



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 01:20 AM BST

PDB ID : 1KLF
Title : FIMH ADHESIN-FIMC CHAPERONE COMPLEX WITH D-MANNOSE
Authors : Hung, C.S.; Bouckaert, J.
Deposited on : 2001-12-11
Resolution : 2.79 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

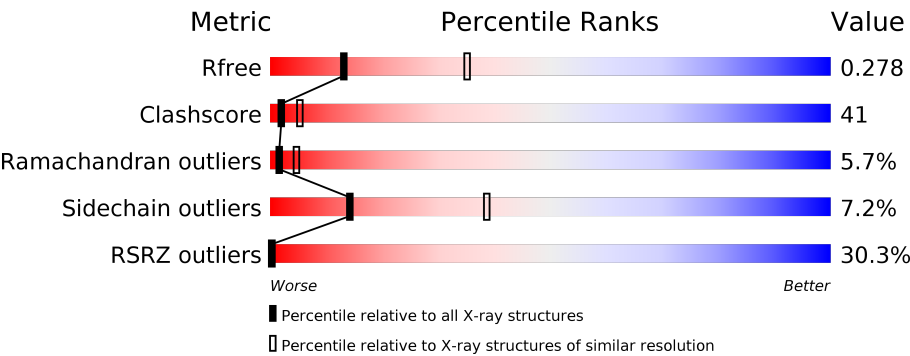
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.79 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	205	<div><div>5%</div><div><div>45%</div><div>47%</div><div>8%</div></div></div>
1	C	205	<div><div>6%</div><div><div>45%</div><div>46%</div><div>8%</div></div></div>
1	E	205	<div><div>%</div><div><div>46%</div><div>46%</div><div>8%</div></div></div>
1	G	205	<div><div>8%</div><div><div>43%</div><div>49%</div><div>8%</div></div></div>
1	I	205	<div><div>71%</div><div><div>38%</div><div>55%</div><div>6%</div></div></div>
1	K	205	<div><div>83%</div><div><div>39%</div><div>54%</div><div>6%</div></div></div>

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Mol	Chain	Length	Quality of chain
1	M	205	 38% 56% 6%
1	O	205	 38% 55% 6%
2	B	279	 57% 35% 8%
2	D	279	 58% 34% 8%
2	F	279	 58% 34% 8%
2	H	279	 56% 36% 8%
2	J	279	 34% 58% 8%
2	L	279	 33% 58% 8%
2	N	279	 34% 57% 8%
2	P	279	 33% 59% 8%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 29775 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			

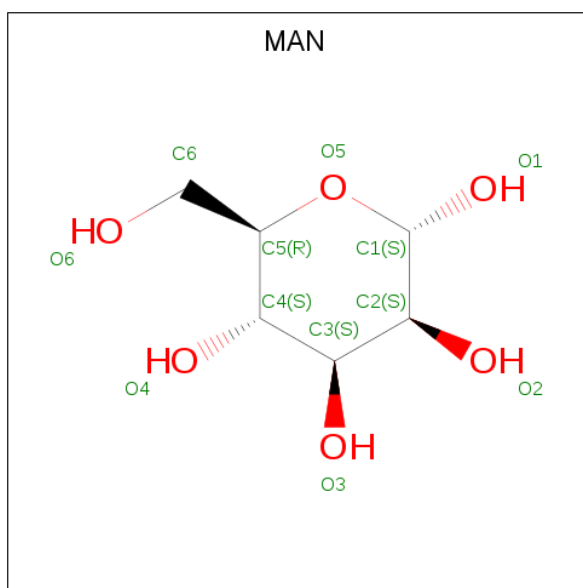
There are 8 discrepancies between the modelled and reference sequences:

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
			2052	1297	342	409	4			
2	D	279	Total	C	N	O	S	0	0	0
			2052	1297	342	409	4			
2	F	279	Total	C	N	O	S	0	0	0
			2052	1297	342	409	4			
2	H	279	Total	C	N	O	S	0	0	0
			2052	1297	342	409	4			
2	J	279	Total	C	N	O	S	0	0	0
			2052	1297	342	409	4			
2	L	279	Total	C	N	O	S	0	0	0
			2052	1297	342	409	4			
2	N	279	Total	C	N	O	S	0	0	0
			2052	1297	342	409	4			
2	P	279	Total	C	N	O	S	0	0	0
			2052	1297	342	409	4			

- Molecule 3 is alpha-D-mannopyranose (three-letter code: MAN) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			12	6	6		
3	D	1	Total	C	O	0	0
			12	6	6		
3	F	1	Total	C	O	0	0
			12	6	6		
3	H	1	Total	C	O	0	0
			12	6	6		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	J	1	Total	C	O	0	0
			12	6	6		
3	L	1	Total	C	O	0	0
			12	6	6		
3	N	1	Total	C	O	0	0
			12	6	6		
3	P	1	Total	C	O	0	0
			12	6	6		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	34	Total	O	0	0
			34	34		
4	B	82	Total	O	0	0
			82	82		
4	C	37	Total	O	0	0
			37	37		
4	D	69	Total	O	0	0
			69	69		
4	E	39	Total	O	0	0
			39	39		
4	F	78	Total	O	0	0
			78	78		
4	G	39	Total	O	0	0
			39	39		
4	H	73	Total	O	0	0
			73	73		
4	I	2	Total	O	0	0
			2	2		
4	J	9	Total	O	0	0
			9	9		
4	K	4	Total	O	0	0
			4	4		
4	L	8	Total	O	0	0
			8	8		
4	M	2	Total	O	0	0
			2	2		
4	N	8	Total	O	0	0
			8	8		
4	O	4	Total	O	0	0
			4	4		

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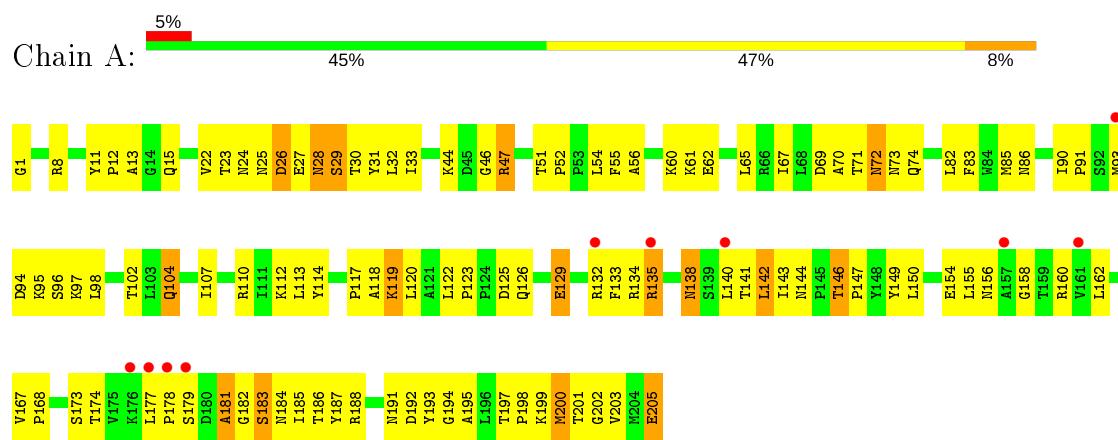
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	P	7	Total	O	0	0
			7	7		

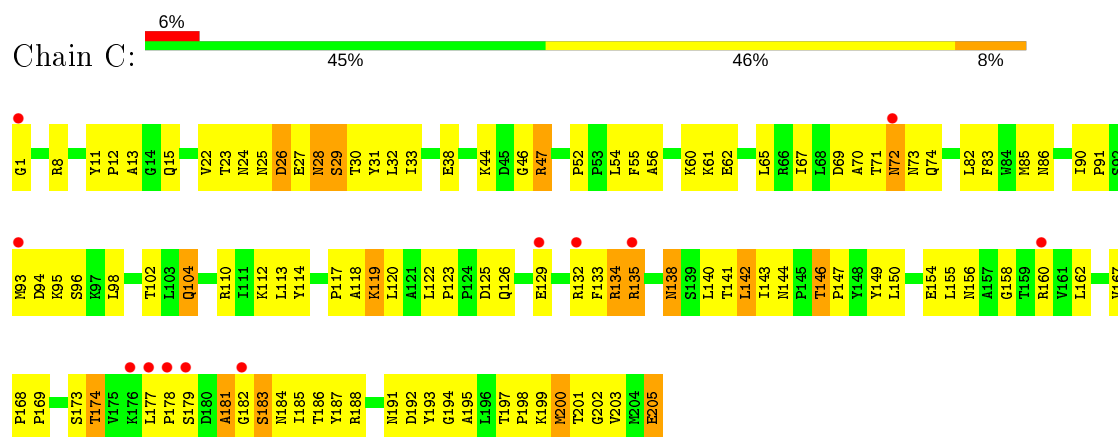
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

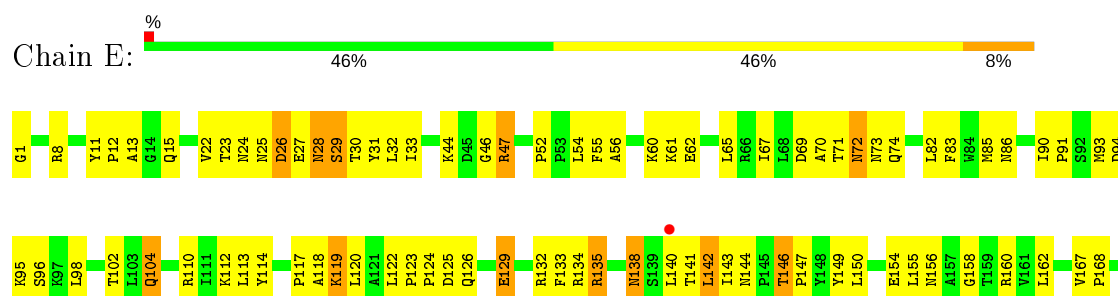
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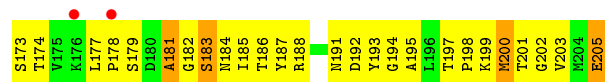


• Molecule 1: CHAPERONE PROTEIN FIMC

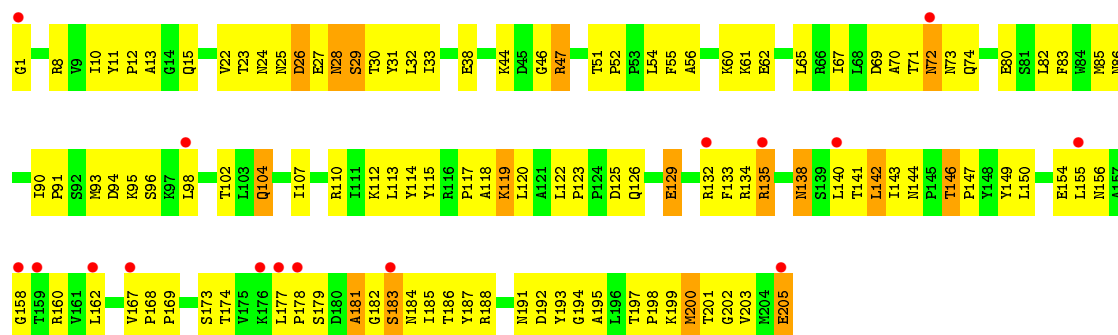
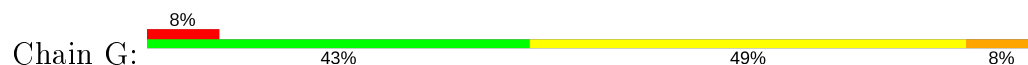


