO	2.4
1	K	83	PHE	2.4
1	K	111	ILE	2.4
1	O	27	GLU	2.4
1	M	170	MET	2.4
1	K	163	GLU	2.4
1	M	10	ILE	2.4
2	P	219	GLN	2.4
2	J	266	GLY	2.4
2	N	200	THR	2.4
2	J	109	LEU	2.4
1	K	169	PRO	2.4
2	L	206	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
2	N	202	ALA	2.4
1	K	132	ARG	2.4
1	K	133	PHE	2.4
1	K	178	PRO	2.4
1	O	63	ASN	2.4
2	L	211	ASN	2.4
1	I	3	ALA	2.4
1	K	160	ARG	2.4
1	K	9	VAL	2.4
1	K	31	TYR	2.4
1	K	113	LEU	2.4
2	L	163	VAL	2.4
1	I	63	ASN	2.3
1	I	48	PHE	2.3
1	K	166	LEU	2.3
1	O	196	LEU	2.3
2	J	162	ASP	2.3
2	L	117	GLY	2.3
1	K	4	LEU	2.3
1	I	106	ALA	2.3
1	O	92	SER	2.3
2	L	102	PRO	2.3
1	I	2	VAL	2.3
1	K	97	LYS	2.3
1	O	155	LEU	2.3
2	N	249	SER	2.3
2	J	228	ASN	2.3
1	K	54	LEU	2.3
2	J	272	ILE	2.3
1	M	156	ASN	2.3
1	M	106	ALA	2.3
1	M	117	PRO	2.3
1	I	154	GLU	2.3
1	K	28	ASN	2.3
2	J	271	ILE	2.3
2	J	261	GLY	2.3
1	M	167	VAL	2.3
1	K	129	GLU	2.3
2	L	28	VAL	2.3
2	N	233	PRO	2.3
1	I	85	MET	2.3
1	M	128	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	I	169	PRO	2.2
1	M	60	LYS	2.2
1	O	175	VAL	2.2
2	P	117	GLY	2.2
1	K	16	LYS	2.2
1	M	155	LEU	2.2
2	P	28	VAL	2.2
2	P	32	GLN	2.2
2	H	165	ALA	2.2
2	J	127	ALA	2.2
1	I	98	LEU	2.2
2	L	123	GLY	2.2
1	M	57	MET	2.2
1	O	97	LYS	2.2
2	J	115	ALA	2.2
1	K	119	LYS	2.2
2	J	211	ASN	2.2
2	L	121	LYS	2.2
1	K	3	ALA	2.2
2	N	20	VAL	2.2
1	O	16	LYS	2.2
2	P	53	THR	2.2
2	N	183	LEU	2.2
1	K	50	VAL	2.2
2	N	126	ILE	2.2
2	L	195	TYR	2.2
1	I	97	LYS	2.2
1	I	198	PRO	2.2
1	K	164	ASN	2.2
2	N	117	GLY	2.2
2	P	199	GLY	2.2
2	J	11	ILE	2.1
2	N	268	VAL	2.1
1	K	192	ASP	2.1
2	J	195	TYR	2.1
2	N	18	ALA	2.1
2	N	53	THR	2.1
1	K	45	ASP	2.1
2	J	243	VAL	2.1
2	J	209	PHE	2.1
2	N	194	GLY	2.1
1	I	166	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
2	J	184	THR	2.1
2	P	209	PHE	2.1
2	P	163	VAL	2.1
1	K	91	PRO	2.1
1	K	155	LEU	2.1
1	M	175	VAL	2.1
1	M	205	GLU	2.1
1	K	99	THR	2.1
2	N	223	VAL	2.1
1	O	93	MET	2.1
2	P	263	VAL	2.1
2	L	219	GLN	2.1
1	K	123	PRO	2.1
2	L	67	VAL	2.1
1	K	183	SER	2.1
2	J	270	SER	2.1
1	G	177	LEU	2.1
1	M	14	GLY	2.1
2	L	273	GLY	2.1
2	L	118	VAL	2.1
1	M	125	ASP	2.0
1	O	119	LYS	2.0
2	N	261	GLY	2.0
1	C	162	LEU	2.0
1	K	150	LEU	2.0
1	O	25	ASN	2.0
2	P	128	VAL	2.0
1	O	33	ILE	2.0
1	A	135	ARG	2.0
1	K	198	PRO	2.0
1	I	179	SER	2.0
2	L	54	ASP	2.0
2	P	260	GLY	2.0
1	K	168	PRO	2.0
1	O	74	GLN	2.0
1	I	109	SER	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)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	MMA	B	500	13/13	0.82	0.36	5.42	36,56,63,64	0
3	MMA	H	603	13/13	0.90	0.31	4.84	32,55,58,59	0
3	MMA	F	502	13/13	0.88	0.31	3.16	34,54,58,58	0
3	MMA	D	601	13/13	0.86	0.29	2.01	39,65,67,68	0
3	MMA	J	605	13/13	0.86	0.35	0.92	116,117,120,121	0
3	MMA	N	506	13/13	0.84	0.28	0.47	93,96,98,100	0
3	MMA	L	504	13/13	0.76	0.28	0.32	102,108,111,112	0
3	MMA	P	607	13/13	0.87	0.26	0.09	112,115,117,117	0

6.5 Other polymers (i)

There are no such residues in this entry.