• Molecule 1: CHAPERONE PROTEIN FIMC

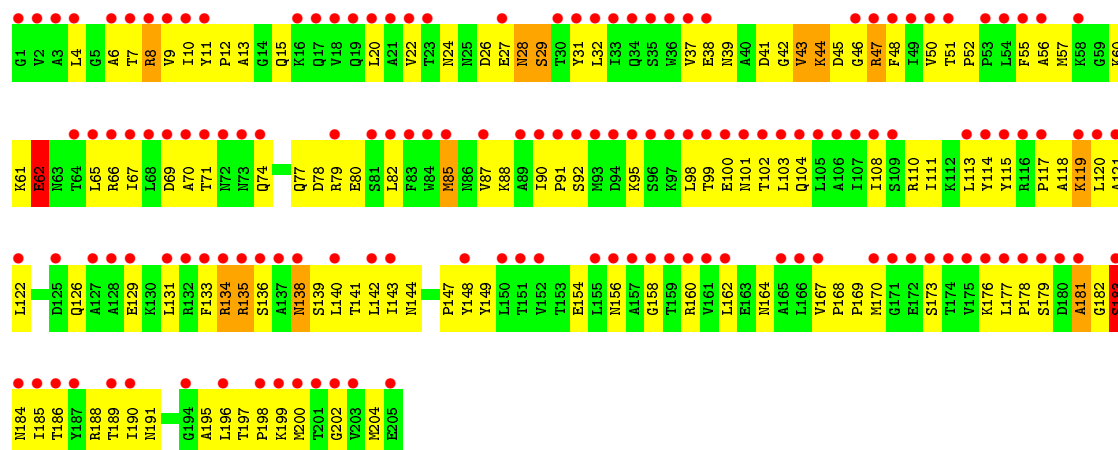




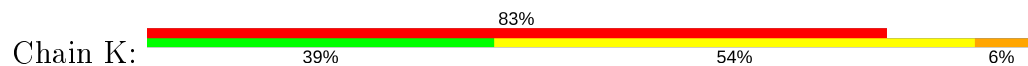
● Molecule 1: CHAPERONE PROTEIN FIMC

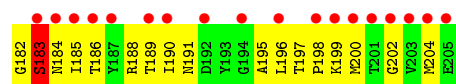


● Molecule 1: CHAPERONE PROTEIN FIMC

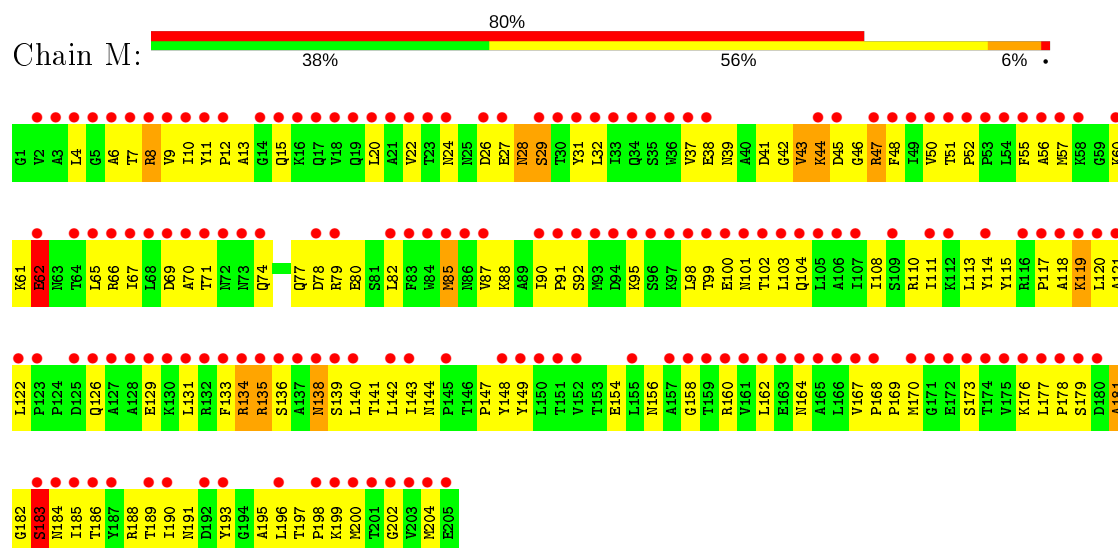


● Molecule 1: CHAPERONE PROTEIN FIMC

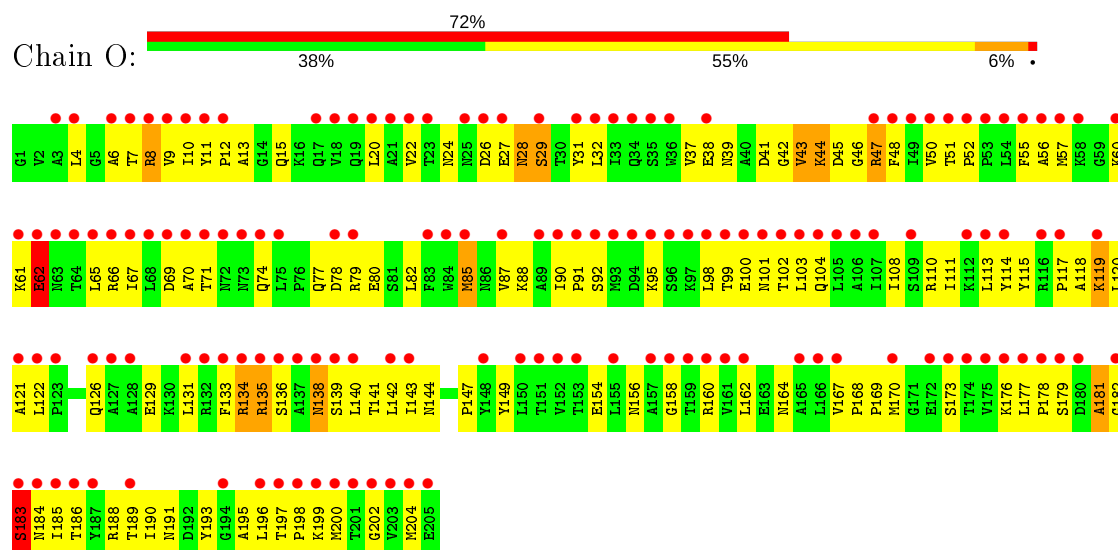




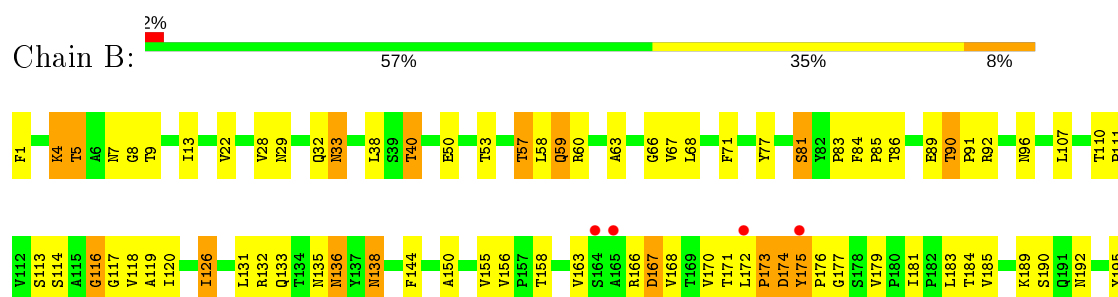
• Molecule 1: CHAPERONE PROTEIN FIMC

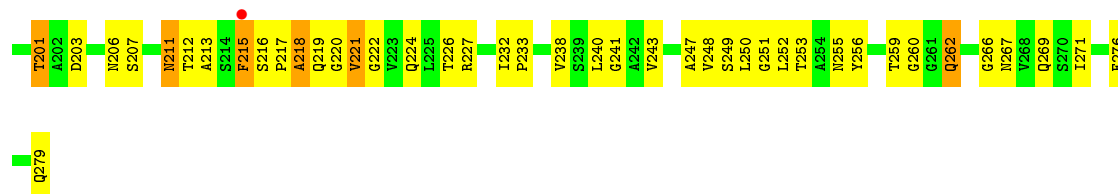


• Molecule 1: CHAPERONE PROTEIN FIMC

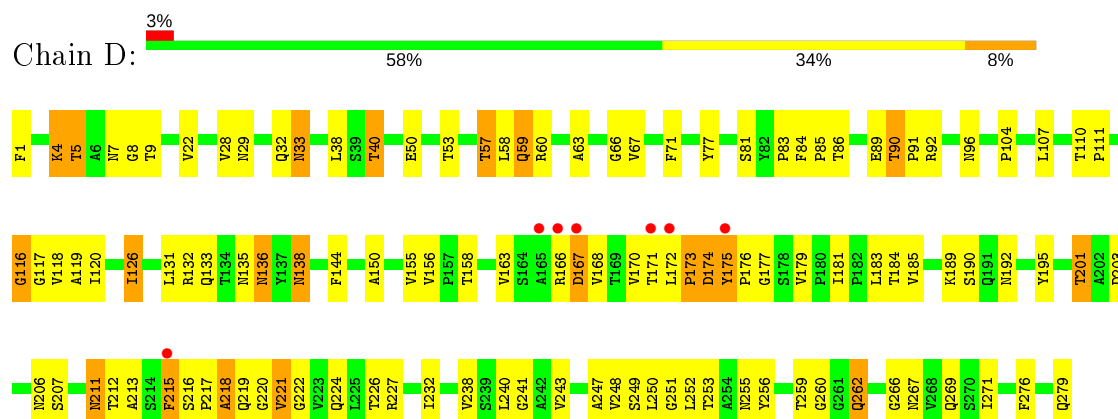


• Molecule 2: FIMH PROTEIN

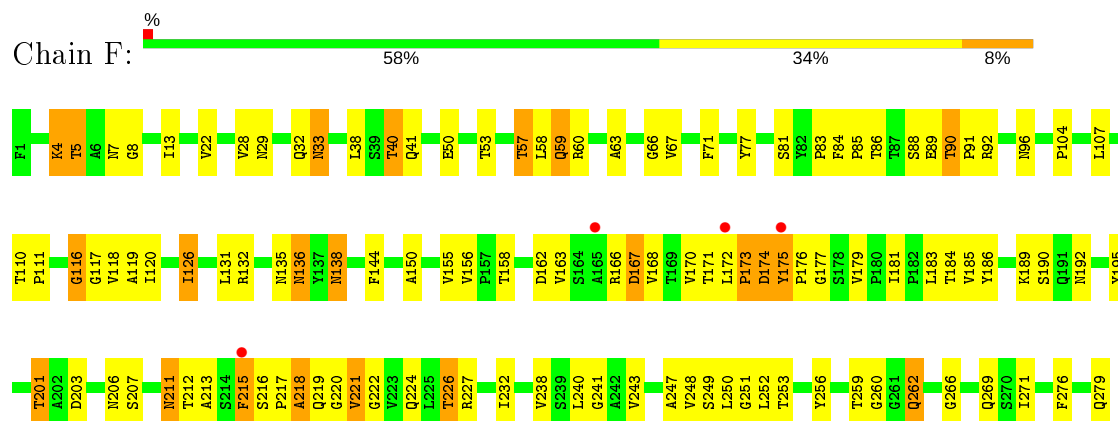




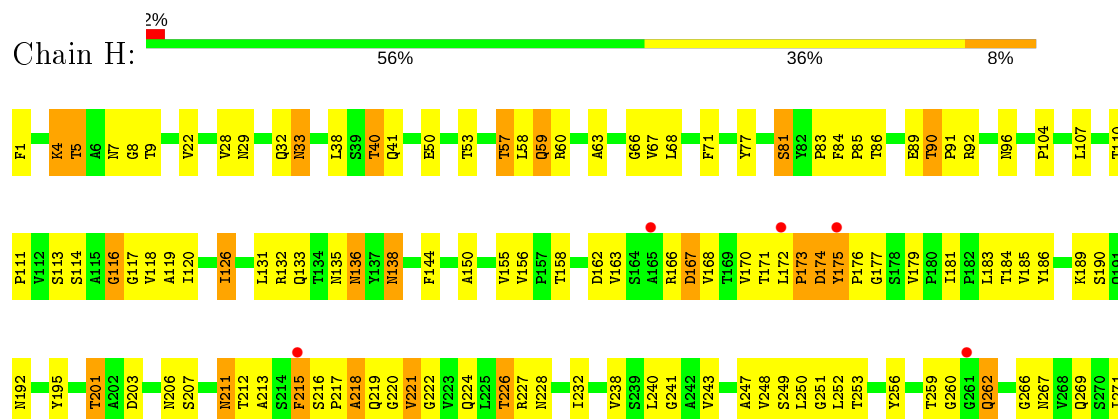
- Molecule 2: FIMH PROTEIN



- Molecule 2: FIMH PROTEIN

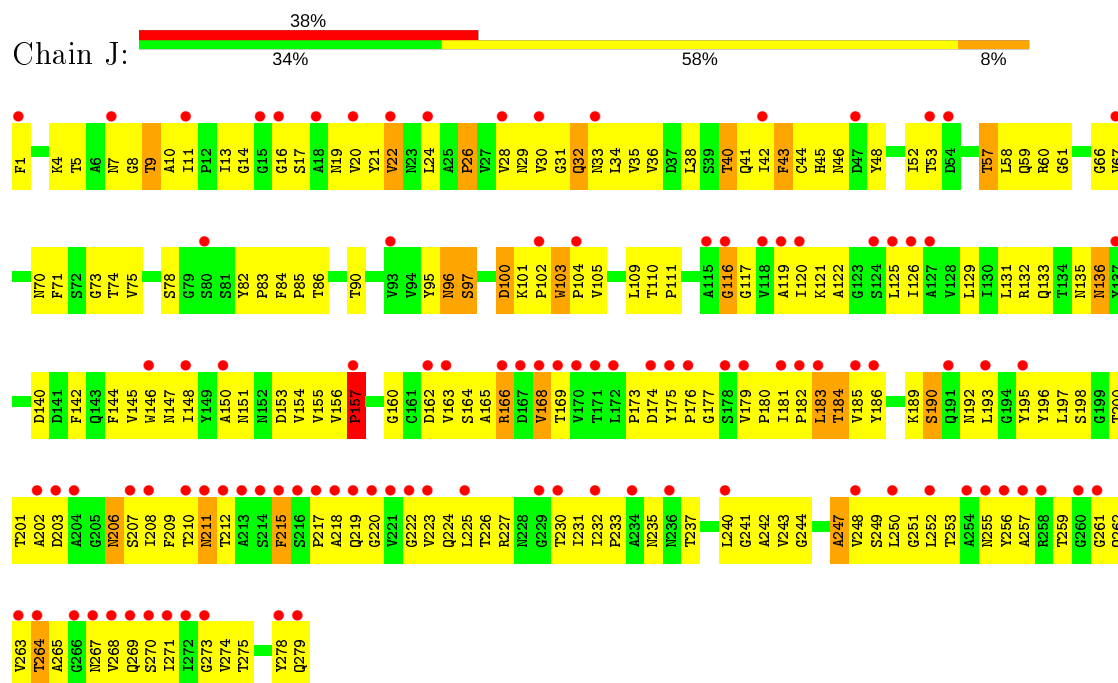


- Molecule 2: FIMH PROTEIN

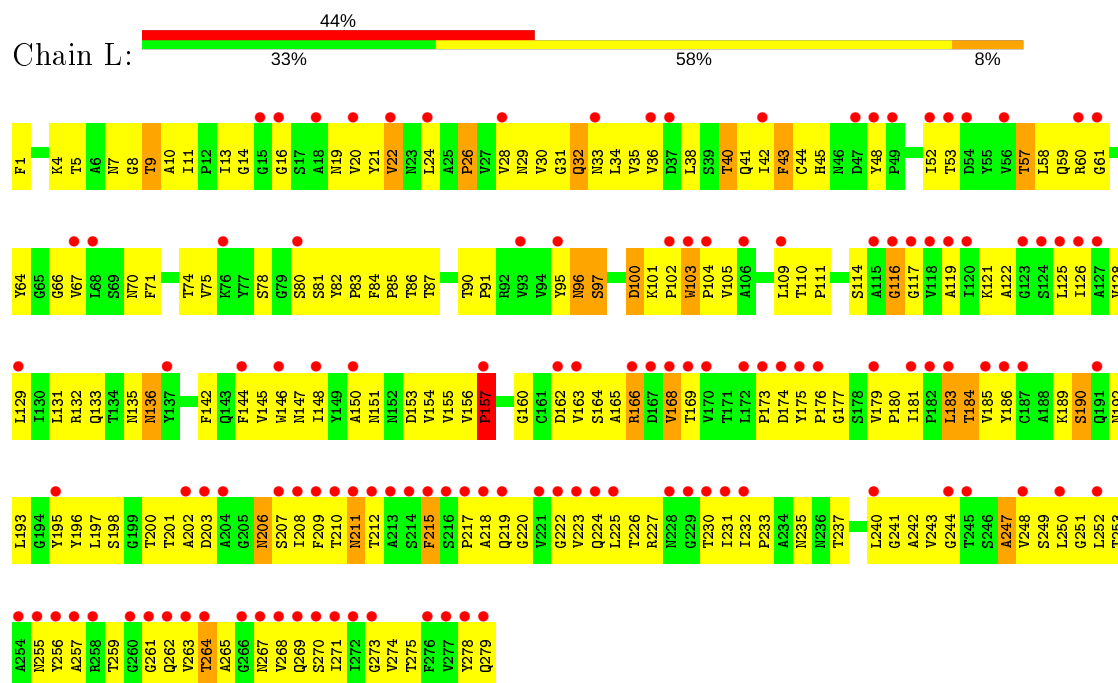




• Molecule 2: FIMH PROTEIN

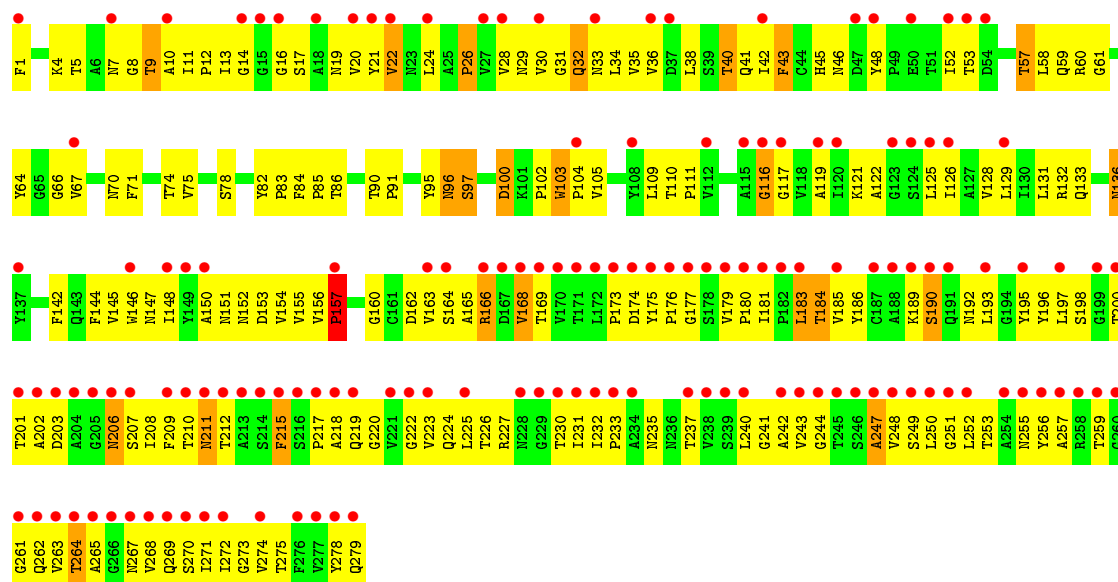


• Molecule 2: FIMH PROTEIN

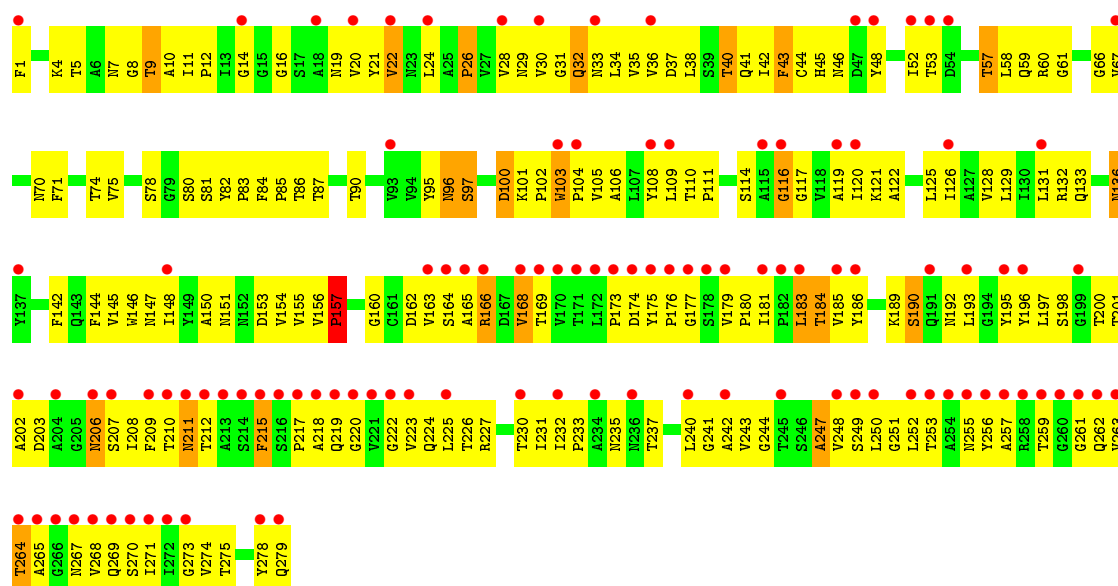


• Molecule 2: FIMH PROTEIN





• Molecule 2: FIMH PROTEIN



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	138.08Å 138.13Å 215.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.68 – 2.79 43.68 – 2.79	Depositor EDS
% Data completeness (in resolution range)	98.9 (43.68-2.79) 99.0 (43.68-2.79)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.86 (at 2.81Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.239 , 0.280 0.240 , 0.278	Depositor DCC
R_{free} test set	9936 reflections (10.02%)	wwPDB-VP
Wilson B-factor (Å ²)	59.1	Xtriage
Anisotropy	0.066	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 68.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.477 for k,h,-l 0.476 for -k,-h,-l 0.477 for -h,-k,l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	29775	wwPDB-VP
Average B, all atoms (Å ²)	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.45% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.74	0/2209
1	C	0.42	0/1625	0.74	0/2209
1	E	0.42	0/1625	0.73	0/2209
1	G	0.42	0/1625	0.74	0/2209
1	I	0.29	0/1625	0.58	0/2209
1	K	0.29	0/1625	0.59	0/2209
1	M	0.29	0/1625	0.59	0/2209
1	O	0.29	0/1625	0.59	0/2209
2	B	0.48	0/2097	0.76	0/2881
2	D	0.48	0/2097	0.76	0/2881
2	F	0.48	0/2097	0.76	0/2881
2	H	0.48	0/2097	0.76	0/2881
2	J	0.31	0/2097	0.59	0/2881
2	L	0.31	0/2097	0.59	0/2881
2	N	0.31	0/2097	0.59	0/2881
2	P	0.31	0/2097	0.59	0/2881
All	All	0.38	0/29776	0.67	0/40720

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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1596	0	1639	133	0
1	C	1596	0	1639	142	0
1	E	1596	0	1639	125	0
1	G	1596	0	1639	135	0
1	I	1596	0	1639	149	0
1	K	1596	0	1639	149	0
1	M	1596	0	1639	152	0
1	O	1596	0	1639	152	0
2	B	2052	0	2007	141	0
2	D	2052	0	2007	142	0
2	F	2052	0	2007	135	0
2	H	2052	0	2007	141	0
2	J	2052	0	2007	200	0
2	L	2052	0	2007	205	0
2	N	2052	0	2007	203	0
2	P	2052	0	2007	208	0
3	B	12	0	12	0	0
3	D	12	0	12	0	0
3	F	12	0	12	0	0
3	H	12	0	12	0	0
3	J	12	0	12	4	0
3	L	12	0	12	2	0
3	N	12	0	12	1	0
3	P	12	0	12	2	0
4	A	34	0	0	3	0
4	B	82	0	0	3	0
4	C	37	0	0	1	0
4	D	69	0	0	4	0
4	E	39	0	0	0	0
4	F	78	0	0	4	0
4	G	39	0	0	3	0
4	H	73	0	0	4	0
4	I	2	0	0	0	0
4	J	9	0	0	1	0
4	K	4	0	0	0	0
4	L	8	0	0	1	0
4	M	2	0	0	0	0
4	N	8	0	0	0	0
4	O	4	0	0	0	0
4	P	7	0	0	0	0
All	All	29775	0	29264	2407	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 41.

All (2407) 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:C:134:ARG:HB3	1:C:141:THR:HG22	1.26	1.14
2:F:126:ILE:HD12	2:F:150:ALA:HB2	1.33	1.10
2:P:224:GLN:HE21	2:P:231:ILE:HG21	1.16	1.10
2:H:126:ILE:HD12	2:H:150:ALA:HB2	1.34	1.09
2:D:126:ILE:HD12	2:D:150:ALA:HB2	1.33	1.09
2:J:224:GLN:HE21	2:J:231:ILE:HG21	1.17	1.08
2:B:126:ILE:HD12	2:B:150:ALA:HB2	1.33	1.07
2:L:201:THR:HG21	2:L:206:ASN:HA	1.38	1.06
2:N:224:GLN:HE21	2:N:231:ILE:HG21	1.17	1.05
2:L:196:TYR:HE1	2:L:198:SER:HB3	1.22	1.05
2:J:196:TYR:HE1	2:J:198:SER:HB3	1.21	1.05
2:L:224:GLN:HE21	2:L:231:ILE:HG21	1.17	1.04
2:N:196:TYR:HE1	2:N:198:SER:HB3	1.22	1.03
2:N:201:THR:HG21	2:N:206:ASN:HA	1.37	1.03
2:J:201:THR:HG21	2:J:206:ASN:HA	1.38	1.03
2:P:196:TYR:HE1	2:P:198:SER:HB3	1.22	1.00
2:B:201:THR:HG21	2:B:206:ASN:HA	1.44	1.00
2:P:201:THR:HG21	2:P:206:ASN:HA	1.38	1.00
2:H:201:THR:HG21	2:H:206:ASN:HA	1.44	1.00
2:D:201:THR:HG21	2:D:206:ASN:HA	1.44	0.99
2:F:201:THR:HG21	2:F:206:ASN:HA	1.45	0.98
1:C:134:ARG:HB3	1:C:141:THR:CG2	1.93	0.98
1:M:47:ARG:HH22	1:M:74:GLN:HE21	1.08	0.97
2:B:170:VAL:HG12	2:B:172:LEU:HB2	1.47	0.97
2:D:170:VAL:HG12	2:D:172:LEU:HB2	1.47	0.96
1:K:47:ARG:HH22	1:K:74:GLN:HE21	1.07	0.96
1:O:47:ARG:HH22	1:O:74:GLN:HE21	1.07	0.96
2:F:120:ILE:HG21	2:F:126:ILE:HD11	1.48	0.96
2:F:170:VAL:HG12	2:F:172:LEU:HB2	1.47	0.96
2:H:170:VAL:HG12	2:H:172:LEU:HB2	1.47	0.95
2:H:5:THR:HG21	4:H:1644:HOH:O	1.68	0.94
2:N:202:ALA:HB2	2:N:210:THR:HG22	1.50	0.94
2:L:57:THR:HG23	2:L:132:ARG:HB3	1.48	0.94
2:P:202:ALA:HB2	2:P:210:THR:HG22	1.50	0.94
2:D:213:ALA:HB2	2:D:269:GLN:HB2	1.50	0.93
2:L:202:ALA:HB2	2:L:210:THR:HG22	1.50	0.93
1:C:47:ARG:HH22	1:C:74:GLN:HE21	0.99	0.93
2:J:202:ALA:HB2	2:J:210:THR:HG22	1.50	0.93
1:E:47:ARG:HH22	1:E:74:GLN:HE21	0.98	0.93
1:G:135:ARG:HH12	1:G:181:ALA:HB1	1.34	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:120:ILE:HG21	2:B:126:ILE:HD11	1.49	0.92
2:D:120:ILE:HG21	2:D:126:ILE:HD11	1.49	0.92
2:J:57:THR:HG23	2:J:132:ARG:HB3	1.49	0.92
2:N:57:THR:HG23	2:N:132:ARG:HB3	1.48	0.92
1:I:47:ARG:HH22	1:I:74:GLN:HE21	1.07	0.92
2:P:57:THR:HG23	2:P:132:ARG:HB3	1.50	0.92
1:G:47:ARG:HH22	1:G:74:GLN:HE21	0.98	0.92
2:H:120:ILE:HG21	2:H:126:ILE:HD11	1.49	0.92
2:F:57:THR:HG22	2:F:132:ARG:HB3	1.52	0.92
2:P:264:THR:HG22	2:P:265:ALA:H	1.35	0.91
1:C:135:ARG:HH12	1:C:181:ALA:HB1	1.33	0.91
2:L:67:VAL:HG21	2:L:126:ILE:HG23	1.51	0.91
1:M:39:ASN:HD21	1:M:43:VAL:HG13	1.35	0.91
2:H:57:THR:HG22	2:H:132:ARG:HB3	1.50	0.91
2:J:264:THR:HG22	2:J:265:ALA:H	1.35	0.91
1:K:39:ASN:HD21	1:K:43:VAL:HG13	1.36	0.91
2:N:163:VAL:HA	2:N:185:VAL:HG22	1.53	0.91
1:A:47:ARG:HH22	1:A:74:GLN:HE21	0.96	0.91
2:L:163:VAL:HA	2:L:185:VAL:HG22	1.52	0.91
1:A:135:ARG:HH12	1:A:181:ALA:HB1	1.34	0.91
1:G:179:SER:C	1:G:181:ALA:H	1.74	0.91
2:H:213:ALA:HB2	2:H:269:GLN:HB2	1.52	0.91
2:N:67:VAL:HG21	2:N:126:ILE:HG23	1.52	0.91
1:E:135:ARG:HH12	1:E:181:ALA:HB1	1.34	0.90
2:J:163:VAL:HA	2:J:185:VAL:HG22	1.53	0.90
2:P:67:VAL:HG21	2:P:126:ILE:HG23	1.51	0.90
2:L:264:THR:HG22	2:L:265:ALA:H	1.35	0.90
1:I:39:ASN:HD21	1:I:43:VAL:HG13	1.36	0.90
1:E:179:SER:C	1:E:181:ALA:H	1.74	0.89
2:J:67:VAL:HG21	2:J:126:ILE:HG23	1.51	0.89
2:P:163:VAL:HA	2:P:185:VAL:HG22	1.52	0.89
1:A:179:SER:C	1:A:181:ALA:H	1.74	0.89
2:F:213:ALA:HB2	2:F:269:GLN:HB2	1.52	0.89
2:B:57:THR:HG21	2:B:89:GLU:OE2	1.73	0.89
2:N:264:THR:HG22	2:N:265:ALA:H	1.36	0.89
1:O:39:ASN:HD21	1:O:43:VAL:HG13	1.36	0.89
2:B:213:ALA:HB2	2:B:269:GLN:HB2	1.53	0.89
2:F:57:THR:HG21	2:F:89:GLU:OE2	1.72	0.89
2:H:167:ASP:CG	2:H:168:VAL:H	1.77	0.88
2:B:167:ASP:CG	2:B:168:VAL:H	1.76	0.88
1:A:133:PHE:HD2	1:A:140:LEU:HD21	1.38	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:57:THR:HG21	2:H:89:GLU:OE2	1.73	0.88
1:M:135:ARG:NH1	1:M:181:ALA:HB1	1.89	0.88
1:C:179:SER:C	1:C:181:ALA:H	1.75	0.88
1:I:176:LYS:H	1:I:176:LYS:HD2	1.38	0.88
1:I:27:GLU:HG2	1:I:60:LYS:HD2	1.55	0.87
1:O:135:ARG:NH1	1:O:181:ALA:HB1	1.89	0.87
2:B:57:THR:HG22	2:B:132:ARG:HB3	1.57	0.87
1:C:133:PHE:HD2	1:C:140:LEU:HD21	1.39	0.87
1:K:134:ARG:HB3	1:K:141:THR:HB	1.56	0.87
1:K:176:LYS:HD2	1:K:176:LYS:H	1.38	0.87
1:M:176:LYS:HD2	1:M:176:LYS:H	1.39	0.87
1:K:135:ARG:NH1	1:K:181:ALA:HB1	1.89	0.86
1:I:134:ARG:HB3	1:I:141:THR:HB	1.56	0.86
1:M:27:GLU:HG2	1:M:60:LYS:HD2	1.55	0.86
1:E:138:ASN:HA	1:E:177:LEU:O	1.76	0.86
2:N:11:ILE:HG23	2:N:16:GLY:HA3	1.57	0.86
1:E:133:PHE:HD2	1:E:140:LEU:HD21	1.38	0.86
1:I:135:ARG:NH1	1:I:181:ALA:HB1	1.89	0.86
1:O:27:GLU:HG2	1:O:60:LYS:HD2	1.55	0.86
2:D:167:ASP:CG	2:D:168:VAL:H	1.76	0.86
1:O:134:ARG:HB3	1:O:141:THR:HB	1.56	0.86
1:C:138:ASN:HA	1:C:177:LEU:O	1.76	0.86
2:D:57:THR:HG21	2:D:89:GLU:OE2	1.75	0.86
2:D:57:THR:HG22	2:D:132:ARG:HB3	1.56	0.86
1:G:133:PHE:HD2	1:G:140:LEU:HD21	1.39	0.86
2:J:58:LEU:H	2:J:90:THR:CG2	1.89	0.86
1:K:27:GLU:HG2	1:K:60:LYS:HD2	1.55	0.86
2:P:11:ILE:HG23	2:P:16:GLY:HA3	1.56	0.85
2:J:11:ILE:HG23	2:J:16:GLY:HA3	1.56	0.85
1:O:135:ARG:HH12	1:O:181:ALA:CB	1.90	0.85
2:D:92:ARG:HH11	2:D:92:ARG:HG3	1.41	0.85
1:G:138:ASN:HA	1:G:177:LEU:O	1.76	0.85
1:M:134:ARG:HB3	1:M:141:THR:HB	1.56	0.85
2:P:58:LEU:H	2:P:90:THR:CG2	1.90	0.85
2:P:58:LEU:H	2:P:90:THR:HG22	1.42	0.85
1:A:138:ASN:HA	1:A:177:LEU:O	1.76	0.84
2:B:92:ARG:HG3	2:B:92:ARG:HH11	1.40	0.84
2:J:5:THR:HG22	2:J:7:ASN:H	1.42	0.84
1:O:176:LYS:H	1:O:176:LYS:HD2	1.38	0.84
2:L:11:ILE:HG23	2:L:16:GLY:HA3	1.56	0.84
2:P:196:TYR:CE1	2:P:198:SER:HB3	2.11	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:135:ARG:HH12	1:C:181:ALA:CB	1.89	0.84
1:E:135:ARG:HH12	1:E:181:ALA:CB	1.90	0.84
2:P:5:THR:HG22	2:P:7:ASN:H	1.43	0.84
1:K:135:ARG:HH12	1:K:181:ALA:CB	1.91	0.84
2:F:167:ASP:CG	2:F:168:VAL:H	1.76	0.84
1:G:135:ARG:HH12	1:G:181:ALA:CB	1.90	0.84
1:M:135:ARG:HH12	1:M:181:ALA:CB	1.90	0.84
1:I:135:ARG:HH12	1:I:181:ALA:CB	1.91	0.84
2:J:196:TYR:CE1	2:J:198:SER:HB3	2.11	0.84
2:N:196:TYR:CE1	2:N:198:SER:HB3	2.11	0.84
2:H:59:GLN:HG2	2:H:132:ARG:HD2	1.60	0.83
2:L:58:LEU:H	2:L:90:THR:HG22	1.42	0.83
1:A:135:ARG:HH12	1:A:181:ALA:CB	1.90	0.83
2:L:196:TYR:CE1	2:L:198:SER:HB3	2.11	0.83
1:C:135:ARG:NH1	1:C:181:ALA:HB1	1.93	0.83
2:N:5:THR:HG22	2:N:7:ASN:H	1.42	0.83
2:J:58:LEU:H	2:J:90:THR:HG22	1.41	0.83
2:N:58:LEU:H	2:N:90:THR:CG2	1.91	0.83
2:L:5:THR:HG22	2:L:7:ASN:H	1.43	0.83
2:B:59:GLN:HG2	2:B:132:ARG:HD2	1.60	0.83
2:L:58:LEU:H	2:L:90:THR:CG2	1.90	0.83
1:G:141:THR:OG1	1:G:174:THR:HG22	1.78	0.82
2:D:192:ASN:HD22	2:D:279:GLN:HE22	1.26	0.82
1:E:47:ARG:NH2	1:E:74:GLN:HE21	1.76	0.82
2:F:92:ARG:HH11	2:F:92:ARG:HG3	1.44	0.82
2:L:226:THR:HB	2:L:231:ILE:HG12	1.62	0.82
1:A:47:ARG:NH2	1:A:74:GLN:HE21	1.75	0.82
2:H:92:ARG:HG3	2:H:92:ARG:HH11	1.42	0.82
2:N:58:LEU:H	2:N:90:THR:HG22	1.42	0.82
2:P:226:THR:HB	2:P:231:ILE:HG12	1.62	0.82
2:N:224:GLN:NE2	2:N:231:ILE:HG21	1.95	0.82
2:H:192:ASN:HD22	2:H:279:GLN:HE22	1.27	0.82
2:F:59:GLN:HG2	2:F:132:ARG:HD2	1.60	0.82
1:G:47:ARG:NH2	1:G:74:GLN:HE21	1.76	0.82
2:D:53:THR:H	2:D:136:ASN:HD21	1.27	0.82
1:I:177:LEU:HD12	1:I:178:PRO:HD2	1.61	0.81
2:N:253:THR:HG22	2:N:255:ASN:HD21	1.45	0.81
1:O:177:LEU:HD12	1:O:178:PRO:HD2	1.61	0.81
2:B:192:ASN:HD22	2:B:279:GLN:HE22	1.26	0.81
2:P:34:LEU:HD12	2:P:35:VAL:H	1.44	0.81
2:J:253:THR:HG22	2:J:255:ASN:HD21	1.44	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:34:LEU:HD12	2:N:35:VAL:H	1.45	0.81
2:D:59:GLN:HG2	2:D:132:ARG:HD2	1.60	0.81
1:I:8:ARG:HB3	1:I:8:ARG:NH2	1.95	0.81
1:M:8:ARG:NH2	1:M:8:ARG:HB3	1.95	0.81
1:E:135:ARG:NH1	1:E:181:ALA:HB1	1.94	0.81
2:H:53:THR:H	2:H:136:ASN:HD21	1.27	0.81
2:P:224:GLN:NE2	2:P:231:ILE:HG21	1.94	0.81
2:P:253:THR:HG22	2:P:255:ASN:HD21	1.45	0.81
1:A:135:ARG:NH1	1:A:181:ALA:HB1	1.94	0.81
2:F:53:THR:H	2:F:136:ASN:HD21	1.26	0.81
2:L:253:THR:HG22	2:L:255:ASN:HD21	1.45	0.81
1:M:177:LEU:HD12	1:M:178:PRO:HD2	1.61	0.81
2:B:53:THR:H	2:B:136:ASN:HD21	1.26	0.81
1:G:135:ARG:NH1	1:G:181:ALA:HB1	1.94	0.81
1:K:177:LEU:HD12	1:K:178:PRO:HD2	1.61	0.81
2:N:208:ILE:HG23	2:N:257:ALA:HB1	1.63	0.81
2:L:34:LEU:HD12	2:L:35:VAL:H	1.45	0.80
1:M:39:ASN:ND2	1:M:43:VAL:HG13	1.95	0.80
2:D:218:ALA:HB2	2:D:266:GLY:C	2.02	0.80
1:I:39:ASN:ND2	1:I:43:VAL:HG13	1.96	0.80
2:F:218:ALA:HB2	2:F:266:GLY:C	2.02	0.80
2:P:208:ILE:HG23	2:P:257:ALA:HB1	1.64	0.80
2:J:226:THR:HB	2:J:231:ILE:HG12	1.62	0.80
2:L:208:ILE:HG23	2:L:257:ALA:HB1	1.63	0.80
1:M:8:ARG:HH21	1:M:8:ARG:HB3	1.47	0.80
1:K:39:ASN:ND2	1:K:43:VAL:HG13	1.96	0.80
1:O:39:ASN:ND2	1:O:43:VAL:HG13	1.96	0.80
1:O:8:ARG:NH2	1:O:8:ARG:HB3	1.95	0.80
1:M:32:LEU:HB2	1:M:90:ILE:HB	1.64	0.80
2:H:218:ALA:HB2	2:H:266:GLY:C	2.02	0.79
2:B:218:ALA:HB2	2:B:266:GLY:C	2.02	0.79
2:J:224:GLN:NE2	2:J:231:ILE:HG21	1.95	0.79
2:J:208:ILE:HG23	2:J:257:ALA:HB1	1.64	0.79
1:K:47:ARG:NH2	1:K:74:GLN:HE21	1.81	0.79
2:N:226:THR:HB	2:N:231:ILE:HG12	1.62	0.79
1:E:47:ARG:HG3	1:E:71:THR:HB	1.65	0.79
1:I:47:ARG:NH2	1:I:74:GLN:HE21	1.81	0.79
2:J:34:LEU:HD12	2:J:35:VAL:H	1.45	0.79
1:K:8:ARG:HB3	1:K:8:ARG:NH2	1.96	0.79
2:F:192:ASN:HD22	2:F:279:GLN:HE22	1.31	0.79
1:O:47:ARG:NH2	1:O:74:GLN:HE21	1.81	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:32:LEU:HB2	1:K:90:ILE:HB	1.64	0.79
2:L:224:GLN:NE2	2:L:231:ILE:HG21	1.95	0.79
1:C:47:ARG:NH2	1:C:74:GLN:HE21	1.78	0.79
1:M:38:GLU:HG2	1:M:44:LYS:HG3	1.65	0.78
1:G:52:PRO:HG2	1:G:55:PHE:CD2	2.18	0.78
1:I:8:ARG:HB3	1:I:8:ARG:HH21	1.47	0.78
2:N:21:TYR:HB3	2:N:151:ASN:HD21	1.49	0.78
1:O:32:LEU:HB2	1:O:90:ILE:HB	1.64	0.78
1:E:188:ARG:HH11	1:E:199:LYS:HB2	1.49	0.78
1:G:188:ARG:HH11	1:G:199:LYS:HB2	1.49	0.78
2:N:59:GLN:HG3	2:N:132:ARG:HB2	1.66	0.78
1:O:8:ARG:HH21	1:O:8:ARG:HB3	1.47	0.78
1:A:188:ARG:HH11	1:A:199:LYS:HB2	1.48	0.78
1:G:47:ARG:HG3	1:G:71:THR:HB	1.65	0.78
2:D:192:ASN:HD22	2:D:279:GLN:NE2	1.82	0.78
1:A:47:ARG:HG3	1:A:71:THR:HB	1.64	0.77
1:C:52:PRO:HG2	1:C:55:PHE:CD2	2.19	0.77
1:K:38:GLU:HG2	1:K:44:LYS:HG3	1.65	0.77
1:C:134:ARG:HD2	1:C:141:THR:CG2	2.14	0.77
1:M:47:ARG:NH2	1:M:74:GLN:HE21	1.81	0.77
2:N:226:THR:HG23	2:N:253:THR:HB	1.66	0.77
1:O:38:GLU:HG2	1:O:44:LYS:HG3	1.65	0.77
2:P:226:THR:HG23	2:P:253:THR:HB	1.67	0.77
1:C:47:ARG:HG3	1:C:71:THR:HB	1.65	0.77
2:J:226:THR:HG23	2:J:253:THR:HB	1.66	0.77
2:P:21:TYR:HB3	2:P:151:ASN:HD21	1.50	0.77
2:D:172:LEU:O	2:D:174:ASP:N	2.18	0.77
1:I:32:LEU:HB2	1:I:90:ILE:HB	1.64	0.77
2:B:192:ASN:HD22	2:B:279:GLN:NE2	1.83	0.77
2:J:21:TYR:HB3	2:J:151:ASN:HD21	1.49	0.77
2:L:226:THR:HG23	2:L:253:THR:HB	1.67	0.77
1:C:134:ARG:HD2	1:C:141:THR:HG21	1.67	0.76
1:K:8:ARG:HB3	1:K:8:ARG:HH21	1.47	0.76
2:L:21:TYR:HB3	2:L:151:ASN:HD21	1.50	0.76
2:L:59:GLN:HG3	2:L:132:ARG:HB2	1.67	0.76
2:H:172:LEU:O	2:H:174:ASP:N	2.18	0.76
2:J:59:GLN:HG3	2:J:132:ARG:HB2	1.66	0.76
1:K:52:PRO:HG2	1:K:55:PHE:CD2	2.20	0.76
1:O:176:LYS:HD2	1:O:176:LYS:N	2.00	0.76
2:B:172:LEU:O	2:B:174:ASP:N	2.18	0.76
2:P:59:GLN:HG3	2:P:132:ARG:HB2	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:197:LEU:HD13	2:P:225:LEU:HD12	1.67	0.76
1:O:52:PRO:HG2	1:O:55:PHE:CD2	2.21	0.76
1:A:32:LEU:HB2	1:A:90:ILE:HB	1.68	0.76
1:C:32:LEU:HB2	1:C:90:ILE:HB	1.67	0.76
2:F:172:LEU:O	2:F:174:ASP:N	2.18	0.76
1:C:188:ARG:HH11	1:C:199:LYS:HB2	1.49	0.76
1:E:52:PRO:HG2	1:E:55:PHE:CD2	2.21	0.75
1:I:52:PRO:HG2	1:I:55:PHE:CD2	2.20	0.75
1:G:112:LYS:HG3	4:G:209:HOH:O	1.86	0.75
1:A:52:PRO:HG2	1:A:55:PHE:CD2	2.21	0.75
1:I:38:GLU:HG2	1:I:44:LYS:HG3	1.65	0.75
1:M:52:PRO:HG2	1:M:55:PHE:CD2	2.21	0.75
1:A:47:ARG:HH22	1:A:74:GLN:NE2	1.80	0.75
2:B:173:PRO:HG3	2:B:179:VAL:HG13	1.69	0.75
2:L:197:LEU:HD13	2:L:225:LEU:HD12	1.68	0.75
1:O:185:ILE:HB	1:O:202:GLY:HA3	1.68	0.75
1:K:176:LYS:HD2	1:K:176:LYS:N	2.00	0.75
2:J:197:LEU:HD13	2:J:225:LEU:HD12	1.67	0.74
2:P:180:PRO:HA	2:P:253:THR:HA	1.70	0.74
1:I:185:ILE:HB	1:I:202:GLY:HA3	1.68	0.74
2:N:197:LEU:HD13	2:N:225:LEU:HD12	1.68	0.74
1:G:32:LEU:HB2	1:G:90:ILE:HB	1.69	0.74
1:M:185:ILE:HB	1:M:202:GLY:HA3	1.68	0.74
2:H:192:ASN:HD22	2:H:279:GLN:NE2	1.85	0.74
2:D:173:PRO:HG3	2:D:179:VAL:HG13	1.69	0.74
1:C:134:ARG:CB	1:C:141:THR:HG22	2.15	0.74
2:N:180:PRO:HA	2:N:253:THR:HA	1.70	0.74
1:E:32:LEU:HB2	1:E:90:ILE:HB	1.70	0.74
2:H:171:THR:C	2:H:173:PRO:HD2	2.08	0.74
1:K:185:ILE:HB	1:K:202:GLY:HA3	1.68	0.74
1:E:47:ARG:HH22	1:E:74:GLN:NE2	1.82	0.73
2:H:173:PRO:HG3	2:H:179:VAL:HG13	1.70	0.73
2:L:180:PRO:HA	2:L:253:THR:HA	1.70	0.73
2:F:171:THR:C	2:F:173:PRO:HD2	2.08	0.73
2:L:180:PRO:HB3	2:L:253:THR:HG23	1.71	0.73
1:M:176:LYS:HD2	1:M:176:LYS:N	2.00	0.73
2:P:180:PRO:HB3	2:P:253:THR:HG23	1.71	0.73
1:A:110:ARG:HD3	4:A:222:HOH:O	1.87	0.73
2:B:171:THR:C	2:B:173:PRO:HD2	2.08	0.73
1:G:47:ARG:HH22	1:G:74:GLN:NE2	1.82	0.73
2:D:226:THR:HG23	4:D:1618:HOH:O	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:29:ASN:HD22	2:D:32:GLN:HE22	1.37	0.73
2:L:186:TYR:HB3	2:L:247:ALA:HA	1.71	0.73
2:J:180:PRO:HA	2:J:253:THR:HA	1.70	0.73
2:N:180:PRO:HB3	2:N:253:THR:HG23	1.71	0.73
2:F:29:ASN:HD22	2:F:32:GLN:HE22	1.36	0.73
2:H:29:ASN:HD22	2:H:32:GLN:HE22	1.36	0.73
2:N:19:ASN:HD21	2:P:219:GLN:NE2	1.85	0.73
2:J:19:ASN:HD21	2:L:219:GLN:NE2	1.87	0.72
1:M:111:ILE:HG22	2:N:278:TYR:HB2	1.72	0.72
2:F:173:PRO:HG3	2:F:179:VAL:HG13	1.70	0.72
2:N:186:TYR:HB3	2:N:247:ALA:HA	1.71	0.72
2:D:201:THR:HG21	2:D:206:ASN:HD22	1.55	0.72
2:H:29:ASN:HD22	2:H:32:GLN:NE2	1.88	0.72
2:H:57:THR:CG2	2:H:132:ARG:HB3	2.19	0.72
2:J:180:PRO:HB3	2:J:253:THR:HG23	1.72	0.72
2:B:29:ASN:HD22	2:B:32:GLN:HE22	1.37	0.72
1:M:101:ASN:HD22	2:N:268:VAL:HG23	1.55	0.72
1:A:112:LYS:HG3	4:A:208:HOH:O	1.90	0.72
1:C:141:THR:HB	1:C:174:THR:HG23	1.72	0.72
1:I:176:LYS:N	1:I:176:LYS:HD2	2.00	0.71
2:P:186:TYR:HB3	2:P:247:ALA:HA	1.71	0.71
1:O:101:ASN:HD22	2:P:268:VAL:HG23	1.56	0.71
2:F:29:ASN:HD22	2:F:32:GLN:NE2	1.87	0.71
1:O:111:ILE:HG22	2:P:278:TYR:HB2	1.72	0.71
2:F:192:ASN:HD22	2:F:279:GLN:NE2	1.87	0.71
1:C:141:THR:O	1:C:141:THR:HG23	1.90	0.71
2:F:201:THR:HG21	2:F:206:ASN:HD22	1.54	0.71
2:J:186:TYR:HB3	2:J:247:ALA:HA	1.71	0.71
2:D:29:ASN:HD22	2:D:32:GLN:NE2	1.89	0.71
2:H:262:GLN:HE21	2:H:262:GLN:HA	1.56	0.71
2:B:201:THR:HG21	2:B:206:ASN:HD22	1.56	0.71
1:C:47:ARG:HH22	1:C:74:GLN:NE2	1.83	0.71
2:D:32:GLN:O	2:D:110:THR:HG23	1.91	0.71
2:D:171:THR:C	2:D:173:PRO:HD2	2.10	0.71
2:F:57:THR:CG2	2:F:132:ARG:HB3	2.21	0.71
1:I:111:ILE:HG22	2:J:278:TYR:HB2	1.72	0.71
2:J:48:TYR:HB2	2:J:52:ILE:HD12	1.73	0.71
2:B:29:ASN:HD22	2:B:32:GLN:NE2	1.89	0.71
2:H:32:GLN:O	2:H:110:THR:HG23	1.90	0.70
2:P:155:VAL:HG12	2:P:157:PRO:HD3	1.73	0.70
2:D:173:PRO:HB2	2:D:177:GLY:HA3	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:32:GLN:O	2:B:110:THR:HG23	1.91	0.70
2:N:155:VAL:HG12	2:N:157:PRO:HD3	1.73	0.70
1:K:101:ASN:HD22	2:L:268:VAL:HG23	1.56	0.70
1:K:111:ILE:HG22	2:L:278:TYR:HB2	1.72	0.70
1:I:101:ASN:HD22	2:J:268:VAL:HG23	1.56	0.70
1:M:12:PRO:HB2	1:M:15:GLN:HG2	1.73	0.70
2:H:201:THR:HG21	2:H:206:ASN:HD22	1.55	0.70
2:L:164:SER:HB2	2:L:184:THR:HG23	1.74	0.70
2:B:262:GLN:HA	2:B:262:GLN:HE21	1.56	0.70
1:M:182:GLY:O	1:M:183:SER:HB2	1.92	0.70
2:P:48:TYR:HB2	2:P:52:ILE:HD12	1.74	0.70
2:F:32:GLN:O	2:F:110:THR:HG23	1.91	0.69
2:F:262:GLN:HA	2:F:262:GLN:HE21	1.56	0.69
2:N:48:TYR:HB2	2:N:52:ILE:HD12	1.74	0.69
2:D:57:THR:CG2	2:D:132:ARG:HB3	2.22	0.69
1:E:12:PRO:HG2	1:E:15:GLN:HE21	1.57	0.69
1:I:12:PRO:HB2	1:I:15:GLN:HG2	1.73	0.69
2:B:173:PRO:HB2	2:B:177:GLY:HA3	1.74	0.69
2:B:81:SER:O	2:P:114:SER:HB2	1.92	0.69
2:F:218:ALA:HB2	2:F:266:GLY:O	1.93	0.69
2:N:164:SER:HB2	2:N:184:THR:HG23	1.75	0.69
2:H:58:LEU:H	2:H:90:THR:HG22	1.57	0.69
1:K:12:PRO:HB2	1:K:15:GLN:HG2	1.73	0.69
1:K:162:LEU:HD21	1:K:178:PRO:HD3	1.75	0.69
1:O:12:PRO:HB2	1:O:15:GLN:HG2	1.73	0.69
1:O:162:LEU:HD21	1:O:178:PRO:HD3	1.75	0.69
2:F:172:LEU:N	2:F:173:PRO:HD2	2.07	0.69
1:G:25:ASN:O	1:G:60:LYS:HG2	1.93	0.69
1:I:162:LEU:HD21	1:I:178:PRO:HD3	1.75	0.69
2:D:262:GLN:HE21	2:D:262:GLN:HA	1.57	0.69
2:L:48:TYR:HB2	2:L:52:ILE:HD12	1.73	0.69
1:C:25:ASN:O	1:C:60:LYS:HG2	1.93	0.69
1:E:112:LYS:HG3	4:F:1506:HOH:O	1.92	0.69
2:H:173:PRO:HB2	2:H:177:GLY:HA3	1.74	0.69
1:I:182:GLY:O	1:I:183:SER:HB2	1.93	0.69
2:J:155:VAL:HG12	2:J:157:PRO:HD3	1.73	0.69
2:L:155:VAL:HG12	2:L:157:PRO:HD3	1.73	0.69
2:D:172:LEU:N	2:D:173:PRO:HD2	2.08	0.69
2:H:172:LEU:N	2:H:173:PRO:HD2	2.06	0.69
1:C:141:THR:CB	1:C:174:THR:HG23	2.22	0.69
2:J:264:THR:HG22	2:J:265:ALA:N	2.08	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:12:PRO:HB2	1:C:15:GLN:CG	2.23	0.69
1:I:82:LEU:HD13	1:I:114:TYR:CE2	2.28	0.69
1:O:88:LYS:HE2	1:O:90:ILE:HG12	1.75	0.69
2:P:164:SER:HB2	2:P:184:THR:HG23	1.75	0.69
1:A:12:PRO:HB2	1:A:15:GLN:CG	2.22	0.68
2:J:164:SER:HB2	2:J:184:THR:HG23	1.74	0.68
2:L:264:THR:HG22	2:L:265:ALA:N	2.08	0.68
1:M:162:LEU:HD21	1:M:178:PRO:HD3	1.75	0.68
1:M:88:LYS:HE2	1:M:90:ILE:HG12	1.75	0.68
2:B:172:LEU:N	2:B:173:PRO:HD2	2.07	0.68
1:C:112:LYS:HG3	4:D:1605:HOH:O	1.94	0.68
1:C:182:GLY:O	1:C:183:SER:HB2	1.92	0.68
2:H:81:SER:O	2:L:114:SER:HB2	1.93	0.68
1:A:12:PRO:HG2	1:A:15:GLN:HE21	1.58	0.68
1:A:182:GLY:O	1:A:183:SER:HB2	1.92	0.68
1:G:182:GLY:O	1:G:183:SER:HB2	1.93	0.68
2:B:218:ALA:HB2	2:B:266:GLY:O	1.94	0.68
2:B:57:THR:CG2	2:B:132:ARG:HB3	2.24	0.68
1:E:86:ASN:HD21	1:E:110:ARG:HE	1.42	0.68
1:G:86:ASN:HD21	1:G:110:ARG:HE	1.41	0.68
1:M:82:LEU:HD13	1:M:114:TYR:CE2	2.28	0.68
1:O:82:LEU:HD13	1:O:114:TYR:CE2	2.28	0.68
2:D:218:ALA:HB2	2:D:266:GLY:O	1.93	0.68
1:G:12:PRO:HG2	1:G:15:GLN:HE21	1.59	0.68
2:H:53:THR:HB	2:H:136:ASN:OD1	1.93	0.68
1:G:27:GLU:HG3	1:G:60:LYS:HD2	1.74	0.68
1:O:135:ARG:NH1	1:O:181:ALA:CB	2.53	0.68
1:E:182:GLY:O	1:E:183:SER:HB2	1.93	0.68
2:F:173:PRO:HB2	2:F:177:GLY:HA3	1.74	0.68
1:K:79:ARG:HB3	1:K:170:MET:CE	2.24	0.68
2:B:116:GLY:HA2	2:B:189:LYS:HE2	1.76	0.68
1:K:135:ARG:NH1	1:K:181:ALA:CB	2.53	0.68
1:M:138:ASN:HA	1:M:177:LEU:O	1.94	0.68
1:A:25:ASN:O	1:A:60:LYS:HG2	1.93	0.68
1:C:12:PRO:HG2	1:C:15:GLN:HE21	1.59	0.68
1:K:82:LEU:HD13	1:K:114:TYR:CE2	2.29	0.68
2:D:53:THR:HB	2:D:136:ASN:OD1	1.94	0.67
1:G:12:PRO:HB2	1:G:15:GLN:CG	2.24	0.67
1:I:79:ARG:HB3	1:I:170:MET:CE	2.24	0.67
1:K:88:LYS:HE2	1:K:90:ILE:HG12	1.76	0.67
1:O:79:ARG:HB3	1:O:170:MET:CE	2.23	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:ASN:HD21	1:A:110:ARG:HE	1.42	0.67
1:A:144:ASN:ND2	1:A:150:LEU:HG	2.10	0.67
2:B:53:THR:H	2:B:136:ASN:ND2	1.92	0.67
1:K:138:ASN:HA	1:K:177:LEU:O	1.94	0.67
2:F:58:LEU:H	2:F:90:THR:HG22	1.59	0.67
1:I:138:ASN:HA	1:I:177:LEU:O	1.94	0.67
1:K:182:GLY:O	1:K:183:SER:HB2	1.93	0.67
2:N:105:VAL:HG11	2:N:129:LEU:HD13	1.77	0.67
2:B:58:LEU:H	2:B:90:THR:HG22	1.58	0.67
1:E:25:ASN:O	1:E:60:LYS:HG2	1.93	0.67
2:P:24:LEU:HD22	2:P:36:VAL:HG22	1.77	0.67
2:B:217:PRO:O	2:B:219:GLN:N	2.28	0.67
2:B:226:THR:HG23	4:B:1508:HOH:O	1.94	0.67
2:D:221:VAL:O	2:D:259:THR:HG23	1.95	0.67
1:G:188:ARG:NH1	1:G:199:LYS:H	1.92	0.67
2:J:186:TYR:HB2	2:J:244:GLY:O	1.95	0.67
1:O:138:ASN:HA	1:O:177:LEU:O	1.94	0.67
1:O:12:PRO:HB2	1:O:15:GLN:CG	2.25	0.67
2:B:53:THR:HB	2:B:136:ASN:OD1	1.94	0.67
2:N:219:GLN:OE1	2:N:262:GLN:HG2	1.95	0.67
1:C:86:ASN:HD21	1:C:110:ARG:HE	1.42	0.67
2:D:53:THR:H	2:D:136:ASN:ND2	1.93	0.67
2:D:116:GLY:HA2	2:D:189:LYS:HE2	1.77	0.67
1:E:27:GLU:HG3	1:E:60:LYS:HD2	1.74	0.67
2:H:211:ASN:HD22	2:H:212:THR:N	1.92	0.67
1:O:182:GLY:O	1:O:183:SER:HB2	1.93	0.67
1:A:12:PRO:HB2	1:A:15:GLN:HG3	1.77	0.67
2:H:218:ALA:HB2	2:H:266:GLY:O	1.93	0.67
1:A:188:ARG:NH1	1:A:199:LYS:H	1.93	0.67
1:C:188:ARG:NH1	1:C:199:LYS:H	1.92	0.67
1:I:88:LYS:HE2	1:I:90:ILE:HG12	1.75	0.67
1:M:79:ARG:HB3	1:M:170:MET:CE	2.24	0.67
1:A:27:GLU:HG3	1:A:60:LYS:HD2	1.76	0.66
1:C:27:GLU:HG3	1:C:60:LYS:HD2	1.75	0.66
1:M:135:ARG:CZ	1:M:181:ALA:HB1	2.25	0.66
2:N:24:LEU:HD22	2:N:36:VAL:HG22	1.77	0.66
1:C:12:PRO:HB2	1:C:15:GLN:HG3	1.77	0.66
1:E:188:ARG:NH1	1:E:199:LYS:H	1.94	0.66
2:H:84:PHE:HA	2:H:85:PRO:C	2.15	0.66
2:N:186:TYR:HB2	2:N:244:GLY:O	1.95	0.66
2:P:219:GLN:OE1	2:P:262:GLN:HG2	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:217:PRO:O	2:H:219:GLN:N	2.28	0.66
1:I:135:ARG:CZ	1:I:181:ALA:HB1	2.25	0.66
1:M:126:GLN:HA	1:M:129:GLU:OE1	1.96	0.66
2:P:264:THR:HG22	2:P:265:ALA:N	2.07	0.66
1:C:110:ARG:HD3	4:C:223:HOH:O	1.95	0.66
1:C:122:LEU:HD11	1:C:126:GLN:O	1.95	0.66
2:H:77:TYR:CD2	2:H:90:THR:HG21	2.30	0.66
1:M:12:PRO:HB2	1:M:15:GLN:CG	2.25	0.66
2:L:219:GLN:OE1	2:L:262:GLN:HG2	1.94	0.66
2:N:264:THR:HG22	2:N:265:ALA:N	2.08	0.66
2:P:186:TYR:HB2	2:P:244:GLY:O	1.96	0.66
2:D:217:PRO:O	2:D:219:GLN:N	2.29	0.66
2:F:211:ASN:HD22	2:F:212:THR:N	1.93	0.66
1:I:102:THR:O	2:J:269:GLN:HA	1.96	0.66
2:L:24:LEU:HD22	2:L:36:VAL:HG22	1.76	0.66
1:O:135:ARG:CZ	1:O:181:ALA:HB1	2.25	0.66
2:B:221:VAL:O	2:B:259:THR:HG23	1.96	0.66
1:I:10:ILE:O	1:I:12:PRO:HD3	1.96	0.66
2:J:219:GLN:OE1	2:J:262:GLN:HG2	1.94	0.66
1:K:103:LEU:HD12	2:L:270:SER:O	1.96	0.66
2:F:116:GLY:HA2	2:F:189:LYS:HE2	1.77	0.66
1:C:144:ASN:ND2	1:C:150:LEU:HG	2.10	0.66
2:D:77:TYR:CD2	2:D:90:THR:HG21	2.30	0.66
1:I:12:PRO:HB2	1:I:15:GLN:CG	2.25	0.66
1:K:126:GLN:HA	1:K:129:GLU:OE1	1.95	0.66
1:M:135:ARG:NH1	1:M:181:ALA:CB	2.53	0.66
2:L:43:PHE:CD2	2:L:102:PRO:HB3	2.31	0.66
2:D:58:LEU:H	2:D:90:THR:HG22	1.60	0.65
2:H:53:THR:H	2:H:136:ASN:ND2	1.94	0.65
2:N:43:PHE:CD2	2:N:102:PRO:HB3	2.31	0.65
1:A:122:LEU:HD11	1:A:126:GLN:O	1.96	0.65
1:G:12:PRO:HB2	1:G:15:GLN:HG3	1.78	0.65
1:I:103:LEU:HD12	2:J:270:SER:O	1.96	0.65
1:M:102:THR:O	2:N:269:GLN:HA	1.96	0.65
1:O:79:ARG:HB3	1:O:170:MET:HE1	1.79	0.65
2:P:43:PHE:CD2	2:P:102:PRO:HB3	2.31	0.65
2:J:24:LEU:HD22	2:J:36:VAL:HG22	1.77	0.65
1:O:126:GLN:HA	1:O:129:GLU:OE1	1.96	0.65
1:K:12:PRO:HB2	1:K:15:GLN:CG	2.25	0.65
1:K:135:ARG:CZ	1:K:181:ALA:HB1	2.25	0.65
1:O:10:ILE:O	1:O:12:PRO:HD3	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:126:GLN:HA	1:I:129:GLU:OE1	1.95	0.65
2:L:116:GLY:HA3	2:L:189:LYS:HG3	1.79	0.65
2:B:77:TYR:CD2	2:B:90:THR:HG21	2.31	0.65
2:F:53:THR:HB	2:F:136:ASN:OD1	1.95	0.65
1:G:144:ASN:ND2	1:G:150:LEU:HG	2.12	0.65
1:G:73:ASN:HA	4:G:222:HOH:O	1.97	0.65
1:E:122:LEU:HD11	1:E:126:GLN:O	1.97	0.65
2:F:53:THR:H	2:F:136:ASN:ND2	1.93	0.65
1:I:79:ARG:HB3	1:I:170:MET:HE1	1.78	0.65
2:L:105:VAL:HG11	2:L:129:LEU:HD13	1.77	0.65
2:N:116:GLY:HA3	2:N:189:LYS:HG3	1.79	0.65
1:O:102:THR:O	2:P:269:GLN:HA	1.96	0.65
2:B:211:ASN:HD22	2:B:212:THR:N	1.94	0.65
2:F:217:PRO:O	2:F:219:GLN:N	2.30	0.65
1:G:122:LEU:HD11	1:G:126:GLN:O	1.96	0.65
2:J:105:VAL:HG11	2:J:129:LEU:HD13	1.77	0.65
1:E:12:PRO:HB2	1:E:15:GLN:CG	2.26	0.65
1:E:144:ASN:ND2	1:E:150:LEU:HG	2.11	0.65
2:F:221:VAL:O	2:F:259:THR:HG23	1.96	0.65
2:L:186:TYR:HB2	2:L:244:GLY:O	1.95	0.65
1:M:103:LEU:HD12	2:N:270:SER:O	1.96	0.65
1:O:103:LEU:HD12	2:P:270:SER:O	1.96	0.65
2:D:84:PHE:HA	2:D:85:PRO:C	2.17	0.65
2:J:58:LEU:N	2:J:90:THR:HG22	2.12	0.65
1:K:10:ILE:O	1:K:12:PRO:HD3	1.96	0.65
1:K:102:THR:O	2:L:269:GLN:HA	1.96	0.65
2:B:90:THR:HG23	2:B:91:PRO:O	1.96	0.64
2:J:38:LEU:C	2:J:40:THR:H	2.00	0.64
2:J:84:PHE:HA	2:J:85:PRO:C	2.18	0.64
2:P:105:VAL:HG11	2:P:129:LEU:HD13	1.78	0.64
2:P:95:TYR:OH	2:P:103:TRP:HA	1.97	0.64
2:F:77:TYR:CD2	2:F:90:THR:HG21	2.31	0.64
2:F:167:ASP:CG	2:F:168:VAL:N	2.50	0.64
2:L:38:LEU:C	2:L:40:THR:H	2.01	0.64
2:P:116:GLY:HA3	2:P:189:LYS:HG3	1.79	0.64
2:D:211:ASN:HD22	2:D:212:THR:N	1.94	0.64
2:D:90:THR:HG23	2:D:91:PRO:O	1.97	0.64
2:F:84:PHE:HA	2:F:85:PRO:C	2.17	0.64
2:J:116:GLY:HA3	2:J:189:LYS:HG3	1.79	0.64
2:J:43:PHE:CD2	2:J:102:PRO:HB3	2.32	0.64
1:M:10:ILE:O	1:M:12:PRO:HD3	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:192:ASN:ND2	2:B:279:GLN:HE22	1.95	0.64
2:B:84:PHE:HA	2:B:85:PRO:C	2.16	0.64
2:H:221:VAL:O	2:H:259:THR:HG23	1.97	0.64
2:J:43:PHE:HA	2:J:102:PRO:HA	1.80	0.64
2:P:58:LEU:N	2:P:90:THR:HG22	2.12	0.64
2:H:116:GLY:HA2	2:H:189:LYS:HE2	1.79	0.64
2:J:95:TYR:OH	2:J:103:TRP:HA	1.97	0.64
1:M:27:GLU:HA	1:M:60:LYS:HG3	1.79	0.64
1:C:134:ARG:CD	1:C:141:THR:HG21	2.28	0.64
2:L:43:PHE:HA	2:L:102:PRO:HA	1.79	0.64
2:N:95:TYR:OH	2:N:103:TRP:HA	1.97	0.64
1:A:97:LYS:HE3	4:B:1573:HOH:O	1.96	0.64
1:E:102:THR:CA	2:F:171:THR:HG22	2.28	0.64
2:N:43:PHE:HA	2:N:102:PRO:HA	1.80	0.64
2:L:67:VAL:HG13	2:L:109:LEU:HD13	1.80	0.63
2:L:84:PHE:HA	2:L:85:PRO:C	2.18	0.63
1:A:156:ASN:HB2	1:A:186:THR:OG1	1.99	0.63
1:A:179:SER:C	1:A:181:ALA:N	2.50	0.63
2:D:167:ASP:CG	2:D:168:VAL:N	2.50	0.63
1:G:102:THR:CA	2:H:171:THR:HG22	2.28	0.63
1:K:27:GLU:HA	1:K:60:LYS:HG3	1.80	0.63
2:L:95:TYR:OH	2:L:103:TRP:HA	1.98	0.63
1:M:4:LEU:HD21	1:M:87:VAL:HG21	1.80	0.63
1:O:135:ARG:NH1	1:O:177:LEU:HD11	2.13	0.63
2:N:67:VAL:HG13	2:N:109:LEU:HD13	1.79	0.63
2:P:38:LEU:C	2:P:40:THR:H	2.01	0.63
1:C:102:THR:CA	2:D:171:THR:HG22	2.27	0.63
2:D:92:ARG:NH1	2:D:92:ARG:HG3	2.10	0.63
1:E:179:SER:C	1:E:181:ALA:N	2.50	0.63
1:M:162:LEU:HD21	1:M:178:PRO:CD	2.29	0.63
2:P:84:PHE:HA	2:P:85:PRO:C	2.17	0.63
2:B:92:ARG:HG3	2:B:92:ARG:NH1	2.09	0.63
1:G:140:LEU:HD23	1:G:141:THR:N	2.14	0.63
2:N:58:LEU:N	2:N:90:THR:HG22	2.13	0.63
2:N:84:PHE:HA	2:N:85:PRO:C	2.18	0.63
1:G:104:GLN:HG3	2:H:168:VAL:HG23	1.81	0.63
1:K:135:ARG:NH1	1:K:177:LEU:HD11	2.13	0.63
2:L:58:LEU:N	2:L:90:THR:HG22	2.13	0.63
1:C:11:TYR:HB2	1:C:113:LEU:HD11	1.81	0.63
1:C:134:ARG:CZ	1:C:141:THR:HG21	2.29	0.63
1:M:27:GLU:CG	1:M:60:LYS:HD2	2.29	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:4:LEU:HD21	1:O:87:VAL:HG21	1.81	0.63
1:A:102:THR:CA	2:B:171:THR:HG22	2.28	0.63
2:F:67:VAL:HG23	2:F:126:ILE:HG12	1.81	0.63
1:G:94:ASP:HB3	1:G:96:SER:OG	1.98	0.63
2:J:32:GLN:O	2:J:110:THR:HG23	1.99	0.63
1:O:162:LEU:HD21	1:O:178:PRO:CD	2.29	0.63
1:G:179:SER:C	1:G:181:ALA:N	2.50	0.62
2:H:90:THR:HG23	2:H:91:PRO:O	1.98	0.62
1:I:27:GLU:HA	1:I:60:LYS:HG3	1.80	0.62
1:I:4:LEU:HD21	1:I:87:VAL:HG21	1.80	0.62
1:M:135:ARG:NH1	1:M:177:LEU:HD11	2.13	0.62
2:N:38:LEU:C	2:N:40:THR:H	2.01	0.62
1:O:27:GLU:HA	1:O:60:LYS:HG3	1.80	0.62
1:A:140:LEU:HD23	1:A:141:THR:N	2.14	0.62
2:P:32:GLN:O	2:P:110:THR:HG23	1.99	0.62
1:A:185:ILE:HB	1:A:202:GLY:HA3	1.82	0.62
1:C:140:LEU:HD23	1:C:141:THR:N	2.15	0.62
1:C:185:ILE:HB	1:C:202:GLY:HA3	1.81	0.62
2:D:192:ASN:ND2	2:D:279:GLN:HE22	1.94	0.62
1:E:12:PRO:HB2	1:E:15:GLN:HG3	1.82	0.62
1:G:185:ILE:HB	1:G:202:GLY:HA3	1.81	0.62
1:I:135:ARG:NH1	1:I:177:LEU:HD11	2.13	0.62
2:D:172:LEU:O	2:D:172:LEU:HD23	1.99	0.62
2:J:20:VAL:HG21	2:J:42:ILE:HD11	1.81	0.62
2:N:184:THR:HA	2:N:249:SER:HA	1.81	0.62
2:N:59:GLN:CG	2:N:132:ARG:HB2	2.28	0.62
2:B:59:GLN:CG	2:B:132:ARG:HD2	2.30	0.62
1:E:156:ASN:HB2	1:E:186:THR:OG1	2.00	0.62
1:G:156:ASN:HB2	1:G:186:THR:OG1	2.00	0.62
1:G:191:ASN:HD21	1:G:195:ALA:HB3	1.64	0.62
2:N:32:GLN:O	2:N:110:THR:HG23	2.00	0.62
2:P:43:PHE:HA	2:P:102:PRO:HA	1.79	0.62
2:P:59:GLN:CG	2:P:132:ARG:HB2	2.29	0.62
1:A:94:ASP:HB3	1:A:96:SER:OG	2.00	0.62
1:C:94:ASP:HB3	1:C:96:SER:OG	1.99	0.62
2:F:90:THR:HG23	2:F:91:PRO:O	1.98	0.62
2:J:59:GLN:CG	2:J:132:ARG:HB2	2.29	0.62
1:K:162:LEU:HD21	1:K:178:PRO:CD	2.29	0.62
2:P:67:VAL:HG13	2:P:109:LEU:HD13	1.80	0.62
2:B:170:VAL:CG1	2:B:172:LEU:HB2	2.27	0.62
1:C:156:ASN:HB2	1:C:186:THR:OG1	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:67:VAL:HG13	2:J:109:LEU:HD13	1.80	0.62
1:K:79:ARG:HB3	1:K:170:MET:HE1	1.80	0.62
2:L:184:THR:HA	2:L:249:SER:HA	1.81	0.62
2:L:59:GLN:CG	2:L:132:ARG:HB2	2.29	0.62
1:A:135:ARG:HH22	1:A:181:ALA:CB	2.13	0.62
2:B:172:LEU:HD23	2:B:172:LEU:O	2.00	0.62
2:J:21:TYR:HB3	2:J:151:ASN:ND2	2.15	0.61
1:K:4:LEU:HD21	1:K:87:VAL:HG21	1.81	0.61
1:C:135:ARG:HH22	1:C:181:ALA:CB	2.13	0.61
1:E:104:GLN:HG3	2:F:168:VAL:HG23	1.82	0.61
2:F:59:GLN:CG	2:F:132:ARG:HD2	2.30	0.61
1:E:135:ARG:HH22	1:E:181:ALA:CB	2.14	0.61
2:H:172:LEU:O	2:H:172:LEU:HD23	2.00	0.61
2:J:201:THR:CG2	2:J:206:ASN:HA	2.24	0.61
2:F:172:LEU:HD23	2:F:172:LEU:O	2.01	0.61
1:G:135:ARG:HH22	1:G:181:ALA:CB	2.13	0.61
1:I:162:LEU:HD21	1:I:178:PRO:CD	2.29	0.61
2:L:32:GLN:O	2:L:110:THR:HG23	1.99	0.61
2:J:19:ASN:HD21	2:L:219:GLN:HE22	1.48	0.61
1:M:79:ARG:HB3	1:M:170:MET:HE1	1.82	0.61
1:E:191:ASN:HD21	1:E:195:ALA:HB3	1.63	0.61
1:E:185:ILE:HB	1:E:202:GLY:HA3	1.82	0.61
2:L:74:THR:HG22	2:L:83:PRO:HA	1.83	0.61
2:H:67:VAL:HG23	2:H:126:ILE:HG12	1.83	0.61
2:B:67:VAL:HG23	2:B:126:ILE:HG12	1.82	0.61
1:E:140:LEU:HD23	1:E:141:THR:N	2.15	0.61
1:G:11:TYR:HB2	1:G:113:LEU:HD11	1.81	0.61
2:H:59:GLN:CG	2:H:132:ARG:HD2	2.30	0.61
1:I:7:THR:O	1:I:111:ILE:HB	2.01	0.61
2:J:184:THR:HA	2:J:249:SER:HA	1.81	0.61
2:N:19:ASN:HD21	2:P:219:GLN:HE22	1.46	0.61
1:A:104:GLN:HG3	2:B:168:VAL:HG23	1.82	0.61
2:F:170:VAL:CG1	2:F:172:LEU:HB2	2.26	0.61
1:I:4:LEU:O	2:J:160:GLY:N	2.33	0.61
2:L:20:VAL:HG21	2:L:42:ILE:HD11	1.82	0.61
2:P:175:TYR:OH	2:P:263:VAL:HB	2.00	0.61
1:C:177:LEU:HD12	1:C:178:PRO:HD2	1.83	0.61
2:N:21:TYR:HB3	2:N:151:ASN:ND2	2.15	0.61
1:A:188:ARG:NH1	1:A:199:LYS:HB2	2.16	0.61
2:N:175:TYR:N	2:N:176:PRO:HD2	2.16	0.61
2:P:184:THR:HA	2:P:249:SER:HA	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:102:THR:HA	2:D:171:THR:HG22	1.82	0.60
2:H:174:ASP:O	2:H:176:PRO:N	2.34	0.60
2:H:92:ARG:HG3	2:H:92:ARG:NH1	2.11	0.60
2:N:193:LEU:HB3	2:N:240:LEU:HD12	1.83	0.60
2:P:20:VAL:HG21	2:P:42:ILE:HD11	1.81	0.60
2:D:175:TYR:O	2:D:256:TYR:CD1	2.54	0.60
2:L:193:LEU:HB3	2:L:240:LEU:HD12	1.82	0.60
1:M:7:THR:O	1:M:111:ILE:HB	2.01	0.60
1:O:27:GLU:CG	1:O:60:LYS:HD2	2.29	0.60
1:C:118:ALA:O	1:C:119:LYS:HB2	2.02	0.60
2:D:207:SER:O	2:D:224:GLN:HG3	2.02	0.60
1:E:188:ARG:NH1	1:E:199:LYS:HB2	2.17	0.60
2:D:170:VAL:CG1	2:D:172:LEU:HB2	2.26	0.60
1:E:102:THR:HA	2:F:171:THR:HG22	1.83	0.60
2:J:74:THR:HG22	2:J:83:PRO:HA	1.82	0.60
1:K:7:THR:O	1:K:111:ILE:HB	2.00	0.60
2:N:20:VAL:HG21	2:N:42:ILE:HD11	1.82	0.60
1:A:11:TYR:HB2	1:A:113:LEU:HD11	1.83	0.60
2:H:192:ASN:ND2	2:H:279:GLN:HE22	1.96	0.60
2:J:175:TYR:OH	2:J:263:VAL:HB	2.01	0.60
2:L:14:GLY:HA2	2:L:142:PHE:CE1	2.37	0.60
2:P:21:TYR:HB3	2:P:151:ASN:ND2	2.15	0.60
2:P:74:THR:HG22	2:P:83:PRO:HA	1.82	0.60
2:J:175:TYR:N	2:J:176:PRO:HD2	2.16	0.60
2:L:125:LEU:HD12	2:L:148:ILE:O	2.02	0.60
1:A:177:LEU:HD12	1:A:178:PRO:HD2	1.83	0.60
1:A:191:ASN:HD21	1:A:195:ALA:HB3	1.66	0.60
1:C:104:GLN:HG3	2:D:168:VAL:HG23	1.84	0.60
2:L:201:THR:CG2	2:L:206:ASN:HA	2.24	0.60
1:O:117:PRO:O	1:O:120:LEU:HG	2.02	0.60
2:F:227:ARG:HB3	2:F:232:ILE:HD11	1.84	0.60
2:L:175:TYR:N	2:L:176:PRO:HD2	2.16	0.60
2:B:167:ASP:OD2	2:B:168:VAL:N	2.35	0.60
2:B:184:THR:HG22	2:B:249:SER:HA	1.82	0.60
2:B:175:TYR:O	2:B:256:TYR:CD1	2.55	0.60
1:G:141:THR:HG23	1:G:174:THR:HG22	1.83	0.60
2:J:193:LEU:HB3	2:J:240:LEU:HD12	1.83	0.60
2:B:174:ASP:O	2:B:176:PRO:N	2.35	0.60
1:E:177:LEU:HD12	1:E:178:PRO:HD2	1.83	0.60
1:E:94:ASP:HB3	1:E:96:SER:OG	2.01	0.60
2:F:174:ASP:O	2:F:176:PRO:N	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:175:TYR:OH	2:L:263:VAL:HB	2.01	0.60
2:P:175:TYR:N	2:P:176:PRO:HD2	2.16	0.60
1:K:4:LEU:O	2:L:160:GLY:N	2.33	0.59
2:L:21:TYR:HB3	2:L:151:ASN:ND2	2.16	0.59
2:N:175:TYR:OH	2:N:263:VAL:HB	2.00	0.59
2:N:74:THR:HG22	2:N:83:PRO:HA	1.82	0.59
2:P:193:LEU:HB3	2:P:240:LEU:HD12	1.82	0.59
2:F:184:THR:HG22	2:F:249:SER:HA	1.83	0.59
1:G:82:LEU:HD12	1:G:83:PHE:N	2.16	0.59
1:I:101:ASN:ND2	2:J:268:VAL:HG23	2.17	0.59
1:M:117:PRO:O	1:M:120:LEU:HG	2.02	0.59
2:P:125:LEU:HD12	2:P:148:ILE:O	2.02	0.59
1:A:102:THR:HA	2:B:171:THR:HG22	1.82	0.59
1:C:82:LEU:HD12	1:C:83:PHE:N	2.17	0.59
2:H:175:TYR:O	2:H:256:TYR:CD1	2.55	0.59
2:H:163:VAL:HG22	2:H:185:VAL:HG12	1.84	0.59
1:I:27:GLU:CG	1:I:60:LYS:HD2	2.29	0.59
1:E:118:ALA:O	1:E:119:LYS:HB2	2.02	0.59
2:H:167:ASP:OD2	2:H:168:VAL:N	2.36	0.59
1:I:117:PRO:O	1:I:120:LEU:HG	2.02	0.59
2:J:14:GLY:HA2	2:J:142:PHE:CE1	2.38	0.59
2:L:177:GLY:HA3	2:L:256:TYR:CE1	2.38	0.59
1:K:101:ASN:ND2	2:L:268:VAL:HG23	2.17	0.59
1:M:188:ARG:HH11	1:M:199:LYS:HB2	1.67	0.59
2:D:174:ASP:O	2:D:176:PRO:N	2.35	0.59
2:D:67:VAL:HG23	2:D:126:ILE:HG12	1.85	0.59
1:E:11:TYR:HB2	1:E:113:LEU:HD11	1.83	0.59
1:G:102:THR:HA	2:H:171:THR:HG22	1.82	0.59
1:G:188:ARG:NH1	1:G:199:LYS:HB2	2.17	0.59
1:K:117:PRO:O	1:K:120:LEU:HG	2.02	0.59
1:A:135:ARG:HH22	1:A:181:ALA:HB1	1.68	0.59
1:G:177:LEU:HD12	1:G:178:PRO:HD2	1.84	0.59
1:K:11:TYR:HB2	1:K:113:LEU:HD11	1.85	0.59
1:M:11:TYR:HB2	1:M:113:LEU:HD11	1.85	0.59
1:O:7:THR:O	1:O:111:ILE:HB	2.01	0.59
2:D:184:THR:HG22	2:D:249:SER:HA	1.85	0.59
1:G:141:THR:CG2	1:G:174:THR:HG22	2.33	0.59
2:N:14:GLY:HA2	2:N:142:PHE:CE1	2.37	0.59
2:P:177:GLY:HA3	2:P:256:TYR:CE1	2.38	0.59
2:H:227:ARG:HB3	2:H:232:ILE:HD11	1.85	0.59
1:O:156:ASN:C	1:O:158:GLY:H	2.06	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:LEU:HD12	1:A:83:PHE:N	2.18	0.59
2:F:13:ILE:HG13	4:F:1539:HOH:O	2.03	0.59
2:F:175:TYR:O	2:F:256:TYR:CD1	2.55	0.59
1:G:118:ALA:O	1:G:119:LYS:HB2	2.02	0.59
2:H:184:THR:HG22	2:H:249:SER:HA	1.84	0.59
1:I:156:ASN:C	1:I:158:GLY:H	2.07	0.59
1:M:4:LEU:O	2:N:160:GLY:N	2.33	0.59
1:C:179:SER:C	1:C:181:ALA:N	2.51	0.59
1:C:191:ASN:HD21	1:C:195:ALA:HB3	1.67	0.59
1:E:82:LEU:HD12	1:E:83:PHE:N	2.17	0.59
2:F:167:ASP:OD2	2:F:168:VAL:N	2.36	0.59
2:N:24:LEU:HD11	2:N:126:ILE:HD11	1.84	0.59
1:I:188:ARG:HH11	1:I:199:LYS:HB2	1.68	0.58
1:K:27:GLU:HG2	1:K:60:LYS:CD	2.32	0.58
2:N:177:GLY:HA3	2:N:256:TYR:CE1	2.37	0.58
2:P:14:GLY:HA2	2:P:142:PHE:CE1	2.37	0.58
1:C:188:ARG:NH1	1:C:199:LYS:HB2	2.17	0.58
1:G:27:GLU:HA	1:G:60:LYS:HG3	1.85	0.58
1:O:79:ARG:HA	1:O:147:PRO:HB2	1.85	0.58
1:A:118:ALA:O	1:A:119:LYS:HB2	2.01	0.58
1:C:27:GLU:HA	1:C:60:LYS:HG3	1.85	0.58
2:F:5:THR:HG22	2:F:8:GLY:H	1.67	0.58
1:G:47:ARG:HH22	1:G:74:GLN:HB2	1.69	0.58
1:I:103:LEU:O	2:J:168:VAL:HG23	2.03	0.58
1:K:27:GLU:CG	1:K:60:LYS:HD2	2.30	0.58
1:A:138:ASN:C	1:A:177:LEU:HB3	2.24	0.58
2:B:227:ARG:HB3	2:B:232:ILE:HD11	1.86	0.58
2:D:59:GLN:CG	2:D:132:ARG:HD2	2.31	0.58
2:H:114:SER:HB3	2:L:80:SER:HB3	1.85	0.58
2:J:24:LEU:HD11	2:J:126:ILE:HD11	1.85	0.58
1:K:188:ARG:HH11	1:K:199:LYS:HB2	1.68	0.58
1:I:11:TYR:HB2	1:I:113:LEU:HD11	1.85	0.58
1:I:135:ARG:NH1	1:I:181:ALA:CB	2.53	0.58
1:M:103:LEU:O	2:N:168:VAL:HG23	2.04	0.58
2:N:125:LEU:HD12	2:N:148:ILE:O	2.02	0.58
2:P:24:LEU:HD11	2:P:126:ILE:HD11	1.85	0.58
2:B:179:VAL:O	2:B:253:THR:HG23	2.03	0.58
2:B:58:LEU:H	2:B:90:THR:CG2	2.16	0.58
1:M:101:ASN:ND2	2:N:268:VAL:HG23	2.17	0.58
1:C:188:ARG:HH12	1:C:199:LYS:H	1.50	0.58
2:F:92:ARG:HG3	2:F:92:ARG:NH1	2.12	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:135:ARG:NH2	1:G:181:ALA:HB1	2.19	0.58
1:G:188:ARG:HH12	1:G:199:LYS:H	1.51	0.58
1:I:197:THR:HB	1:I:198:PRO:HD2	1.86	0.58
2:N:131:LEU:HB3	2:N:144:PHE:HB2	1.86	0.58
2:N:84:PHE:CD1	2:N:85:PRO:HA	2.39	0.58
1:O:11:TYR:HB2	1:O:113:LEU:HD11	1.85	0.58
1:O:103:LEU:O	2:P:168:VAL:HG23	2.04	0.58
2:F:192:ASN:ND2	2:F:279:GLN:HE22	1.99	0.58
1:G:135:ARG:HH22	1:G:181:ALA:HB1	1.68	0.58
2:H:170:VAL:CG1	2:H:172:LEU:HB2	2.27	0.58
2:H:58:LEU:H	2:H:90:THR:CG2	2.16	0.58
2:N:201:THR:CG2	2:N:206:ASN:HA	2.24	0.58
1:C:135:ARG:HH22	1:C:181:ALA:HB1	1.68	0.58
1:E:135:ARG:NH2	1:E:181:ALA:HB1	2.19	0.58
1:G:1:GLY:H1	1:G:26:ASP:CG	2.07	0.58
1:K:122:LEU:HD11	1:K:126:GLN:O	2.04	0.58
1:O:122:LEU:HD11	1:O:126:GLN:O	2.04	0.58
2:L:223:VAL:HG12	2:L:224:GLN:N	2.19	0.58
1:M:27:GLU:HG2	1:M:60:LYS:CD	2.32	0.58
1:M:79:ARG:HA	1:M:147:PRO:HB2	1.85	0.58
1:A:27:GLU:HA	1:A:60:LYS:HG3	1.86	0.57
2:B:167:ASP:CG	2:B:168:VAL:N	2.50	0.57
2:B:68:LEU:O	2:P:87:THR:HG21	2.03	0.57
2:D:167:ASP:OD2	2:D:168:VAL:N	2.35	0.57
1:E:138:ASN:C	1:E:177:LEU:HB3	2.24	0.57
2:F:58:LEU:H	2:F:90:THR:CG2	2.16	0.57
2:J:177:GLY:HA3	2:J:256:TYR:CE1	2.38	0.57
1:K:6:ALA:HB3	1:K:20:LEU:HD11	1.86	0.57
2:H:68:LEU:O	2:L:87:THR:HG21	2.04	0.57
1:O:197:THR:HB	1:O:198:PRO:HD2	1.86	0.57
1:O:4:LEU:O	2:P:160:GLY:N	2.33	0.57
2:P:201:THR:CG2	2:P:206:ASN:HA	2.24	0.57
1:A:24:ASN:O	1:A:60:LYS:HA	2.05	0.57
1:E:27:GLU:HA	1:E:60:LYS:HG3	1.87	0.57
1:G:158:GLY:HA2	1:G:184:ASN:HD22	1.69	0.57
1:G:135:ARG:CZ	1:G:181:ALA:HB1	2.34	0.57
1:I:122:LEU:HD11	1:I:126:GLN:O	2.04	0.57
1:I:27:GLU:HG2	1:I:60:LYS:CD	2.32	0.57
1:K:79:ARG:HA	1:K:147:PRO:HB2	1.85	0.57
1:O:6:ALA:HB3	1:O:20:LEU:HD11	1.86	0.57
1:C:138:ASN:C	1:C:177:LEU:HB3	2.24	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:131:LEU:HB3	2:L:144:PHE:HB2	1.87	0.57
1:O:188:ARG:HH11	1:O:199:LYS:HB2	1.68	0.57
1:O:101:ASN:ND2	2:P:268:VAL:HG23	2.17	0.57
2:B:120:ILE:CG2	2:B:126:ILE:HD11	2.31	0.57
1:C:135:ARG:NH2	1:C:181:ALA:HB1	2.19	0.57
2:L:84:PHE:CD1	2:L:85:PRO:HA	2.40	0.57
2:P:84:PHE:CD1	2:P:85:PRO:HA	2.39	0.57
1:C:134:ARG:CD	1:C:141:THR:CG2	2.83	0.57
2:D:5:THR:HG22	2:D:8:GLY:H	1.69	0.57
1:G:138:ASN:C	1:G:177:LEU:HB3	2.25	0.57
2:J:125:LEU:HD12	2:J:148:ILE:O	2.03	0.57
1:K:156:ASN:C	1:K:158:GLY:H	2.07	0.57
1:M:156:ASN:C	1:M:158:GLY:H	2.06	0.57
1:A:135:ARG:NH2	1:A:181:ALA:HB1	2.19	0.57
1:C:135:ARG:CZ	1:C:181:ALA:HB1	2.34	0.57
1:C:158:GLY:HA2	1:C:184:ASN:HD22	1.69	0.57
1:E:197:THR:HB	1:E:198:PRO:HD2	1.87	0.57
2:F:179:VAL:O	2:F:253:THR:HG23	2.03	0.57
1:K:103:LEU:O	2:L:168:VAL:HG23	2.04	0.57
2:L:24:LEU:HD11	2:L:126:ILE:HD11	1.84	0.57
2:L:71:PHE:CE2	2:L:111:PRO:HG3	2.39	0.57
2:N:71:PHE:CE2	2:N:111:PRO:HG3	2.39	0.57
2:B:114:SER:HB3	2:P:80:SER:HB3	1.85	0.57
2:D:163:VAL:HG22	2:D:185:VAL:HG12	1.87	0.57
2:F:163:VAL:HG22	2:F:185:VAL:HG12	1.86	0.57
1:I:79:ARG:HA	1:I:147:PRO:HB2	1.85	0.57
2:J:131:LEU:HB3	2:J:144:PHE:HB2	1.87	0.57
2:J:71:PHE:CE2	2:J:111:PRO:HG3	2.40	0.57
2:L:96:ASN:HD22	2:L:96:ASN:H	1.53	0.57
1:M:197:THR:HB	1:M:198:PRO:HD2	1.86	0.57
1:M:6:ALA:HB3	1:M:20:LEU:HD11	1.87	0.57
2:N:66:GLY:O	2:N:70:ASN:HB2	2.05	0.57
1:C:134:ARG:NH1	1:C:141:THR:HG21	2.19	0.57
2:D:58:LEU:H	2:D:90:THR:CG2	2.18	0.57
2:P:71:PHE:CE2	2:P:111:PRO:HG3	2.40	0.57
2:P:131:LEU:HB3	2:P:144:PHE:HB2	1.87	0.57
2:P:227:ARG:HH22	2:P:230:THR:HG21	1.70	0.57
2:B:5:THR:HG22	2:B:8:GLY:H	1.69	0.57
2:J:223:VAL:HG12	2:J:224:GLN:N	2.19	0.57
2:L:227:ARG:HH22	2:L:230:THR:HG21	1.70	0.57
2:L:267:ASN:HB3	2:L:269:GLN:HG3	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:28:ASN:HD22	1:M:28:ASN:N	2.03	0.57
2:N:224:GLN:HG2	2:N:231:ILE:CG2	2.35	0.57
1:A:135:ARG:CZ	1:A:181:ALA:HB1	2.34	0.57
1:C:188:ARG:NH1	1:C:199:LYS:N	2.53	0.57
1:E:135:ARG:HH22	1:E:181:ALA:HB1	1.68	0.57
2:H:5:THR:HG22	2:H:8:GLY:H	1.70	0.57
2:J:84:PHE:CD1	2:J:85:PRO:HA	2.40	0.57
1:M:122:LEU:HD11	1:M:126:GLN:O	2.04	0.57
1:E:158:GLY:HA2	1:E:184:ASN:HD22	1.69	0.56
1:E:135:ARG:CZ	1:E:181:ALA:HB1	2.34	0.56
2:J:96:ASN:H	2:J:96:ASN:HD22	1.53	0.56
1:K:197:THR:HB	1:K:198:PRO:HD2	1.86	0.56
1:O:11:TYR:CE2	1:O:69:ASP:HB2	2.40	0.56
2:P:224:GLN:HG2	2:P:231:ILE:CG2	2.35	0.56
2:D:136:ASN:C	2:D:136:ASN:HD22	2.08	0.56
1:K:28:ASN:N	1:K:28:ASN:HD22	2.03	0.56
2:B:219:GLN:HG2	2:B:220:GLY:N	2.20	0.56
2:D:179:VAL:O	2:D:253:THR:HG23	2.05	0.56
1:E:24:ASN:O	1:E:60:LYS:HA	2.05	0.56
1:G:193:TYR:O	2:H:158:THR:HG22	2.06	0.56
2:J:66:GLY:O	2:J:70:ASN:HB2	2.05	0.56
1:M:11:TYR:CE2	1:M:69:ASP:HB2	2.40	0.56
1:A:158:GLY:HA2	1:A:184:ASN:HD22	1.69	0.56
2:D:219:GLN:HG2	2:D:220:GLY:N	2.19	0.56
1:E:193:TYR:O	2:F:158:THR:HG22	2.06	0.56
2:H:28:VAL:O	2:H:156:VAL:HA	2.06	0.56
2:H:219:GLN:HG2	2:H:220:GLY:N	2.20	0.56
2:J:250:LEU:HB2	2:J:252:LEU:HG	1.87	0.56
2:L:11:ILE:HD12	2:L:146:TRP:CZ2	2.40	0.56
2:P:267:ASN:HB3	2:P:269:GLN:HG3	1.87	0.56
1:A:188:ARG:NH1	1:A:199:LYS:N	2.53	0.56
2:F:226:THR:HG22	2:F:253:THR:HB	1.88	0.56
2:H:179:VAL:O	2:H:253:THR:HG23	2.05	0.56
1:I:11:TYR:CE2	1:I:69:ASP:HB2	2.40	0.56
2:N:11:ILE:HD12	2:N:146:TRP:CZ2	2.40	0.56
2:N:227:ARG:HH22	2:N:230:THR:HG21	1.70	0.56
1:O:154:GLU:OE2	1:O:188:ARG:HD3	2.06	0.56
2:D:227:ARG:HB3	2:D:232:ILE:HD11	1.88	0.56
1:G:188:ARG:NH1	1:G:199:LYS:N	2.54	0.56
2:H:120:ILE:HD13	2:H:126:ILE:HD11	1.87	0.56
2:J:30:VAL:HA	2:J:111:PRO:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:224:GLN:HG2	2:N:231:ILE:HG21	1.87	0.56
2:P:264:THR:CG2	2:P:265:ALA:H	2.15	0.56
1:C:47:ARG:HH22	1:C:74:GLN:HB2	1.70	0.56
1:E:188:ARG:HH12	1:E:199:LYS:H	1.52	0.56
1:I:6:ALA:HB3	1:I:20:LEU:HD11	1.86	0.56
2:J:227:ARG:HH22	2:J:230:THR:HG21	1.70	0.56
1:K:189:THR:O	1:K:196:LEU:HA	2.06	0.56
1:O:189:THR:O	1:O:196:LEU:HA	2.06	0.56
2:P:223:VAL:HG12	2:P:224:GLN:N	2.19	0.56
2:B:163:VAL:HG22	2:B:185:VAL:HG12	1.88	0.56
1:C:193:TYR:O	2:D:158:THR:HG22	2.06	0.56
1:G:197:THR:HB	1:G:198:PRO:HD2	1.88	0.56
1:I:162:LEU:CD2	1:I:178:PRO:HD3	2.36	0.56
1:I:135:ARG:HH12	1:I:181:ALA:HB2	1.69	0.56
2:J:224:GLN:HG2	2:J:231:ILE:CG2	2.35	0.56
1:K:80:GLU:HG3	1:K:147:PRO:O	2.05	0.56
2:L:224:GLN:HG2	2:L:231:ILE:CG2	2.35	0.56
2:N:267:ASN:HB3	2:N:269:GLN:HG3	1.87	0.56
2:B:28:VAL:O	2:B:156:VAL:HA	2.05	0.56
1:E:142:LEU:CD2	1:E:142:LEU:H	2.19	0.56
2:J:11:ILE:HD12	2:J:146:TRP:CZ2	2.41	0.56
1:M:22:VAL:CG2	1:M:65:LEU:HG	2.36	0.56
1:O:27:GLU:HG2	1:O:60:LYS:CD	2.32	0.56
1:O:80:GLU:HG3	1:O:147:PRO:O	2.06	0.56
2:P:60:ARG:HG3	2:P:61:GLY:N	2.21	0.56
2:P:66:GLY:O	2:P:70:ASN:HB2	2.06	0.56
1:E:188:ARG:NH1	1:E:199:LYS:N	2.54	0.56
1:K:11:TYR:CE2	1:K:69:ASP:HB2	2.40	0.56
2:N:223:VAL:HG12	2:N:224:GLN:N	2.20	0.56
2:P:224:GLN:HG2	2:P:231:ILE:HG21	1.88	0.56
1:A:188:ARG:HH12	1:A:199:LYS:H	1.51	0.56
2:B:226:THR:HG22	2:B:253:THR:HB	1.88	0.56
2:F:28:VAL:O	2:F:156:VAL:HA	2.05	0.56
2:F:219:GLN:HG2	2:F:220:GLY:N	2.20	0.56
2:L:60:ARG:HG3	2:L:61:GLY:N	2.21	0.56
1:A:197:THR:HB	1:A:198:PRO:HD2	1.88	0.55
2:D:28:VAL:O	2:D:156:VAL:HA	2.07	0.55
1:E:47:ARG:HH22	1:E:74:GLN:HB2	1.69	0.55
1:G:141:THR:CB	1:G:174:THR:HG22	2.35	0.55
2:H:207:SER:O	2:H:224:GLN:HG3	2.06	0.55
2:J:267:ASN:HB3	2:J:269:GLN:HG3	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:162:LEU:CD2	1:K:178:PRO:HD3	2.36	0.55
1:K:22:VAL:CG2	1:K:65:LEU:HG	2.36	0.55
2:L:20:VAL:HG12	2:L:22:VAL:HG13	1.88	0.55
1:M:80:GLU:HG3	1:M:147:PRO:O	2.06	0.55
2:P:250:LEU:HB2	2:P:252:LEU:HG	1.87	0.55
2:P:30:VAL:HA	2:P:111:PRO:HB2	1.89	0.55
1:A:47:ARG:HH22	1:A:74:GLN:HB2	1.71	0.55
2:F:71:PHE:CE2	2:F:111:PRO:HG3	2.41	0.55
1:I:154:GLU:OE2	1:I:188:ARG:HD3	2.06	0.55
2:N:264:THR:CG2	2:N:265:ALA:H	2.16	0.55
2:B:207:SER:O	2:B:224:GLN:HG3	2.06	0.55
2:D:120:ILE:HD13	2:D:126:ILE:HD11	1.87	0.55
2:F:131:LEU:C	2:F:131:LEU:HD23	2.27	0.55
2:H:226:THR:HG22	2:H:253:THR:HB	1.88	0.55
1:I:22:VAL:CG2	1:I:65:LEU:HG	2.37	0.55
2:N:220:GLY:HA2	2:N:259:THR:OG1	2.07	0.55
1:O:28:ASN:N	1:O:28:ASN:HD22	2.03	0.55
1:O:22:VAL:CG2	1:O:65:LEU:HG	2.36	0.55
2:P:220:GLY:HA2	2:P:259:THR:OG1	2.07	0.55
2:P:96:ASN:H	2:P:96:ASN:HD22	1.54	0.55
1:A:142:LEU:H	1:A:142:LEU:CD2	2.20	0.55
2:B:201:THR:CG2	2:B:206:ASN:HA	2.29	0.55
2:F:201:THR:CG2	2:F:206:ASN:HD22	2.18	0.55
2:F:83:PRO:O	2:F:86:THR:HA	2.07	0.55
1:G:142:LEU:CD2	1:G:142:LEU:H	2.19	0.55
1:I:104:GLN:O	2:J:271:ILE:HA	2.07	0.55
2:L:66:GLY:O	2:L:70:ASN:HB2	2.05	0.55
2:N:20:VAL:HG12	2:N:22:VAL:HG13	1.89	0.55
2:P:11:ILE:HD12	2:P:146:TRP:CZ2	2.40	0.55
1:I:28:ASN:HD22	1:I:28:ASN:N	2.03	0.55
2:L:30:VAL:HA	2:L:111:PRO:HB2	1.87	0.55
1:M:162:LEU:CD2	1:M:178:PRO:HD3	2.36	0.55
2:N:19:ASN:ND2	2:P:219:GLN:NE2	2.53	0.55
1:M:104:GLN:O	2:N:271:ILE:HA	2.07	0.55
2:P:117:GLY:O	2:P:155:VAL:HA	2.06	0.55
2:B:136:ASN:C	2:B:136:ASN:HD22	2.09	0.55
2:H:131:LEU:HD23	2:H:131:LEU:C	2.27	0.55
2:J:28:VAL:O	2:J:156:VAL:HA	2.07	0.55
2:F:120:ILE:CG2	2:F:126:ILE:HD11	2.29	0.55
1:I:189:THR:O	1:I:196:LEU:HA	2.07	0.55
1:I:28:ASN:N	1:I:28:ASN:ND2	2.54	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:80:GLU:HG3	1:I:147:PRO:O	2.06	0.55
2:J:73:GLY:HA2	4:J:1611:HOH:O	2.06	0.55
1:M:154:GLU:OE2	1:M:188:ARG:HD3	2.06	0.55
1:M:184:ASN:O	1:M:186:THR:HG23	2.07	0.55
2:N:250:LEU:HB2	2:N:252:LEU:HG	1.88	0.55
1:O:135:ARG:HH12	1:O:181:ALA:HB2	1.68	0.55
1:C:142:LEU:CD2	1:C:142:LEU:H	2.20	0.55
2:F:117:GLY:O	2:F:155:VAL:HA	2.07	0.55
2:J:117:GLY:O	2:J:155:VAL:HA	2.07	0.55
2:L:4:LYS:HA	2:L:10:ALA:HA	1.89	0.55
2:J:19:ASN:ND2	2:L:219:GLN:NE2	2.54	0.55
1:M:28:ASN:H	1:M:28:ASN:HD22	1.54	0.55
2:H:201:THR:CG2	2:H:206:ASN:HD22	2.18	0.55
2:L:71:PHE:HE2	2:L:111:PRO:HG3	1.72	0.55
2:D:201:THR:CG2	2:D:206:ASN:HD22	2.18	0.55
1:E:140:LEU:HB2	1:E:177:LEU:HD22	1.89	0.55
2:L:250:LEU:HB2	2:L:252:LEU:HG	1.87	0.55
1:M:28:ASN:N	1:M:28:ASN:ND2	2.54	0.55
2:H:71:PHE:CE2	2:H:111:PRO:HG3	2.42	0.54
2:J:224:GLN:HG2	2:J:231:ILE:HG21	1.88	0.54
1:K:28:ASN:HD22	1:K:28:ASN:H	1.54	0.54
1:O:184:ASN:O	1:O:186:THR:HG23	2.08	0.54
1:A:174:THR:HG23	1:A:174:THR:O	2.06	0.54
2:F:136:ASN:C	2:F:136:ASN:HD22	2.09	0.54
2:J:4:LYS:HA	2:J:10:ALA:HA	1.89	0.54
1:M:115:TYR:O	1:M:117:PRO:HD3	2.08	0.54
2:D:131:LEU:C	2:D:131:LEU:HD23	2.28	0.54
1:K:115:TYR:O	1:K:117:PRO:HD3	2.07	0.54
1:K:184:ASN:O	1:K:186:THR:HG23	2.07	0.54
1:K:28:ASN:N	1:K:28:ASN:ND2	2.54	0.54
2:L:200:THR:O	2:L:209:PHE:HA	2.07	0.54
1:M:189:THR:O	1:M:196:LEU:HA	2.06	0.54
2:P:28:VAL:O	2:P:156:VAL:HA	2.07	0.54
2:P:200:THR:O	2:P:209:PHE:HA	2.07	0.54
1:C:24:ASN:O	1:C:60:LYS:HA	2.06	0.54
2:F:120:ILE:HD13	2:F:126:ILE:HD11	1.89	0.54
2:F:170:VAL:C	2:F:172:LEU:H	2.10	0.54
2:J:200:THR:O	2:J:209:PHE:HA	2.07	0.54
2:L:162:ASP:O	2:L:185:VAL:HG13	2.07	0.54
1:K:104:GLN:O	2:L:271:ILE:HA	2.07	0.54
2:H:117:GLY:O	2:H:155:VAL:HA	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:162:ASP:O	2:J:185:VAL:HG13	2.07	0.54
2:L:224:GLN:HG2	2:L:231:ILE:HG21	1.88	0.54
2:D:71:PHE:CE2	2:D:111:PRO:HG3	2.42	0.54
2:F:172:LEU:O	2:F:173:PRO:C	2.46	0.54
1:I:185:ILE:HD12	1:I:204:MET:SD	2.48	0.54
2:N:200:THR:O	2:N:209:PHE:HA	2.08	0.54
2:N:60:ARG:HG3	2:N:61:GLY:N	2.22	0.54
1:O:162:LEU:CD2	1:O:178:PRO:HD3	2.36	0.54
2:F:5:THR:HG23	2:F:7:ASN:H	1.72	0.54
1:G:24:ASN:O	1:G:60:LYS:HA	2.07	0.54
1:I:115:TYR:O	1:I:117:PRO:HD3	2.07	0.54
2:J:201:THR:HA	2:J:209:PHE:HA	1.90	0.54
2:J:20:VAL:HG12	2:J:22:VAL:HG13	1.88	0.54
2:J:264:THR:CG2	2:J:265:ALA:H	2.16	0.54
1:K:135:ARG:HH12	1:K:181:ALA:HB2	1.69	0.54
2:L:264:THR:CG2	2:L:265:ALA:H	2.15	0.54
2:L:74:THR:HB	2:L:82:TYR:O	2.07	0.54
2:N:96:ASN:H	2:N:96:ASN:HD22	1.55	0.54
1:O:28:ASN:HD22	1:O:28:ASN:H	1.55	0.54
1:I:28:ASN:H	1:I:28:ASN:HD22	1.54	0.54
1:K:154:GLU:OE2	1:K:188:ARG:HD3	2.06	0.54
2:N:117:GLY:O	2:N:155:VAL:HA	2.07	0.54
2:P:162:ASP:O	2:P:185:VAL:HG13	2.07	0.54
2:D:83:PRO:O	2:D:86:THR:HA	2.07	0.54
2:H:136:ASN:C	2:H:136:ASN:HD22	2.09	0.54
1:I:131:LEU:HD12	1:I:143:ILE:O	2.08	0.54
2:J:220:GLY:HA2	2:J:259:THR:OG1	2.07	0.54
1:K:185:ILE:HD12	1:K:204:MET:SD	2.48	0.54
2:L:201:THR:HA	2:L:209:PHE:HA	1.90	0.54
2:L:40:THR:O	2:L:40:THR:HG22	2.08	0.54
2:N:28:VAL:O	2:N:156:VAL:HA	2.07	0.54
2:N:74:THR:HB	2:N:82:TYR:O	2.07	0.54
1:O:28:ASN:N	1:O:28:ASN:ND2	2.54	0.54
2:B:201:THR:CG2	2:B:206:ASN:HD22	2.20	0.54
1:E:183:SER:C	1:E:185:ILE:H	2.12	0.54
2:F:207:SER:O	2:F:224:GLN:HG3	2.08	0.54
1:G:186:THR:HG21	1:G:199:LYS:HZ1	1.73	0.54
2:H:201:THR:CG2	2:H:206:ASN:HA	2.29	0.54
1:O:104:GLN:O	2:P:271:ILE:HA	2.07	0.54
1:O:115:TYR:O	1:O:117:PRO:HD3	2.08	0.54
1:O:133:PHE:CE1	1:O:202:GLY:HA2	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:TYR:O	2:B:158:THR:HG22	2.06	0.53
1:C:134:ARG:HD2	1:C:141:THR:HG22	1.91	0.53
1:G:133:PHE:CD2	1:G:140:LEU:HD21	2.31	0.53
1:G:140:LEU:HB2	1:G:177:LEU:HD22	1.90	0.53
1:K:131:LEU:HD12	1:K:143:ILE:O	2.08	0.53
1:M:185:ILE:HD12	1:M:204:MET:SD	2.48	0.53
2:P:192:ASN:HB2	2:P:279:GLN:NE2	2.23	0.53
2:P:71:PHE:HE2	2:P:111:PRO:HG3	1.74	0.53
1:A:183:SER:C	1:A:185:ILE:H	2.12	0.53
2:B:71:PHE:CE2	2:B:111:PRO:HG3	2.43	0.53
1:G:183:SER:C	1:G:185:ILE:H	2.12	0.53
2:J:192:ASN:HB2	2:J:279:GLN:NE2	2.24	0.53
2:N:162:ASP:O	2:N:185:VAL:HG13	2.07	0.53
2:N:192:ASN:HB2	2:N:279:GLN:NE2	2.23	0.53
1:O:185:ILE:HD12	1:O:204:MET:SD	2.48	0.53
1:E:174:THR:HG23	1:E:174:THR:O	2.07	0.53
2:J:224:GLN:NE2	2:J:231:ILE:HD13	2.23	0.53
2:J:74:THR:HB	2:J:82:TYR:O	2.08	0.53
2:L:117:GLY:O	2:L:155:VAL:HA	2.08	0.53
2:N:30:VAL:HA	2:N:111:PRO:HB2	1.88	0.53
2:N:224:GLN:NE2	2:N:231:ILE:HD13	2.24	0.53
2:N:40:THR:HG22	2:N:40:THR:O	2.09	0.53
2:P:74:THR:HB	2:P:82:TYR:O	2.08	0.53
1:C:140:LEU:HB2	1:C:177:LEU:HD22	1.90	0.53
1:C:184:ASN:O	1:C:186:THR:HG23	2.09	0.53
2:D:120:ILE:CG2	2:D:126:ILE:HD11	2.30	0.53
2:H:5:THR:HG23	2:H:7:ASN:H	1.73	0.53
2:J:174:ASP:HB3	2:J:176:PRO:HD2	1.91	0.53
1:K:101:ASN:ND2	2:L:268:VAL:H	2.07	0.53
1:M:101:ASN:ND2	2:N:268:VAL:H	2.07	0.53
2:P:224:GLN:NE2	2:P:231:ILE:HD13	2.24	0.53
2:P:40:THR:O	2:P:40:THR:HG22	2.08	0.53
2:B:131:LEU:C	2:B:131:LEU:HD23	2.29	0.53
2:B:170:VAL:C	2:B:172:LEU:H	2.11	0.53
2:L:28:VAL:O	2:L:156:VAL:HA	2.08	0.53
1:A:140:LEU:HB2	1:A:177:LEU:HD22	1.91	0.53
1:C:205:GLU:OXT	1:C:205:GLU:HG3	2.09	0.53
1:G:205:GLU:HG3	1:G:205:GLU:OXT	2.09	0.53
2:H:172:LEU:O	2:H:173:PRO:C	2.46	0.53
2:J:60:ARG:HG3	2:J:61:GLY:N	2.23	0.53
2:H:173:PRO:HG3	2:H:179:VAL:CG1	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:83:PRO:O	2:H:86:THR:HA	2.08	0.53
1:I:133:PHE:CE1	1:I:202:GLY:HA2	2.43	0.53
1:K:133:PHE:CE1	1:K:202:GLY:HA2	2.44	0.53
2:N:71:PHE:HE2	2:N:111:PRO:HG3	1.73	0.53
2:P:4:LYS:HA	2:P:10:ALA:HA	1.90	0.53
2:P:20:VAL:HG12	2:P:22:VAL:HG13	1.89	0.53
1:C:186:THR:HG21	1:C:199:LYS:NZ	2.23	0.53
2:D:170:VAL:C	2:D:172:LEU:H	2.12	0.53
2:D:63:ALA:HB1	2:D:67:VAL:HG12	1.89	0.53
2:L:174:ASP:HB3	2:L:176:PRO:HD2	1.91	0.53
2:B:172:LEU:O	2:B:173:PRO:C	2.47	0.53
1:C:197:THR:HB	1:C:198:PRO:HD2	1.90	0.53
2:D:211:ASN:C	2:D:211:ASN:HD22	2.12	0.53
1:G:184:ASN:O	1:G:186:THR:HG23	2.08	0.53
2:H:7:ASN:HB2	4:H:1661:HOH:O	2.09	0.53
1:I:101:ASN:ND2	2:J:268:VAL:H	2.07	0.53
2:L:192:ASN:HB2	2:L:279:GLN:NE2	2.24	0.53
2:L:220:GLY:HA2	2:L:259:THR:OG1	2.06	0.53
1:M:191:ASN:HD21	1:M:195:ALA:HB3	1.74	0.53
1:E:186:THR:HG21	1:E:199:LYS:NZ	2.24	0.53
1:M:133:PHE:CE1	1:M:202:GLY:HA2	2.44	0.53
2:N:4:LYS:HA	2:N:10:ALA:HA	1.90	0.53
2:N:201:THR:HA	2:N:209:PHE:HA	1.90	0.53
1:O:46:GLY:O	1:O:70:ALA:HB3	2.09	0.53
2:P:174:ASP:HB3	2:P:176:PRO:HD2	1.91	0.53
2:P:34:LEU:HD12	2:P:35:VAL:N	2.20	0.53
2:F:211:ASN:C	2:F:211:ASN:HD22	2.11	0.52
2:H:211:ASN:HD22	2:H:211:ASN:C	2.10	0.52
2:L:224:GLN:NE2	2:L:231:ILE:HD13	2.24	0.52
1:M:28:ASN:O	1:M:29:SER:HB3	2.09	0.52
2:N:174:ASP:HB3	2:N:176:PRO:HD2	1.91	0.52
2:L:78:SER:H	2:L:104:PRO:HB2	1.74	0.52
1:M:46:GLY:O	1:M:70:ALA:HB3	2.10	0.52
2:J:71:PHE:HE2	2:J:111:PRO:HG3	1.73	0.52
2:B:185:VAL:HG23	2:B:243:VAL:HG11	1.90	0.52
1:C:183:SER:C	1:C:185:ILE:H	2.12	0.52
1:E:22:VAL:CG2	1:E:65:LEU:HG	2.39	0.52
2:H:167:ASP:CG	2:H:168:VAL:N	2.50	0.52
2:J:78:SER:H	2:J:104:PRO:HB2	1.75	0.52
1:O:131:LEU:HD12	1:O:143:ILE:O	2.09	0.52
2:P:78:SER:H	2:P:104:PRO:HB2	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:207:SER:O	2:P:224:GLN:HG3	2.10	0.52
2:P:201:THR:HA	2:P:209:PHE:HA	1.90	0.52
2:B:120:ILE:HD13	2:B:126:ILE:HD11	1.90	0.52
2:D:117:GLY:O	2:D:155:VAL:HA	2.08	0.52
2:L:208:ILE:HG21	2:L:259:THR:HG22	1.91	0.52
1:A:184:ASN:O	1:A:186:THR:HG23	2.08	0.52
2:D:22:VAL:HG23	2:D:22:VAL:O	2.09	0.52
1:I:184:ASN:O	1:I:186:THR:HG23	2.08	0.52
1:I:46:GLY:O	1:I:70:ALA:HB3	2.09	0.52
1:M:135:ARG:HH12	1:M:181:ALA:HB2	1.68	0.52
1:O:101:ASN:ND2	2:P:268:VAL:H	2.07	0.52
2:B:174:ASP:O	2:B:176:PRO:CD	2.58	0.52
1:C:122:LEU:CD1	1:C:126:GLN:HB3	2.40	0.52
2:D:174:ASP:O	2:D:176:PRO:CD	2.58	0.52
1:E:184:ASN:O	1:E:186:THR:HG23	2.08	0.52
1:G:186:THR:HG21	1:G:199:LYS:NZ	2.23	0.52
2:H:185:VAL:HG23	2:H:243:VAL:HG11	1.92	0.52
1:I:140:LEU:HD23	1:I:141:THR:N	2.25	0.52
1:K:28:ASN:O	1:K:29:SER:HB3	2.09	0.52
2:N:13:ILE:HG23	3:N:1506:MAN:C2	2.40	0.52
2:N:208:ILE:HG21	2:N:259:THR:HG22	1.92	0.52
1:O:191:ASN:HD21	1:O:195:ALA:HB3	1.74	0.52
2:B:83:PRO:O	2:B:86:THR:HA	2.08	0.52
1:M:131:LEU:HD12	1:M:143:ILE:O	2.08	0.52
2:N:14:GLY:HA2	2:N:142:PHE:CD1	2.45	0.52
1:O:140:LEU:HD23	1:O:141:THR:N	2.25	0.52
2:H:174:ASP:O	2:H:176:PRO:CD	2.58	0.52
1:K:191:ASN:HD21	1:K:195:ALA:HB3	1.74	0.52
1:K:46:GLY:O	1:K:70:ALA:HB3	2.09	0.52
2:L:43:PHE:N	2:L:43:PHE:CD1	2.78	0.52
1:O:28:ASN:O	1:O:29:SER:HB3	2.09	0.52
2:B:211:ASN:HD22	2:B:211:ASN:C	2.12	0.52
2:B:5:THR:HG23	2:B:7:ASN:H	1.73	0.52
2:J:40:THR:O	2:J:40:THR:HG22	2.09	0.52
1:K:140:LEU:HD23	1:K:141:THR:N	2.25	0.52
2:P:14:GLY:HA2	2:P:142:PHE:CD1	2.45	0.52
2:B:173:PRO:HG3	2:B:179:VAL:CG1	2.39	0.51
1:C:186:THR:HG21	1:C:199:LYS:HZ1	1.75	0.51
1:E:205:GLU:HG3	1:E:205:GLU:OXT	2.09	0.51
1:I:191:ASN:HD21	1:I:195:ALA:HB3	1.74	0.51
1:M:79:ARG:HB3	1:M:170:MET:HE3	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:164:SER:HB2	2:N:184:THR:O	2.10	0.51
1:A:85:MET:O	1:A:110:ARG:HA	2.10	0.51
1:A:186:THR:HG21	1:A:199:LYS:NZ	2.25	0.51
1:C:144:ASN:OD1	1:C:146:THR:HG23	2.10	0.51
2:D:172:LEU:O	2:D:173:PRO:C	2.47	0.51
2:F:33:ASN:ND2	2:F:110:THR:OG1	2.44	0.51
2:F:185:VAL:HG23	2:F:243:VAL:HG11	1.91	0.51
2:H:170:VAL:C	2:H:172:LEU:H	2.12	0.51
2:H:63:ALA:HB1	2:H:67:VAL:HG12	1.91	0.51
2:L:14:GLY:HA2	2:L:142:PHE:CD1	2.45	0.51
2:N:34:LEU:HD12	2:N:35:VAL:N	2.20	0.51
2:N:78:SER:H	2:N:104:PRO:HB2	1.75	0.51
1:O:160:ARG:CG	1:O:178:PRO:HG3	2.41	0.51
1:A:133:PHE:CD2	1:A:140:LEU:HD21	2.30	0.51
1:E:85:MET:O	1:E:110:ARG:HA	2.10	0.51
1:M:160:ARG:CG	1:M:178:PRO:HG3	2.41	0.51
1:A:144:ASN:OD1	1:A:146:THR:HG23	2.10	0.51
1:E:122:LEU:CD1	1:E:126:GLN:HB3	2.40	0.51
1:E:1:GLY:H1	1:E:26:ASP:CG	2.14	0.51
2:F:50:GLU:H	2:F:50:GLU:CD	2.14	0.51
1:G:144:ASN:OD1	1:G:146:THR:HG23	2.11	0.51
2:H:211:ASN:ND2	2:H:269:GLN:H	2.09	0.51
1:I:28:ASN:O	1:I:29:SER:HB3	2.09	0.51
2:L:215:PHE:CD2	2:L:215:PHE:C	2.84	0.51
2:N:207:SER:O	2:N:224:GLN:HG3	2.10	0.51
2:P:208:ILE:HG21	2:P:259:THR:HG22	1.92	0.51
1:A:1:GLY:H1	1:A:26:ASP:CG	2.14	0.51
2:D:211:ASN:HD21	2:D:269:GLN:H	1.58	0.51
2:H:50:GLU:CD	2:H:50:GLU:H	2.14	0.51
1:A:122:LEU:CD1	1:A:126:GLN:HB3	2.40	0.51
2:B:117:GLY:O	2:B:155:VAL:HA	2.09	0.51
1:C:13:ALA:HB3	1:C:118:ALA:H	1.76	0.51
2:F:211:ASN:HD21	2:F:269:GLN:H	1.57	0.51
1:K:160:ARG:CG	1:K:178:PRO:HG3	2.41	0.51
2:N:43:PHE:CD1	2:N:43:PHE:N	2.78	0.51
2:H:120:ILE:CG2	2:H:126:ILE:HD11	2.31	0.51
2:J:208:ILE:HG21	2:J:259:THR:HG22	1.91	0.51
2:J:67:VAL:HG21	2:J:126:ILE:CG2	2.35	0.51
1:A:22:VAL:CG2	1:A:65:LEU:HG	2.41	0.51
2:F:67:VAL:CG2	2:F:126:ILE:HG12	2.41	0.51
1:I:66:ARG:HH11	1:I:66:ARG:HG2	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:43:PHE:N	2:J:43:PHE:CD1	2.79	0.51
1:M:140:LEU:HD23	1:M:141:THR:N	2.25	0.51
1:M:66:ARG:HH11	1:M:66:ARG:HG2	1.76	0.51
2:P:190:SER:HA	2:P:244:GLY:HA2	1.93	0.51
1:C:22:VAL:CG2	1:C:65:LEU:HG	2.41	0.51
2:D:5:THR:HG23	2:D:7:ASN:H	1.76	0.51
2:F:174:ASP:O	2:F:176:PRO:CD	2.59	0.51
2:H:211:ASN:HD21	2:H:269:GLN:H	1.57	0.51
1:K:66:ARG:HH11	1:K:66:ARG:HG2	1.76	0.51
2:P:43:PHE:CD1	2:P:43:PHE:N	2.78	0.51
1:A:205:GLU:OXT	1:A:205:GLU:HG3	2.10	0.51
2:D:174:ASP:O	2:D:176:PRO:HD2	2.11	0.51
2:H:174:ASP:O	2:H:176:PRO:HD2	2.11	0.51
1:I:160:ARG:CG	1:I:178:PRO:HG3	2.41	0.51
1:O:67:ILE:N	1:O:67:ILE:HD12	2.26	0.51
2:P:164:SER:HB2	2:P:184:THR:O	2.11	0.51
2:B:163:VAL:CG1	2:B:183:LEU:HD21	2.41	0.50
1:G:122:LEU:CD1	1:G:126:GLN:HB3	2.40	0.50
2:L:96:ASN:ND2	2:L:96:ASN:N	2.58	0.50
1:M:47:ARG:HH22	1:M:74:GLN:HB2	1.76	0.50
2:N:190:SER:HA	2:N:244:GLY:HA2	1.93	0.50
2:N:96:ASN:N	2:N:96:ASN:ND2	2.60	0.50
2:B:131:LEU:HB3	2:B:144:PHE:HB2	1.93	0.50
2:B:227:ARG:HA	2:B:251:GLY:O	2.11	0.50
2:D:226:THR:HG22	2:D:253:THR:HB	1.94	0.50
1:I:9:VAL:O	1:I:113:LEU:HA	2.11	0.50
2:L:163:VAL:HA	2:L:185:VAL:CG2	2.35	0.50
1:A:13:ALA:HB3	1:A:118:ALA:H	1.76	0.50
2:B:174:ASP:O	2:B:176:PRO:HD2	2.11	0.50
1:E:133:PHE:CD2	1:E:140:LEU:HD21	2.31	0.50
2:H:33:ASN:ND2	2:H:110:THR:OG1	2.44	0.50
2:H:184:THR:HG22	2:H:249:SER:CA	2.41	0.50
2:J:215:PHE:C	2:J:215:PHE:CD2	2.84	0.50
2:J:96:ASN:N	2:J:96:ASN:ND2	2.59	0.50
2:L:202:ALA:HB2	2:L:210:THR:CG2	2.34	0.50
2:P:96:ASN:ND2	2:P:96:ASN:N	2.59	0.50
1:C:94:ASP:CG	2:D:168:VAL:HG11	2.32	0.50
1:E:144:ASN:OD1	1:E:146:THR:HG23	2.12	0.50
2:J:14:GLY:HA2	2:J:142:PHE:CD1	2.47	0.50
2:J:207:SER:O	2:J:224:GLN:HG3	2.10	0.50
1:K:67:ILE:N	1:K:67:ILE:HD12	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:47:ARG:HH22	1:K:74:GLN:HB2	1.76	0.50
2:L:66:GLY:HA3	2:L:119:ALA:O	2.11	0.50
2:B:184:THR:HG22	2:B:249:SER:CA	2.40	0.50
2:D:211:ASN:ND2	2:D:269:GLN:H	2.10	0.50
1:E:132:ARG:HB3	1:E:205:GLU:HB3	1.92	0.50
1:G:85:MET:O	1:G:110:ARG:HA	2.11	0.50
1:I:101:ASN:HD22	2:J:268:VAL:CG2	2.24	0.50
2:N:66:GLY:HA3	2:N:119:ALA:O	2.11	0.50
2:N:215:PHE:C	2:N:215:PHE:CD2	2.84	0.50
1:A:194:GLY:O	2:B:158:THR:HG21	2.11	0.50
1:C:133:PHE:CD2	1:C:140:LEU:HD21	2.31	0.50
1:C:194:GLY:O	2:D:158:THR:HG21	2.12	0.50
2:F:184:THR:HG22	2:F:249:SER:CA	2.42	0.50
1:G:114:TYR:CE2	1:G:149:TYR:HB2	2.47	0.50
2:H:163:VAL:CG1	2:H:183:LEU:HD21	2.41	0.50
1:O:66:ARG:HG2	1:O:66:ARG:HH11	1.77	0.50
2:H:166:ARG:O	2:H:167:ASP:HB2	2.12	0.50
1:I:67:ILE:N	1:I:67:ILE:HD12	2.26	0.50
2:B:126:ILE:CD1	2:B:150:ALA:HB2	2.24	0.50
1:A:94:ASP:CG	2:B:168:VAL:HG11	2.32	0.50
1:C:85:MET:O	1:C:110:ARG:HA	2.11	0.50
1:E:12:PRO:HD2	1:E:15:GLN:HG3	1.92	0.50
1:E:194:GLY:O	2:F:158:THR:HG21	2.12	0.50
2:F:211:ASN:ND2	2:F:269:GLN:H	2.10	0.50
1:G:186:THR:CG2	1:G:199:LYS:NZ	2.75	0.50
2:H:22:VAL:HG23	2:H:22:VAL:O	2.12	0.50
2:J:66:GLY:HA3	2:J:119:ALA:O	2.11	0.50
2:L:207:SER:O	2:L:224:GLN:HG3	2.10	0.50
1:M:149:TYR:CD2	1:M:168:PRO:HA	2.47	0.50
2:D:185:VAL:HG23	2:D:243:VAL:HG11	1.93	0.50
2:D:50:GLU:H	2:D:50:GLU:CD	2.15	0.50
2:F:174:ASP:O	2:F:176:PRO:HD2	2.12	0.50
2:H:67:VAL:CG2	2:H:126:ILE:HG12	2.42	0.50
2:J:190:SER:HA	2:J:244:GLY:HA2	1.93	0.50
1:K:9:VAL:O	1:K:113:LEU:HA	2.11	0.50
1:O:47:ARG:HH22	1:O:74:GLN:HB2	1.76	0.50
1:O:9:VAL:O	1:O:113:LEU:HA	2.11	0.50
2:P:126:ILE:HD12	2:P:148:ILE:HG22	1.94	0.50
2:B:211:ASN:HD21	2:B:269:GLN:H	1.57	0.49
2:B:211:ASN:ND2	2:B:269:GLN:H	2.10	0.49
1:C:11:TYR:CE2	1:C:69:ASP:HB2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:132:ARG:HB3	1:C:205:GLU:HB3	1.92	0.49
2:F:173:PRO:HG3	2:F:179:VAL:CG1	2.39	0.49
1:G:22:VAL:CG2	1:G:65:LEU:HG	2.42	0.49
1:O:149:TYR:CD2	1:O:168:PRO:HA	2.47	0.49
2:B:22:VAL:O	2:B:22:VAL:HG23	2.11	0.49
2:B:50:GLU:CD	2:B:50:GLU:H	2.14	0.49
1:E:142:LEU:HD22	1:E:142:LEU:H	1.77	0.49
1:K:79:ARG:HB3	1:K:170:MET:HE3	1.93	0.49
2:L:190:SER:HA	2:L:244:GLY:HA2	1.93	0.49
1:M:67:ILE:N	1:M:67:ILE:HD12	2.26	0.49
1:A:12:PRO:HD2	1:A:15:GLN:HG3	1.93	0.49
2:B:163:VAL:HG13	2:B:183:LEU:HD21	1.95	0.49
1:E:94:ASP:CG	2:F:168:VAL:HG11	2.32	0.49
2:F:227:ARG:HA	2:F:251:GLY:O	2.12	0.49
1:G:94:ASP:CG	2:H:168:VAL:HG11	2.33	0.49
1:I:149:TYR:CD2	1:I:168:PRO:HA	2.47	0.49
1:I:47:ARG:HH22	1:I:74:GLN:HB2	1.76	0.49
2:J:225:LEU:O	2:J:231:ILE:HG23	2.12	0.49
2:L:271:ILE:N	2:L:271:ILE:HD12	2.28	0.49
1:C:186:THR:CG2	1:C:199:LYS:NZ	2.75	0.49
2:J:145:VAL:HG12	2:J:146:TRP:N	2.27	0.49
2:J:253:THR:HG22	2:J:255:ASN:ND2	2.21	0.49
2:J:75:VAL:HG13	2:J:75:VAL:O	2.11	0.49
1:K:149:TYR:CD2	1:K:168:PRO:HA	2.47	0.49
1:K:11:TYR:CZ	1:K:69:ASP:HB2	2.47	0.49
2:N:208:ILE:HG23	2:N:257:ALA:CB	2.40	0.49
2:N:227:ARG:HA	2:N:251:GLY:O	2.13	0.49
2:P:145:VAL:HG12	2:P:146:TRP:N	2.27	0.49
2:P:271:ILE:N	2:P:271:ILE:HD12	2.28	0.49
1:A:156:ASN:C	1:A:158:GLY:H	2.16	0.49
1:G:194:GLY:O	2:H:158:THR:HG21	2.11	0.49
2:H:163:VAL:HG13	2:H:183:LEU:HD21	1.94	0.49
2:J:164:SER:HB2	2:J:184:THR:O	2.11	0.49
1:K:41:ASP:HB2	1:K:43:VAL:HG12	1.94	0.49
2:L:21:TYR:CB	2:L:151:ASN:HD21	2.24	0.49
1:M:9:VAL:O	1:M:113:LEU:HA	2.11	0.49
2:N:225:LEU:O	2:N:231:ILE:HG23	2.12	0.49
1:O:41:ASP:HB2	1:O:43:VAL:HG12	1.94	0.49
1:A:132:ARG:HB3	1:A:205:GLU:HB3	1.93	0.49
2:D:163:VAL:CG1	2:D:183:LEU:HD21	2.43	0.49
1:I:11:TYR:CZ	1:I:69:ASP:HB2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:164:SER:HB2	2:L:184:THR:O	2.11	0.49
1:M:140:LEU:HD22	1:M:142:LEU:HD22	1.95	0.49
1:M:98:LEU:HD13	1:M:98:LEU:C	2.33	0.49
2:N:145:VAL:HG12	2:N:146:TRP:N	2.27	0.49
1:O:11:TYR:CZ	1:O:69:ASP:HB2	2.47	0.49
2:P:66:GLY:HA3	2:P:119:ALA:O	2.12	0.49
2:P:227:ARG:HA	2:P:251:GLY:O	2.13	0.49
1:E:13:ALA:HB3	1:E:118:ALA:H	1.76	0.49
1:G:132:ARG:HB3	1:G:205:GLU:HB3	1.93	0.49
1:M:101:ASN:HD22	2:N:268:VAL:CG2	2.23	0.49
1:A:12:PRO:HB2	1:A:15:GLN:HG2	1.93	0.49
2:D:185:VAL:HG11	2:D:276:PHE:CE2	2.48	0.49
1:E:1:GLY:N	1:E:26:ASP:CG	2.66	0.49
2:J:126:ILE:HD12	2:J:148:ILE:HG22	1.94	0.49
2:J:45:HIS:HB3	2:J:100:ASP:HA	1.95	0.49
1:K:140:LEU:HD22	1:K:142:LEU:HD22	1.95	0.49
2:N:271:ILE:HD12	2:N:271:ILE:N	2.27	0.49
1:O:140:LEU:HD22	1:O:142:LEU:HD22	1.95	0.49
1:O:39:ASN:CG	1:O:43:VAL:HG13	2.33	0.49
2:B:67:VAL:CG2	2:B:126:ILE:HG12	2.42	0.49
2:F:185:VAL:HG11	2:F:276:PHE:CE2	2.48	0.49
2:H:185:VAL:HG11	2:H:276:PHE:CE2	2.48	0.49
2:D:163:VAL:HG13	2:D:183:LEU:HD21	1.95	0.49
2:F:173:PRO:O	2:F:256:TYR:HE1	1.96	0.49
2:F:163:VAL:CG1	2:F:183:LEU:HD21	2.42	0.49
1:G:156:ASN:C	1:G:158:GLY:H	2.16	0.49
1:I:47:ARG:HH22	1:I:74:GLN:NE2	1.92	0.49
2:J:271:ILE:HD12	2:J:271:ILE:N	2.27	0.49
1:K:98:LEU:HD13	1:K:98:LEU:C	2.33	0.49
2:L:270:SER:C	2:L:271:ILE:HD12	2.33	0.49
1:M:11:TYR:CZ	1:M:69:ASP:HB2	2.47	0.49
2:P:163:VAL:HA	2:P:185:VAL:CG2	2.35	0.49
2:P:225:LEU:O	2:P:231:ILE:HG23	2.13	0.49
1:C:12:PRO:HD2	1:C:15:GLN:HG3	1.94	0.48
2:F:66:GLY:HA3	2:F:119:ALA:O	2.13	0.48
2:H:211:ASN:ND2	2:H:211:ASN:C	2.66	0.48
2:H:227:ARG:HA	2:H:251:GLY:O	2.13	0.48
1:I:140:LEU:HD22	1:I:142:LEU:HD22	1.95	0.48
1:I:39:ASN:CG	1:I:43:VAL:HG13	2.32	0.48
1:I:27:GLU:HA	1:I:60:LYS:CG	2.43	0.48
2:J:270:SER:C	2:J:271:ILE:HD12	2.33	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:34:LEU:HD12	2:J:35:VAL:N	2.21	0.48
2:L:131:LEU:HD23	2:L:131:LEU:C	2.33	0.48
1:M:39:ASN:HB3	1:M:45:ASP:OD2	2.13	0.48
2:N:267:ASN:HB3	2:N:269:GLN:HE21	1.78	0.48
1:G:13:ALA:HB3	1:G:118:ALA:H	1.76	0.48
2:H:66:GLY:HA3	2:H:119:ALA:O	2.14	0.48
2:J:202:ALA:HB2	2:J:210:THR:CG2	2.34	0.48
1:K:101:ASN:HD22	2:L:268:VAL:CG2	2.24	0.48
1:K:39:ASN:HB3	1:K:45:ASP:OD2	2.13	0.48
2:L:126:ILE:HD12	2:L:148:ILE:HG22	1.95	0.48
2:N:164:SER:O	2:N:183:LEU:HD23	2.13	0.48
2:P:267:ASN:HB3	2:P:269:GLN:HE21	1.78	0.48
2:P:75:VAL:O	2:P:75:VAL:HG13	2.13	0.48
1:A:142:LEU:H	1:A:142:LEU:HD22	1.78	0.48
2:B:63:ALA:HB1	2:B:67:VAL:HG12	1.94	0.48
2:D:166:ARG:O	2:D:167:ASP:HB2	2.14	0.48
2:F:211:ASN:ND2	2:F:211:ASN:C	2.66	0.48
1:G:93:MET:CE	1:G:98:LEU:HD23	2.43	0.48
1:I:41:ASP:HB2	1:I:43:VAL:HG12	1.94	0.48
2:L:267:ASN:HB3	2:L:269:GLN:HE21	1.79	0.48
1:M:6:ALA:HB3	1:M:20:LEU:CD1	2.44	0.48
2:N:270:SER:C	2:N:271:ILE:HD12	2.33	0.48
1:O:101:ASN:HD22	2:P:268:VAL:CG2	2.23	0.48
2:P:270:SER:C	2:P:271:ILE:HD12	2.33	0.48
2:B:166:ARG:O	2:B:167:ASP:HB2	2.13	0.48
1:E:11:TYR:CE2	1:E:69:ASP:HB2	2.49	0.48
2:H:131:LEU:HB3	2:H:144:PHE:HB2	1.96	0.48
2:H:181:ILE:HB	2:H:252:LEU:HB2	1.96	0.48
1:I:39:ASN:HB3	1:I:45:ASP:OD2	2.13	0.48
2:J:96:ASN:N	2:J:96:ASN:HD22	2.10	0.48
2:L:145:VAL:HG12	2:L:146:TRP:N	2.28	0.48
2:P:215:PHE:CD2	2:P:215:PHE:C	2.84	0.48
2:D:66:GLY:HA3	2:D:119:ALA:O	2.13	0.48
2:D:33:ASN:ND2	2:D:110:THR:OG1	2.46	0.48
2:H:172:LEU:N	2:H:173:PRO:CD	2.75	0.48
1:M:39:ASN:CG	1:M:43:VAL:HG13	2.33	0.48
2:P:45:HIS:HB3	2:P:100:ASP:HA	1.96	0.48
2:P:38:LEU:C	2:P:40:THR:N	2.67	0.48
1:A:71:THR:HG23	1:A:71:THR:O	2.14	0.48
2:B:33:ASN:ND2	2:B:110:THR:OG1	2.46	0.48
2:B:66:GLY:HA3	2:B:119:ALA:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:181:ILE:HB	2:B:252:LEU:HB2	1.95	0.48
2:D:136:ASN:C	2:D:136:ASN:ND2	2.67	0.48
1:G:11:TYR:CE2	1:G:69:ASP:HB2	2.48	0.48
2:J:17:SER:HB2	2:L:262:GLN:OE1	2.13	0.48
1:K:6:ALA:HB3	1:K:20:LEU:CD1	2.43	0.48
2:N:131:LEU:C	2:N:131:LEU:HD23	2.34	0.48
1:O:39:ASN:HB3	1:O:45:ASP:OD2	2.13	0.48
1:O:98:LEU:HD13	1:O:98:LEU:C	2.33	0.48
2:P:253:THR:HG22	2:P:255:ASN:ND2	2.22	0.48
2:B:172:LEU:N	2:B:173:PRO:CD	2.76	0.48
1:C:140:LEU:H	1:C:177:LEU:HB2	1.79	0.48
2:F:166:ARG:O	2:F:167:ASP:HB2	2.14	0.48
2:L:45:HIS:HB3	2:L:100:ASP:HA	1.96	0.48
2:L:225:LEU:O	2:L:231:ILE:HG23	2.12	0.48
2:L:227:ARG:CD	2:L:232:ILE:HD11	2.44	0.48
2:L:38:LEU:C	2:L:40:THR:N	2.67	0.48
1:M:37:VAL:HG11	1:M:48:PHE:HB2	1.96	0.48
1:M:27:GLU:HA	1:M:60:LYS:CG	2.43	0.48
2:N:227:ARG:CD	2:N:232:ILE:HD11	2.44	0.48
2:N:17:SER:HB2	2:P:262:GLN:OE1	2.13	0.48
2:D:173:PRO:O	2:D:256:TYR:HE1	1.97	0.48
2:D:77:TYR:CE2	2:D:90:THR:HG21	2.49	0.48
1:E:140:LEU:H	1:E:177:LEU:HB2	1.78	0.48
1:E:186:THR:HG21	1:E:199:LYS:HZ1	1.79	0.48
1:G:140:LEU:H	1:G:177:LEU:HB2	1.78	0.48
2:L:227:ARG:HA	2:L:251:GLY:O	2.13	0.48
1:O:79:ARG:HB3	1:O:170:MET:HE3	1.94	0.48
1:A:186:THR:CG2	1:A:199:LYS:NZ	2.76	0.48
2:D:173:PRO:HG3	2:D:179:VAL:CG1	2.40	0.48
1:E:1:GLY:N	1:E:26:ASP:OD1	2.46	0.48
2:J:267:ASN:HB3	2:J:269:GLN:HE21	1.78	0.48
1:K:37:VAL:HG11	1:K:48:PHE:HB2	1.96	0.48
2:N:218:ALA:HA	2:N:264:THR:HB	1.96	0.48
2:N:96:ASN:N	2:N:96:ASN:HD22	2.12	0.48
2:P:164:SER:O	2:P:183:LEU:HD23	2.13	0.48
2:D:227:ARG:HA	2:D:251:GLY:O	2.13	0.48
1:I:133:PHE:HD2	1:I:140:LEU:HD21	1.79	0.48
2:L:75:VAL:O	2:L:75:VAL:HG13	2.14	0.48
2:L:96:ASN:ND2	2:L:96:ASN:H	2.11	0.48
2:N:45:HIS:HB3	2:N:100:ASP:HA	1.95	0.48
1:E:156:ASN:C	1:E:158:GLY:H	2.17	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:186:THR:CG2	1:E:199:LYS:NZ	2.76	0.47
1:G:1:GLY:N	1:G:26:ASP:CG	2.68	0.47
1:G:71:THR:HG23	1:G:71:THR:O	2.13	0.47
2:H:173:PRO:O	2:H:256:TYR:HE1	1.97	0.47
2:L:164:SER:O	2:L:183:LEU:HD23	2.13	0.47
1:M:135:ARG:HH22	1:M:181:ALA:CB	2.27	0.47
1:M:41:ASP:HB2	1:M:43:VAL:HG12	1.94	0.47
2:B:173:PRO:O	2:B:256:TYR:HE1	1.98	0.47
1:C:134:ARG:NE	1:C:141:THR:HG21	2.28	0.47
1:C:71:THR:O	1:C:71:THR:HG23	2.14	0.47
2:D:181:ILE:HB	2:D:252:LEU:HB2	1.96	0.47
1:I:135:ARG:HH22	1:I:181:ALA:CB	2.27	0.47
1:I:98:LEU:HD13	1:I:98:LEU:C	2.33	0.47
2:J:131:LEU:HD23	2:J:131:LEU:C	2.34	0.47
2:J:164:SER:O	2:J:183:LEU:HD23	2.14	0.47
1:K:135:ARG:HH22	1:K:181:ALA:CB	2.27	0.47
1:K:39:ASN:CG	1:K:43:VAL:HG13	2.33	0.47
1:A:1:GLY:N	1:A:26:ASP:OD1	2.47	0.47
1:C:1:GLY:N	1:C:26:ASP:OD1	2.47	0.47
2:F:163:VAL:HG13	2:F:183:LEU:HD21	1.96	0.47
2:H:77:TYR:CE2	2:H:90:THR:HG21	2.49	0.47
2:J:38:LEU:C	2:J:40:THR:N	2.66	0.47
2:N:126:ILE:HD12	2:N:148:ILE:HG22	1.94	0.47
1:O:135:ARG:HH22	1:O:181:ALA:CB	2.27	0.47
2:P:155:VAL:HG12	2:P:157:PRO:CD	2.43	0.47
2:P:48:TYR:H	3:P:1607:MAN:H62	1.80	0.47
1:A:186:THR:HG21	1:A:199:LYS:HZ1	1.79	0.47
2:D:184:THR:HG22	2:D:249:SER:CA	2.43	0.47
1:I:6:ALA:HB3	1:I:20:LEU:CD1	2.44	0.47
1:M:47:ARG:NH2	1:M:74:GLN:NE2	2.59	0.47
2:N:75:VAL:O	2:N:75:VAL:HG13	2.14	0.47
2:P:227:ARG:CD	2:P:232:ILE:HD11	2.44	0.47
2:P:267:ASN:CB	2:P:269:GLN:HE21	2.28	0.47
1:C:114:TYR:CE2	1:C:149:TYR:HB2	2.50	0.47
1:E:114:TYR:CE2	1:E:149:TYR:HB2	2.49	0.47
1:E:12:PRO:HB2	1:E:15:GLN:HG2	1.96	0.47
1:E:71:THR:HG23	1:E:71:THR:O	2.15	0.47
2:F:181:ILE:HB	2:F:252:LEU:HB2	1.97	0.47
2:L:218:ALA:HA	2:L:264:THR:HB	1.96	0.47
2:N:163:VAL:HA	2:N:185:VAL:CG2	2.36	0.47
1:O:133:PHE:HD2	1:O:140:LEU:HD21	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:27:GLU:HA	1:O:60:LYS:CG	2.43	0.47
1:O:6:ALA:HB3	1:O:20:LEU:CD1	2.44	0.47
2:P:131:LEU:HD23	2:P:131:LEU:C	2.33	0.47
2:P:218:ALA:HA	2:P:264:THR:HB	1.96	0.47
1:A:11:TYR:CE2	1:A:69:ASP:HB2	2.50	0.47
2:B:60:ARG:CZ	2:B:60:ARG:HB2	2.45	0.47
2:B:77:TYR:CE2	2:B:90:THR:HG21	2.50	0.47
1:I:185:ILE:O	1:I:202:GLY:N	2.35	0.47
2:J:227:ARG:CD	2:J:232:ILE:HD11	2.44	0.47
1:K:178:PRO:O	1:K:179:SER:HB3	2.15	0.47
2:L:66:GLY:HA2	2:L:70:ASN:HD22	1.79	0.47
2:P:53:THR:H	2:P:136:ASN:ND2	2.13	0.47
1:C:141:THR:HB	1:C:174:THR:CG2	2.41	0.47
1:C:142:LEU:HD22	1:C:142:LEU:H	1.78	0.47
1:C:33:ILE:O	1:C:54:LEU:HA	2.15	0.47
2:D:240:LEU:HD21	2:D:250:LEU:HD22	1.96	0.47
1:I:47:ARG:NH2	1:I:74:GLN:NE2	2.58	0.47
2:J:218:ALA:HA	2:J:264:THR:HB	1.96	0.47
1:K:27:GLU:HA	1:K:60:LYS:CG	2.44	0.47
1:K:47:ARG:HH22	1:K:74:GLN:NE2	1.92	0.47
2:L:179:VAL:HG23	2:L:179:VAL:O	2.15	0.47
1:K:102:THR:H	2:L:269:GLN:HG2	1.80	0.47
1:M:11:TYR:OH	1:M:69:ASP:HB2	2.14	0.47
2:N:226:THR:CG2	2:N:253:THR:HB	2.42	0.47
1:O:178:PRO:O	1:O:179:SER:HB3	2.15	0.47
1:A:30:THR:HG22	1:A:31:TYR:N	2.30	0.47
1:A:95:LYS:N	1:A:95:LYS:HD3	2.30	0.47
1:E:30:THR:HG22	1:E:31:TYR:N	2.30	0.47
1:E:95:LYS:HD3	1:E:95:LYS:N	2.30	0.47
2:F:136:ASN:ND2	2:F:136:ASN:C	2.68	0.47
1:G:140:LEU:C	1:G:140:LEU:HD23	2.35	0.47
2:J:227:ARG:HA	2:J:251:GLY:O	2.13	0.47
2:P:226:THR:CG2	2:P:253:THR:HB	2.43	0.47
2:P:66:GLY:HA2	2:P:70:ASN:HD22	1.79	0.47
2:D:201:THR:HG23	2:D:203:ASP:H	1.79	0.47
2:D:195:TYR:CE1	2:D:238:VAL:HB	2.50	0.47
2:F:41:GLN:NE2	4:F:1523:HOH:O	2.48	0.47
1:G:142:LEU:HD22	1:G:142:LEU:H	1.78	0.47
1:G:1:GLY:N	1:G:26:ASP:OD1	2.48	0.47
2:H:41:GLN:NE2	4:H:1627:HOH:O	2.47	0.47
1:I:11:TYR:OH	1:I:69:ASP:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:267:ASN:CB	2:J:269:GLN:HE21	2.28	0.47
1:K:11:TYR:OH	1:K:69:ASP:HB2	2.14	0.47
1:K:133:PHE:HD2	1:K:140:LEU:HD21	1.79	0.47
2:L:13:ILE:HG23	3:L:1504:MAN:C2	2.45	0.47
1:M:178:PRO:O	1:M:179:SER:HB3	2.15	0.47
2:N:1:PHE:HD1	2:N:144:PHE:CZ	2.33	0.47
2:N:179:VAL:HG23	2:N:179:VAL:O	2.15	0.47
1:A:140:LEU:C	1:A:140:LEU:HD23	2.35	0.47
2:D:211:ASN:C	2:D:211:ASN:ND2	2.67	0.47
2:L:224:GLN:HE21	2:L:231:ILE:HD13	1.80	0.47
1:M:160:ARG:HG3	1:M:178:PRO:HG3	1.97	0.47
1:M:95:LYS:HD3	1:M:95:LYS:N	2.30	0.47
1:A:140:LEU:H	1:A:177:LEU:HB2	1.79	0.47
2:B:195:TYR:CE1	2:B:238:VAL:HB	2.50	0.47
2:B:185:VAL:HG11	2:B:276:PHE:CE2	2.50	0.47
1:C:156:ASN:C	1:C:158:GLY:H	2.17	0.47
2:D:192:ASN:HA	2:D:241:GLY:O	2.15	0.47
2:H:201:THR:HG23	2:H:203:ASP:H	1.80	0.47
1:I:37:VAL:HG11	1:I:48:PHE:HB2	1.96	0.47
2:J:103:TRP:CE2	2:J:105:VAL:HG21	2.50	0.47
1:M:61:LYS:O	1:M:62:GLU:HB2	2.15	0.47
1:O:37:VAL:HG11	1:O:48:PHE:HB2	1.96	0.47
2:D:201:THR:CG2	2:D:206:ASN:HA	2.29	0.46
2:F:22:VAL:HG23	2:F:22:VAL:O	2.13	0.46
1:G:12:PRO:HD2	1:G:15:GLN:HG3	1.95	0.46
2:H:29:ASN:HA	4:H:1629:HOH:O	2.13	0.46
2:J:96:ASN:H	2:J:96:ASN:ND2	2.12	0.46
2:L:1:PHE:HD1	2:L:144:PHE:CZ	2.33	0.46
2:L:250:LEU:HD13	2:L:252:LEU:HD11	1.97	0.46
2:L:253:THR:HG22	2:L:255:ASN:ND2	2.22	0.46
1:M:133:PHE:HD2	1:M:140:LEU:HD21	1.79	0.46
2:N:96:ASN:ND2	2:N:96:ASN:H	2.13	0.46
2:B:211:ASN:C	2:B:211:ASN:ND2	2.68	0.46
1:G:141:THR:HG23	1:G:174:THR:CG2	2.45	0.46
1:G:160:ARG:HG2	1:G:178:PRO:HG3	1.97	0.46
2:H:136:ASN:C	2:H:136:ASN:ND2	2.68	0.46
2:H:215:PHE:O	2:H:216:SER:C	2.54	0.46
2:H:60:ARG:HB2	2:H:60:ARG:CZ	2.45	0.46
1:I:178:PRO:O	1:I:179:SER:HB3	2.15	0.46
1:I:95:LYS:N	1:I:95:LYS:HD3	2.30	0.46
2:J:1:PHE:HD1	2:J:144:PHE:CZ	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:53:THR:H	2:N:136:ASN:ND2	2.13	0.46
2:N:38:LEU:C	2:N:40:THR:N	2.67	0.46
2:N:66:GLY:HA2	2:N:70:ASN:HD22	1.80	0.46
1:O:11:TYR:OH	1:O:69:ASP:HB2	2.14	0.46
1:A:72:ASN:O	1:A:74:GLN:HG3	2.16	0.46
2:F:63:ALA:HB1	2:F:67:VAL:HG12	1.96	0.46
1:G:12:PRO:HB2	1:G:15:GLN:HG2	1.96	0.46
2:J:21:TYR:CB	2:J:151:ASN:HD21	2.24	0.46
1:O:160:ARG:HG3	1:O:178:PRO:HG3	1.98	0.46
1:A:12:PRO:CB	1:A:15:GLN:HG3	2.45	0.46
1:A:94:ASP:C	1:A:96:SER:H	2.18	0.46
2:B:113:SER:OG	2:P:81:SER:N	2.47	0.46
2:B:136:ASN:C	2:B:136:ASN:ND2	2.68	0.46
1:C:1:GLY:H1	1:C:26:ASP:CG	2.19	0.46
1:E:86:ASN:ND2	1:E:110:ARG:HB2	2.30	0.46
2:F:77:TYR:CE2	2:F:90:THR:HG21	2.51	0.46
1:G:33:ILE:O	1:G:54:LEU:HA	2.15	0.46
2:H:195:TYR:CE1	2:H:238:VAL:HB	2.49	0.46
1:I:142:LEU:HB2	1:I:173:SER:O	2.16	0.46
2:L:195:TYR:O	2:L:237:THR:HA	2.15	0.46
2:P:195:TYR:O	2:P:237:THR:HA	2.15	0.46
1:A:28:ASN:O	1:A:29:SER:HB3	2.16	0.46
1:A:33:ILE:O	1:A:54:LEU:HA	2.15	0.46
1:C:12:PRO:HB2	1:C:15:GLN:HG2	1.95	0.46
1:C:30:THR:HG22	1:C:31:TYR:N	2.30	0.46
1:E:33:ILE:O	1:E:54:LEU:HA	2.14	0.46
2:F:60:ARG:HB2	2:F:60:ARG:CZ	2.45	0.46
2:F:88:SER:HA	4:F:1572:HOH:O	2.16	0.46
1:K:47:ARG:NH2	1:K:74:GLN:NE2	2.58	0.46
1:O:47:ARG:HH22	1:O:74:GLN:NE2	1.92	0.46
2:P:1:PHE:HD1	2:P:144:PHE:CZ	2.33	0.46
2:P:197:LEU:CD1	2:P:225:LEU:HD12	2.42	0.46
1:C:140:LEU:HD23	1:C:140:LEU:C	2.35	0.46
1:C:95:LYS:HD3	1:C:95:LYS:N	2.30	0.46
1:C:93:MET:CE	1:C:98:LEU:HD23	2.45	0.46
1:E:93:MET:CE	1:E:98:LEU:HD23	2.45	0.46
2:F:201:THR:HG23	2:F:203:ASP:H	1.80	0.46
1:I:102:THR:H	2:J:269:GLN:HG2	1.80	0.46
2:J:24:LEU:O	2:J:26:PRO:N	2.49	0.46
2:L:83:PRO:O	2:L:86:THR:HA	2.15	0.46
1:M:102:THR:H	2:N:269:GLN:HG2	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:19:ASN:HD21	2:P:219:GLN:CD	2.19	0.46
1:O:177:LEU:HD12	1:O:178:PRO:CD	2.40	0.46
2:P:250:LEU:HD13	2:P:252:LEU:HD11	1.97	0.46
1:A:138:ASN:CA	1:A:177:LEU:HB3	2.46	0.46
2:B:135:ASN:HD21	2:B:138:ASN:HD21	1.63	0.46
2:B:215:PHE:O	2:B:216:SER:C	2.54	0.46
1:C:72:ASN:O	1:C:74:GLN:HG3	2.16	0.46
1:C:102:THR:C	2:D:171:THR:HG22	2.36	0.46
2:D:172:LEU:N	2:D:173:PRO:CD	2.77	0.46
1:E:181:ALA:HB1	1:E:182:GLY:H	1.53	0.46
1:G:95:LYS:HD3	1:G:95:LYS:N	2.31	0.46
1:I:79:ARG:HB3	1:I:170:MET:HE3	1.96	0.46
2:J:179:VAL:O	2:J:179:VAL:HG23	2.15	0.46
2:J:208:ILE:HG23	2:J:257:ALA:CB	2.40	0.46
2:J:250:LEU:HD13	2:J:252:LEU:HD11	1.96	0.46
2:J:53:THR:H	2:J:136:ASN:ND2	2.13	0.46
2:J:66:GLY:HA2	2:J:70:ASN:HD22	1.80	0.46
1:K:136:SER:HB2	1:K:139:SER:H	1.81	0.46
1:K:39:ASN:HD21	1:K:43:VAL:CG1	2.18	0.46
2:N:203:ASP:OD1	2:N:208:ILE:HD12	2.16	0.46
2:P:203:ASP:OD1	2:P:208:ILE:HD12	2.16	0.46
2:P:224:GLN:HE21	2:P:231:ILE:HD13	1.81	0.46
2:B:13:ILE:HG13	4:B:1545:HOH:O	2.15	0.46
1:C:160:ARG:HG2	1:C:178:PRO:HG3	1.98	0.46
2:D:131:LEU:HB3	2:D:144:PHE:HB2	1.97	0.46
1:G:86:ASN:ND2	1:G:110:ARG:HB2	2.31	0.46
2:J:203:ASP:OD1	2:J:208:ILE:HD12	2.16	0.46
1:K:12:PRO:HB2	1:K:15:GLN:HG3	1.97	0.46
1:K:95:LYS:N	1:K:95:LYS:HD3	2.30	0.46
2:L:184:THR:OG1	2:L:247:ALA:HB1	2.16	0.46
1:M:136:SER:HB2	1:M:139:SER:H	1.81	0.46
2:N:103:TRP:CE2	2:N:105:VAL:HG21	2.51	0.46
2:P:96:ASN:H	2:P:96:ASN:ND2	2.12	0.46
1:A:46:GLY:O	1:A:70:ALA:HB3	2.16	0.46
1:A:93:MET:CE	1:A:98:LEU:HD23	2.44	0.46
2:D:67:VAL:CG2	2:D:126:ILE:HG12	2.46	0.46
1:E:140:LEU:C	1:E:140:LEU:HD23	2.36	0.46
2:F:215:PHE:O	2:F:216:SER:C	2.54	0.46
2:J:175:TYR:N	2:J:176:PRO:CD	2.79	0.46
2:L:203:ASP:OD1	2:L:208:ILE:HD12	2.15	0.46
2:L:60:ARG:HG2	4:L:1505:HOH:O	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:78:ASP:O	1:M:170:MET:HE1	2.16	0.46
2:N:195:TYR:O	2:N:237:THR:HA	2.16	0.46
2:N:24:LEU:O	2:N:26:PRO:N	2.49	0.46
1:O:102:THR:H	2:P:269:GLN:HG2	1.80	0.46
2:P:24:LEU:O	2:P:26:PRO:N	2.49	0.46
2:P:83:PRO:O	2:P:86:THR:HA	2.16	0.46
1:A:160:ARG:HG2	1:A:178:PRO:HG3	1.98	0.46
1:C:1:GLY:N	1:C:26:ASP:CG	2.70	0.46
1:E:94:ASP:C	1:E:96:SER:H	2.19	0.46
1:G:129:GLU:HG3	1:G:129:GLU:H	1.52	0.46
1:G:72:ASN:O	1:G:74:GLN:HG3	2.16	0.46
1:K:142:LEU:HB2	1:K:173:SER:O	2.16	0.46
2:N:267:ASN:CB	2:N:269:GLN:HE21	2.28	0.46
1:O:57:MET:HA	1:O:61:LYS:CE	2.46	0.46
1:O:95:LYS:N	1:O:95:LYS:HD3	2.30	0.46
2:P:103:TRP:CE2	2:P:105:VAL:HG21	2.51	0.46
2:P:179:VAL:O	2:P:179:VAL:HG23	2.15	0.46
1:A:86:ASN:ND2	1:A:110:ARG:HB2	2.31	0.45
1:C:28:ASN:O	1:C:29:SER:HB3	2.15	0.45
1:E:160:ARG:HG2	1:E:178:PRO:HG3	1.98	0.45
1:E:191:ASN:ND2	1:E:195:ALA:HB3	2.31	0.45
1:E:72:ASN:O	1:E:74:GLN:HG3	2.16	0.45
1:I:57:MET:HA	1:I:61:LYS:CE	2.46	0.45
2:L:250:LEU:CD1	2:L:252:LEU:HD11	2.47	0.45
2:L:267:ASN:CB	2:L:269:GLN:HE21	2.28	0.45
1:M:57:MET:HA	1:M:61:LYS:CE	2.46	0.45
2:N:250:LEU:HD13	2:N:252:LEU:HD11	1.97	0.45
2:N:83:PRO:O	2:N:86:THR:HA	2.17	0.45
2:P:184:THR:OG1	2:P:247:ALA:HB1	2.16	0.45
2:P:208:ILE:HG23	2:P:257:ALA:CB	2.40	0.45
1:C:94:ASP:C	1:C:96:SER:H	2.19	0.45
1:E:28:ASN:O	1:E:29:SER:HB3	2.17	0.45
2:J:250:LEU:CD1	2:J:252:LEU:HD11	2.47	0.45
1:K:57:MET:HA	1:K:61:LYS:CE	2.46	0.45
2:L:34:LEU:HD12	2:L:35:VAL:N	2.21	0.45
1:A:186:THR:HB	1:A:199:LYS:NZ	2.32	0.45
1:C:141:THR:HA	1:C:174:THR:HA	1.98	0.45
2:D:215:PHE:O	2:D:216:SER:C	2.54	0.45
2:D:184:THR:HB	2:D:247:ALA:HB1	1.98	0.45
2:F:131:LEU:HB3	2:F:144:PHE:HB2	1.98	0.45
1:G:28:ASN:O	1:G:28:ASN:ND2	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:240:LEU:HD21	2:H:250:LEU:HD22	1.98	0.45
1:I:136:SER:HB2	1:I:139:SER:H	1.81	0.45
2:J:224:GLN:HE21	2:J:231:ILE:HD13	1.80	0.45
2:J:83:PRO:O	2:J:86:THR:HA	2.16	0.45
2:L:53:THR:H	2:L:136:ASN:ND2	2.13	0.45
2:N:96:ASN:O	2:N:97:SER:HB2	2.17	0.45
2:P:175:TYR:N	2:P:176:PRO:CD	2.80	0.45
1:C:86:ASN:ND2	1:C:110:ARG:HB2	2.32	0.45
1:C:162:LEU:HD21	1:C:178:PRO:CD	2.47	0.45
2:F:167:ASP:CG	2:F:168:VAL:HG12	2.37	0.45
2:F:201:THR:CG2	2:F:206:ASN:HA	2.31	0.45
2:F:195:TYR:CE1	2:F:238:VAL:HB	2.51	0.45
1:G:186:THR:HB	1:G:199:LYS:NZ	2.31	0.45
1:I:12:PRO:HB2	1:I:15:GLN:HG3	1.97	0.45
1:I:177:LEU:HD12	1:I:178:PRO:CD	2.40	0.45
2:J:155:VAL:HG12	2:J:157:PRO:CD	2.43	0.45
1:M:142:LEU:HB2	1:M:173:SER:O	2.16	0.45
2:P:154:VAL:HG12	2:P:155:VAL:N	2.32	0.45
1:A:114:TYR:CE2	1:A:149:TYR:HB2	2.51	0.45
1:A:156:ASN:O	1:A:185:ILE:HA	2.16	0.45
1:A:154:GLU:OE2	1:A:188:ARG:HD3	2.16	0.45
2:D:158:THR:HG23	4:D:1617:HOH:O	2.15	0.45
2:D:60:ARG:CZ	2:D:60:ARG:HB2	2.47	0.45
2:D:5:THR:CG2	2:D:8:GLY:H	2.29	0.45
1:E:186:THR:CG2	1:E:199:LYS:HZ2	2.30	0.45
1:G:46:GLY:O	1:G:70:ALA:HB3	2.16	0.45
2:L:103:TRP:CE2	2:L:105:VAL:HG21	2.51	0.45
1:M:12:PRO:HB2	1:M:15:GLN:HG3	1.97	0.45
2:N:184:THR:OG1	2:N:247:ALA:HB1	2.16	0.45
2:N:195:TYR:HB2	2:N:275:THR:O	2.17	0.45
1:O:142:LEU:HB2	1:O:173:SER:O	2.16	0.45
2:P:250:LEU:CD1	2:P:252:LEU:HD11	2.47	0.45
1:G:102:THR:C	2:H:171:THR:HG22	2.37	0.45
1:I:160:ARG:HG3	1:I:178:PRO:HG3	1.98	0.45
2:J:226:THR:CG2	2:J:253:THR:HB	2.42	0.45
1:O:61:LYS:O	1:O:62:GLU:HB2	2.15	0.45
2:B:184:THR:HB	2:B:247:ALA:HB1	1.98	0.45
1:C:167:VAL:HA	1:C:168:PRO:HD2	1.77	0.45
1:C:138:ASN:CA	1:C:177:LEU:HB3	2.47	0.45
1:E:138:ASN:CA	1:E:177:LEU:HB3	2.47	0.45
2:F:167:ASP:OD1	2:F:168:VAL:HG12	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:122:LEU:HD12	1:G:122:LEU:C	2.37	0.45
1:G:94:ASP:C	1:G:96:SER:H	2.18	0.45
1:I:61:LYS:O	1:I:62:GLU:HB2	2.16	0.45
1:K:160:ARG:HG3	1:K:178:PRO:HG3	1.98	0.45
1:O:144:ASN:HB3	1:O:167:VAL:HG12	1.99	0.45
1:C:46:GLY:O	1:C:70:ALA:HB3	2.16	0.45
2:D:4:LYS:NZ	2:D:4:LYS:HB2	2.31	0.45
1:E:102:THR:C	2:F:171:THR:HG22	2.36	0.45
1:G:125:ASP:OD1	1:G:126:GLN:N	2.50	0.45
1:I:144:ASN:HB3	1:I:167:VAL:HG12	1.99	0.45
2:J:195:TYR:HB2	2:J:275:THR:O	2.16	0.45
2:J:195:TYR:O	2:J:237:THR:HA	2.16	0.45
1:O:144:ASN:HB3	1:O:167:VAL:CG1	2.47	0.45
2:B:240:LEU:HD21	2:B:250:LEU:HD22	1.97	0.45
1:C:201:THR:O	1:C:203:VAL:HG23	2.17	0.45
2:D:38:LEU:C	2:D:40:THR:N	2.69	0.45
1:E:186:THR:HB	1:E:199:LYS:NZ	2.32	0.45
2:F:118:VAL:O	2:F:118:VAL:HG12	2.17	0.45
2:H:167:ASP:CG	2:H:168:VAL:HG12	2.38	0.45
2:J:96:ASN:O	2:J:97:SER:HB2	2.17	0.45
1:K:61:LYS:O	1:K:62:GLU:HB2	2.16	0.45
1:M:149:TYR:CD1	1:M:169:PRO:HD3	2.52	0.45
1:M:47:ARG:HH22	1:M:74:GLN:NE2	1.92	0.45
2:N:227:ARG:NE	2:N:232:ILE:HD11	2.32	0.45
1:A:1:GLY:N	1:A:26:ASP:CG	2.69	0.45
1:C:144:ASN:HB3	1:C:167:VAL:HG12	1.98	0.45
1:G:141:THR:HA	1:G:174:THR:HA	1.99	0.45
2:H:201:THR:CB	2:H:206:ASN:ND2	2.81	0.45
2:L:24:LEU:O	2:L:26:PRO:N	2.49	0.45
2:L:96:ASN:O	2:L:97:SER:HB2	2.17	0.45
1:O:136:SER:HB2	1:O:139:SER:H	1.81	0.45
1:O:47:ARG:NH2	1:O:74:GLN:NE2	2.58	0.45
1:A:186:THR:CG2	1:A:199:LYS:HZ2	2.30	0.44
1:C:82:LEU:HD12	1:C:83:PHE:H	1.82	0.44
1:E:156:ASN:O	1:E:185:ILE:HA	2.17	0.44
1:E:46:GLY:O	1:E:70:ALA:HB3	2.17	0.44
2:F:38:LEU:C	2:F:40:THR:N	2.70	0.44
1:G:30:THR:HG22	1:G:31:TYR:N	2.31	0.44
2:N:197:LEU:CD1	2:N:225:LEU:HD12	2.43	0.44
2:N:42:ILE:HG23	2:N:146:TRP:CH2	2.52	0.44
2:P:195:TYR:HB2	2:P:275:THR:O	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:227:ARG:NE	2:P:232:ILE:HD11	2.32	0.44
1:A:144:ASN:HB3	1:A:167:VAL:HG12	1.98	0.44
1:A:102:THR:C	2:B:171:THR:HG22	2.37	0.44
1:C:156:ASN:O	1:C:185:ILE:HA	2.16	0.44
1:C:154:GLU:OE2	1:C:188:ARG:HD3	2.17	0.44
1:E:201:THR:O	1:E:203:VAL:HG23	2.18	0.44
1:E:71:THR:O	1:E:73:ASN:N	2.51	0.44
2:F:136:ASN:N	2:F:136:ASN:HD22	2.15	0.44
1:G:144:ASN:HB3	1:G:167:VAL:HG12	1.98	0.44
1:G:28:ASN:O	1:G:29:SER:HB3	2.16	0.44
2:J:154:VAL:HG12	2:J:155:VAL:N	2.32	0.44
2:J:184:THR:OG1	2:J:247:ALA:HB1	2.17	0.44
2:N:253:THR:HG22	2:N:255:ASN:ND2	2.22	0.44
1:O:82:LEU:HB2	1:O:149:TYR:CE1	2.53	0.44
2:P:96:ASN:O	2:P:97:SER:HB2	2.17	0.44
1:I:144:ASN:HB3	1:I:167:VAL:CG1	2.48	0.44
1:I:39:ASN:OD1	1:I:43:VAL:HG13	2.18	0.44
1:I:57:MET:HA	1:I:61:LYS:HE3	2.00	0.44
2:J:42:ILE:HG23	2:J:146:TRP:CH2	2.53	0.44
1:K:177:LEU:HD12	1:K:178:PRO:CD	2.40	0.44
1:K:71:THR:HG23	1:K:71:THR:O	2.17	0.44
1:K:85:MET:O	1:K:110:ARG:HA	2.17	0.44
2:N:154:VAL:HG12	2:N:155:VAL:N	2.32	0.44
2:N:175:TYR:N	2:N:176:PRO:CD	2.80	0.44
2:N:224:GLN:HE21	2:N:231:ILE:HD13	1.80	0.44
1:O:85:MET:O	1:O:110:ARG:HA	2.17	0.44
2:B:201:THR:HG23	2:B:203:ASP:H	1.82	0.44
2:F:172:LEU:N	2:F:173:PRO:CD	2.76	0.44
1:G:201:THR:O	1:G:203:VAL:HG23	2.18	0.44
2:H:135:ASN:HD21	2:H:138:ASN:HD21	1.64	0.44
1:I:85:MET:O	1:I:110:ARG:HA	2.17	0.44
1:I:190:ILE:HD12	2:J:279:GLN:HG2	1.99	0.44
2:L:155:VAL:HG12	2:L:157:PRO:CD	2.43	0.44
2:N:250:LEU:CD1	2:N:252:LEU:HD11	2.47	0.44
2:N:59:GLN:HG3	2:N:132:ARG:HD3	2.00	0.44
1:O:186:THR:HB	1:O:199:LYS:NZ	2.32	0.44
1:A:47:ARG:NH2	1:A:74:GLN:HB2	2.33	0.44
1:C:28:ASN:O	1:C:28:ASN:ND2	2.51	0.44
1:E:141:THR:HA	1:E:174:THR:HA	2.00	0.44
1:I:82:LEU:HB2	1:I:149:TYR:CE1	2.52	0.44
2:L:267:ASN:OD1	2:L:269:GLN:NE2	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:144:ASN:HB3	1:M:167:VAL:CG1	2.47	0.44
1:M:190:ILE:HD12	2:N:279:GLN:HG2	2.00	0.44
1:O:12:PRO:HD2	1:O:15:GLN:HG3	1.99	0.44
2:P:61:GLY:HA3	2:P:86:THR:HG23	2.00	0.44
1:A:177:LEU:HA	1:A:178:PRO:HD2	1.88	0.44
1:E:122:LEU:HD12	1:E:122:LEU:C	2.38	0.44
1:G:138:ASN:CA	1:G:177:LEU:HB3	2.48	0.44
1:G:154:GLU:OE2	1:G:188:ARG:HD3	2.17	0.44
1:I:186:THR:HB	1:I:199:LYS:NZ	2.32	0.44
2:L:195:TYR:HB2	2:L:275:THR:O	2.17	0.44
1:M:82:LEU:HB2	1:M:149:TYR:CE1	2.53	0.44
2:N:168:VAL:O	2:N:168:VAL:HG13	2.18	0.44
1:O:71:THR:O	1:O:71:THR:HG23	2.18	0.44
2:P:58:LEU:H	2:P:90:THR:HG21	1.79	0.44
2:B:184:THR:HA	2:B:248:VAL:O	2.18	0.44
1:C:71:THR:O	1:C:73:ASN:N	2.51	0.44
2:D:5:THR:HG22	2:D:9:THR:N	2.32	0.44
1:E:123:PRO:HA	1:E:124:PRO:HD2	1.84	0.44
1:E:47:ARG:NH2	1:E:74:GLN:HB2	2.32	0.44
2:H:192:ASN:HA	2:H:241:GLY:O	2.18	0.44
2:H:4:LYS:HB2	2:H:4:LYS:NZ	2.33	0.44
1:I:71:THR:HG23	1:I:71:THR:O	2.18	0.44
2:J:168:VAL:HG13	2:J:168:VAL:O	2.18	0.44
2:J:211:ASN:HD22	2:J:212:THR:N	2.16	0.44
2:J:44:CYS:O	2:J:101:LYS:N	2.50	0.44
2:J:61:GLY:HA3	2:J:86:THR:HG23	1.99	0.44
1:K:78:ASP:O	1:K:170:MET:HE1	2.18	0.44
1:K:179:SER:C	1:K:181:ALA:H	2.20	0.44
1:K:39:ASN:OD1	1:K:43:VAL:HG13	2.18	0.44
1:M:186:THR:HB	1:M:199:LYS:NZ	2.33	0.44
1:M:45:ASP:OD1	1:M:47:ARG:HB2	2.18	0.44
2:N:267:ASN:OD1	2:N:269:GLN:NE2	2.51	0.44
1:O:12:PRO:HB2	1:O:15:GLN:HG3	1.98	0.44
1:O:149:TYR:CD1	1:O:169:PRO:HD3	2.52	0.44
2:P:42:ILE:HG23	2:P:146:TRP:CH2	2.53	0.44
2:P:202:ALA:HB2	2:P:210:THR:CG2	2.34	0.44
2:P:211:ASN:HD22	2:P:212:THR:N	2.16	0.44
2:P:267:ASN:OD1	2:P:269:GLN:NE2	2.50	0.44
1:A:122:LEU:C	1:A:122:LEU:HD12	2.38	0.44
1:A:191:ASN:ND2	1:A:195:ALA:HB3	2.33	0.44
2:B:167:ASP:OD1	2:B:168:VAL:HG12	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:12:PRO:CB	1:C:15:GLN:HG3	2.45	0.44
1:C:186:THR:HB	1:C:199:LYS:NZ	2.32	0.44
2:D:167:ASP:OD1	2:D:168:VAL:HG12	2.18	0.44
1:G:162:LEU:HD21	1:G:178:PRO:CD	2.48	0.44
1:K:190:ILE:HD12	2:L:279:GLN:HG2	2.00	0.44
2:L:211:ASN:HD22	2:L:212:THR:N	2.16	0.44
1:M:144:ASN:HB3	1:M:167:VAL:HG12	1.99	0.44
1:O:190:ILE:HD12	2:P:279:GLN:HG2	2.00	0.44
2:P:59:GLN:HG3	2:P:132:ARG:HD3	2.00	0.44
2:P:21:TYR:CB	2:P:151:ASN:HD21	2.24	0.44
1:A:187:TYR:C	1:A:187:TYR:CD1	2.91	0.44
1:E:154:GLU:OE2	1:E:188:ARG:HD3	2.18	0.44
2:F:184:THR:HB	2:F:247:ALA:HB1	1.98	0.44
1:G:156:ASN:O	1:G:185:ILE:HA	2.17	0.44
2:H:38:LEU:C	2:H:40:THR:N	2.71	0.44
1:I:160:ARG:HG2	1:I:178:PRO:HG3	2.00	0.44
2:J:95:TYR:HH	2:J:103:TRP:HA	1.83	0.44
1:K:149:TYR:CD1	1:K:169:PRO:HD3	2.52	0.44
1:K:144:ASN:HB3	1:K:167:VAL:HG12	1.99	0.44
1:K:45:ASP:OD1	1:K:47:ARG:HB2	2.18	0.44
2:L:227:ARG:NE	2:L:232:ILE:HD11	2.32	0.44
2:L:42:ILE:HG23	2:L:146:TRP:CH2	2.53	0.44
2:L:59:GLN:HG3	2:L:132:ARG:HD3	2.00	0.44
1:M:71:THR:O	1:M:71:THR:HG23	2.18	0.44
1:A:162:LEU:HD21	1:A:178:PRO:CD	2.47	0.43
1:C:47:ARG:NH2	1:C:74:GLN:HB2	2.33	0.43
1:E:162:LEU:HD21	1:E:178:PRO:CD	2.48	0.43
2:J:19:ASN:HD21	2:L:219:GLN:CD	2.21	0.43
1:K:186:THR:HB	1:K:199:LYS:NZ	2.32	0.43
1:K:24:ASN:HB2	1:K:57:MET:HE3	2.00	0.43
2:L:154:VAL:HG12	2:L:155:VAL:N	2.32	0.43
2:L:175:TYR:N	2:L:176:PRO:CD	2.80	0.43
2:L:8:GLY:O	2:L:9:THR:C	2.57	0.43
2:N:61:GLY:HA3	2:N:86:THR:HG23	2.00	0.43
2:D:184:THR:HA	2:D:248:VAL:O	2.18	0.43
1:E:155:LEU:HD12	1:E:187:TYR:HB3	2.01	0.43
1:E:31:TYR:O	1:E:56:ALA:HA	2.18	0.43
2:H:118:VAL:HG12	2:H:118:VAL:O	2.18	0.43
2:H:184:THR:HB	2:H:247:ALA:HB1	1.99	0.43
2:J:41:GLN:O	2:J:42:ILE:HG13	2.18	0.43
1:K:82:LEU:HB2	1:K:149:TYR:CE1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:135:ASN:ND2	3:L:1504:MAN:O4	2.52	0.43
2:N:211:ASN:HD22	2:N:212:THR:N	2.16	0.43
1:O:160:ARG:HG2	1:O:178:PRO:HG3	2.00	0.43
2:F:201:THR:CB	2:F:206:ASN:ND2	2.81	0.43
2:H:184:THR:HA	2:H:248:VAL:O	2.18	0.43
2:J:1:PHE:CD1	2:J:133:GLN:HG3	2.53	0.43
2:J:267:ASN:OD1	2:J:269:GLN:NE2	2.51	0.43
2:L:67:VAL:HG21	2:L:126:ILE:CG2	2.35	0.43
2:N:58:LEU:H	2:N:90:THR:HG21	1.80	0.43
2:P:1:PHE:CD1	2:P:133:GLN:HG3	2.53	0.43
2:P:192:ASN:HA	2:P:241:GLY:O	2.18	0.43
1:A:125:ASP:OD1	1:A:126:GLN:N	2.51	0.43
2:D:262:GLN:CA	2:D:262:GLN:HE21	2.25	0.43
2:H:5:THR:CG2	2:H:8:GLY:H	2.31	0.43
1:K:185:ILE:O	1:K:202:GLY:N	2.35	0.43
2:L:30:VAL:HG23	2:L:156:VAL:CG1	2.49	0.43
2:L:41:GLN:O	2:L:42:ILE:HG13	2.18	0.43
1:M:50:VAL:HG12	1:M:51:THR:N	2.34	0.43
2:N:30:VAL:HG23	2:N:156:VAL:CG1	2.49	0.43
1:O:57:MET:HA	1:O:61:LYS:HE3	2.00	0.43
2:D:167:ASP:CG	2:D:168:VAL:HG12	2.37	0.43
1:E:144:ASN:HB3	1:E:167:VAL:HG12	1.98	0.43
2:J:30:VAL:HG23	2:J:156:VAL:CG1	2.48	0.43
1:K:144:ASN:HB3	1:K:167:VAL:CG1	2.47	0.43
1:K:52:PRO:HG2	1:K:55:PHE:CE2	2.53	0.43
1:M:85:MET:O	1:M:110:ARG:HA	2.18	0.43
1:O:39:ASN:OD1	1:O:43:VAL:HG13	2.18	0.43
1:O:78:ASP:O	1:O:170:MET:HE1	2.18	0.43
1:A:201:THR:O	1:A:203:VAL:HG23	2.18	0.43
1:A:28:ASN:ND2	1:A:28:ASN:O	2.51	0.43
2:B:221:VAL:HG12	2:B:222:GLY:N	2.33	0.43
1:G:132:ARG:C	1:G:133:PHE:CD1	2.92	0.43
1:G:168:PRO:HA	1:G:169:PRO:HD3	1.87	0.43
1:G:155:LEU:HD12	1:G:187:TYR:HB3	2.01	0.43
2:H:167:ASP:OD1	2:H:168:VAL:HG12	2.18	0.43
2:H:5:THR:HG22	2:H:9:THR:N	2.33	0.43
1:I:149:TYR:CG	1:I:169:PRO:HD3	2.54	0.43
1:I:149:TYR:CD1	1:I:169:PRO:HD3	2.52	0.43
1:I:135:ARG:NH2	1:I:181:ALA:CB	2.82	0.43
2:J:227:ARG:NE	2:J:232:ILE:HD11	2.33	0.43
1:M:182:GLY:O	1:M:183:SER:CB	2.65	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:39:ASN:OD1	1:M:43:VAL:HG13	2.18	0.43
2:N:21:TYR:CB	2:N:151:ASN:HD21	2.24	0.43
2:N:41:GLN:O	2:N:42:ILE:HG13	2.19	0.43
2:P:41:GLN:O	2:P:42:ILE:HG13	2.18	0.43
1:A:141:THR:HA	1:A:174:THR:HA	1.99	0.43
2:B:38:LEU:C	2:B:40:THR:N	2.72	0.43
1:C:186:THR:CG2	1:C:199:LYS:HZ2	2.32	0.43
1:E:125:ASP:OD1	1:E:126:GLN:N	2.51	0.43
2:F:184:THR:HA	2:F:248:VAL:O	2.18	0.43
2:J:122:ALA:N	2:J:153:ASP:OD1	2.52	0.43
2:J:192:ASN:HA	2:J:241:GLY:O	2.19	0.43
2:J:241:GLY:O	2:J:243:VAL:HG23	2.19	0.43
1:K:135:ARG:NH2	1:K:181:ALA:CB	2.82	0.43
1:K:135:ARG:NH2	1:K:181:ALA:HB1	2.34	0.43
2:L:208:ILE:HG23	2:L:257:ALA:CB	2.40	0.43
2:L:192:ASN:HA	2:L:241:GLY:O	2.19	0.43
2:N:155:VAL:HG12	2:N:157:PRO:CD	2.43	0.43
2:N:30:VAL:HG12	2:N:31:GLY:N	2.33	0.43
1:O:13:ALA:HB3	1:O:118:ALA:H	1.84	0.43
1:O:135:ARG:NH2	1:O:181:ALA:CB	2.81	0.43
1:O:188:ARG:NH1	1:O:199:LYS:N	2.67	0.43
2:P:168:VAL:HG13	2:P:168:VAL:O	2.18	0.43
1:A:132:ARG:C	1:A:133:PHE:CD1	2.92	0.43
1:A:31:TYR:O	1:A:56:ALA:HA	2.19	0.43
1:A:47:ARG:NH2	1:A:74:GLN:NE2	2.54	0.43
1:E:187:TYR:CD1	1:E:187:TYR:C	2.92	0.43
1:G:31:TYR:O	1:G:56:ALA:HA	2.19	0.43
1:G:47:ARG:NH2	1:G:74:GLN:HB2	2.31	0.43
1:G:93:MET:HE1	1:G:98:LEU:HD23	2.00	0.43
1:I:52:PRO:HG2	1:I:55:PHE:CE2	2.53	0.43
1:K:41:ASP:C	1:K:43:VAL:H	2.22	0.43
2:L:241:GLY:O	2:L:243:VAL:HG23	2.19	0.43
2:N:241:GLY:O	2:N:243:VAL:HG23	2.19	0.43
2:N:95:TYR:OH	2:N:103:TRP:CA	2.66	0.43
2:B:167:ASP:CG	2:B:168:VAL:HG12	2.38	0.43
2:B:1:PHE:CG	2:B:133:GLN:HG3	2.54	0.43
2:B:5:THR:CG2	2:B:8:GLY:H	2.32	0.43
1:C:187:TYR:CD1	1:C:187:TYR:C	2.92	0.43
1:C:31:TYR:O	1:C:56:ALA:HA	2.18	0.43
1:E:122:LEU:HD12	1:E:123:PRO:N	2.34	0.43
2:J:197:LEU:CD1	2:J:225:LEU:HD12	2.42	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:177:LEU:HA	1:K:178:PRO:HD2	1.79	0.43
1:M:135:ARG:NH2	1:M:181:ALA:CB	2.81	0.43
1:M:57:MET:HA	1:M:61:LYS:HE3	2.00	0.43
1:O:45:ASP:OD1	1:O:47:ARG:HB2	2.19	0.43
1:O:52:PRO:HG2	1:O:55:PHE:CE2	2.54	0.43
2:B:212:THR:O	2:B:269:GLN:HB2	2.19	0.43
2:B:4:LYS:NZ	2:B:4:LYS:HB2	2.34	0.43
1:C:125:ASP:OD1	1:C:126:GLN:N	2.52	0.43
2:D:38:LEU:C	2:D:40:THR:H	2.21	0.43
1:E:28:ASN:ND2	1:E:28:ASN:O	2.52	0.43
1:G:122:LEU:HD12	1:G:123:PRO:N	2.34	0.43
2:H:116:GLY:HA2	2:H:189:LYS:CE	2.48	0.43
2:J:13:ILE:HG23	3:J:1605:MAN:C2	2.48	0.43
1:K:160:ARG:HG2	1:K:178:PRO:HG3	2.00	0.43
2:L:53:THR:H	2:L:136:ASN:HD21	1.67	0.43
1:M:179:SER:C	1:M:181:ALA:H	2.20	0.43
1:M:135:ARG:NH2	1:M:181:ALA:HB1	2.34	0.43
2:B:111:PRO:HB3	2:B:156:VAL:HG21	2.01	0.42
1:G:187:TYR:C	1:G:187:TYR:CD1	2.92	0.42
1:G:38:GLU:OE1	1:G:110:ARG:NH2	2.46	0.42
1:G:67:ILE:HD12	1:G:67:ILE:N	2.34	0.42
2:H:221:VAL:HG12	2:H:222:GLY:N	2.34	0.42
1:I:12:PRO:HD2	1:I:15:GLN:HG3	2.00	0.42
2:J:135:ASN:ND2	3:J:1605:MAN:O4	2.52	0.42
2:L:126:ILE:HD11	2:L:150:ALA:HB2	2.01	0.42
1:M:160:ARG:HG2	1:M:178:PRO:HG3	2.01	0.42
1:M:24:ASN:HB2	1:M:57:MET:HE3	2.00	0.42
1:M:77:GLN:NE2	1:M:77:GLN:HA	2.34	0.42
1:O:135:ARG:NH2	1:O:181:ALA:HB1	2.34	0.42
2:P:126:ILE:HD11	2:P:150:ALA:HB2	2.01	0.42
2:P:207:SER:HB3	2:P:233:PRO:HB3	2.01	0.42
2:H:126:ILE:CD1	2:H:150:ALA:HB2	2.26	0.42
1:I:136:SER:C	1:I:177:LEU:HD23	2.39	0.42
2:J:59:GLN:HG3	2:J:132:ARG:HD3	2.00	0.42
1:K:149:TYR:CG	1:K:169:PRO:HD3	2.54	0.42
2:L:29:ASN:OD1	2:L:157:PRO:HD2	2.19	0.42
1:M:39:ASN:HD21	1:M:43:VAL:CG1	2.18	0.42
1:M:52:PRO:HG2	1:M:55:PHE:CE2	2.54	0.42
2:N:29:ASN:OD1	2:N:157:PRO:HD2	2.19	0.42
1:O:31:TYR:O	1:O:56:ALA:HA	2.19	0.42
1:O:41:ASP:C	1:O:43:VAL:H	2.22	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:122:ALA:N	2:P:153:ASP:OD1	2.52	0.42
1:A:155:LEU:HD12	1:A:187:TYR:HB3	2.01	0.42
1:C:117:PRO:O	1:C:120:LEU:HG	2.19	0.42
2:D:226:THR:HG22	2:D:255:ASN:HD21	1.84	0.42
2:F:4:LYS:NZ	2:F:4:LYS:HB2	2.34	0.42
1:G:117:PRO:O	1:G:120:LEU:HG	2.19	0.42
2:H:201:THR:HB	2:H:206:ASN:ND2	2.34	0.42
1:I:13:ALA:HB3	1:I:118:ALA:H	1.84	0.42
2:J:41:GLN:C	2:J:42:ILE:HG13	2.40	0.42
1:K:136:SER:C	1:K:177:LEU:HD23	2.39	0.42
2:L:168:VAL:HG13	2:L:168:VAL:O	2.18	0.42
1:O:24:ASN:HB2	1:O:57:MET:HE3	2.00	0.42
1:O:50:VAL:HG12	1:O:51:THR:N	2.34	0.42
2:D:226:THR:CG2	2:D:255:ASN:HD21	2.32	0.42
2:F:240:LEU:HD21	2:F:250:LEU:HD22	2.00	0.42
1:G:10:ILE:O	1:G:12:PRO:HD3	2.19	0.42
1:G:191:ASN:ND2	1:G:195:ALA:HB3	2.32	0.42
2:H:33:ASN:HA	2:H:33:ASN:HD22	1.59	0.42
2:J:181:ILE:HA	2:J:182:PRO:HD3	1.93	0.42
2:J:223:VAL:CG1	2:J:224:GLN:N	2.82	0.42
2:J:8:GLY:O	2:J:9:THR:C	2.57	0.42
1:K:13:ALA:HB3	1:K:118:ALA:H	1.84	0.42
1:K:50:VAL:HG12	1:K:51:THR:N	2.34	0.42
2:L:61:GLY:HA3	2:L:86:THR:HG23	2.00	0.42
1:O:134:ARG:HD2	1:O:141:THR:OG1	2.20	0.42
1:O:188:ARG:NH1	1:O:199:LYS:H	2.17	0.42
2:P:136:ASN:N	2:P:136:ASN:HD22	2.17	0.42
2:P:29:ASN:OD1	2:P:157:PRO:HD2	2.20	0.42
2:P:223:VAL:CG1	2:P:224:GLN:N	2.82	0.42
2:P:30:VAL:HG23	2:P:156:VAL:CG1	2.49	0.42
2:P:41:GLN:C	2:P:42:ILE:HG13	2.40	0.42
1:A:117:PRO:O	1:A:120:LEU:HG	2.19	0.42
1:C:155:LEU:HD12	1:C:187:TYR:HB3	2.01	0.42
2:D:7:ASN:HB2	4:D:1654:HOH:O	2.19	0.42
1:E:93:MET:HE1	1:E:98:LEU:HD23	2.01	0.42
2:F:192:ASN:HA	2:F:241:GLY:O	2.19	0.42
2:H:113:SER:OG	2:L:81:SER:N	2.47	0.42
2:H:136:ASN:N	2:H:136:ASN:HD22	2.18	0.42
1:I:45:ASP:OD1	1:I:47:ARG:HB2	2.18	0.42
1:K:13:ALA:CB	1:K:117:PRO:HA	2.50	0.42
1:K:188:ARG:NH1	1:K:199:LYS:N	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:250:LEU:CB	2:L:252:LEU:HG	2.50	0.42
1:M:12:PRO:HD2	1:M:15:GLN:HG3	2.00	0.42
1:M:188:ARG:NH1	1:M:199:LYS:N	2.67	0.42
1:M:41:ASP:C	1:M:43:VAL:H	2.22	0.42
2:N:122:ALA:N	2:N:153:ASP:OD1	2.53	0.42
2:N:192:ASN:HA	2:N:241:GLY:O	2.19	0.42
1:O:179:SER:C	1:O:181:ALA:H	2.21	0.42
2:P:241:GLY:O	2:P:243:VAL:HG23	2.19	0.42
2:B:116:GLY:HA2	2:B:189:LYS:CE	2.47	0.42
1:C:132:ARG:C	1:C:133:PHE:CD1	2.93	0.42
2:D:118:VAL:HG12	2:D:118:VAL:O	2.19	0.42
2:D:126:ILE:CD1	2:D:150:ALA:HB2	2.24	0.42
1:I:28:ASN:O	1:I:29:SER:CB	2.68	0.42
1:I:39:ASN:HD21	1:I:43:VAL:CG1	2.18	0.42
2:J:20:VAL:CG1	2:J:22:VAL:HG13	2.50	0.42
2:J:184:THR:HA	2:J:248:VAL:O	2.19	0.42
2:J:30:VAL:HG12	2:J:31:GLY:N	2.34	0.42
2:L:1:PHE:CD1	2:L:133:GLN:HG3	2.55	0.42
1:M:134:ARG:HD2	1:M:141:THR:OG1	2.20	0.42
1:M:149:TYR:CG	1:M:169:PRO:HD3	2.54	0.42
1:M:31:TYR:O	1:M:56:ALA:HA	2.20	0.42
2:N:126:ILE:HD11	2:N:150:ALA:HB2	2.02	0.42
2:N:11:ILE:HA	2:N:12:PRO:HD2	1.89	0.42
2:P:169:THR:OG1	2:P:181:ILE:HG23	2.19	0.42
1:A:122:LEU:HD12	1:A:123:PRO:N	2.35	0.42
1:A:142:LEU:N	1:A:142:LEU:HD22	2.35	0.42
1:A:67:ILE:N	1:A:67:ILE:HD12	2.34	0.42
2:D:135:ASN:HD21	2:D:138:ASN:HD21	1.66	0.42
2:D:212:THR:O	2:D:269:GLN:HB2	2.20	0.42
1:E:142:LEU:HD22	1:E:142:LEU:N	2.34	0.42
1:I:135:ARG:CZ	1:I:177:LEU:HD21	2.50	0.42
1:I:50:VAL:HG12	1:I:51:THR:N	2.34	0.42
1:K:156:ASN:C	1:K:158:GLY:N	2.73	0.42
2:L:95:TYR:OH	2:L:103:TRP:CA	2.66	0.42
1:M:177:LEU:HD12	1:M:178:PRO:CD	2.40	0.42
2:N:8:GLY:O	2:N:9:THR:C	2.57	0.42
1:A:107:ILE:HG12	4:A:213:HOH:O	2.19	0.42
1:C:122:LEU:C	1:C:122:LEU:HD12	2.38	0.42
1:C:177:LEU:HA	1:C:178:PRO:HD2	1.87	0.42
2:D:201:THR:CB	2:D:206:ASN:ND2	2.83	0.42
2:F:136:ASN:H	2:F:136:ASN:ND2	2.17	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:212:THR:O	2:F:269:GLN:HB2	2.20	0.42
1:I:117:PRO:O	1:I:119:LYS:N	2.53	0.42
1:I:122:LEU:CD1	1:I:126:GLN:HB3	2.50	0.42
1:I:135:ARG:NH2	1:I:181:ALA:HB1	2.34	0.42
1:I:188:ARG:NH1	1:I:199:LYS:H	2.18	0.42
2:J:13:ILE:HG23	3:J:1605:MAN:O2	2.20	0.42
2:J:58:LEU:H	2:J:90:THR:HG21	1.79	0.42
1:K:57:MET:HA	1:K:61:LYS:HE3	2.00	0.42
2:L:30:VAL:HG12	2:L:31:GLY:N	2.34	0.42
2:L:48:TYR:HB2	2:L:52:ILE:CD1	2.48	0.42
1:M:135:ARG:CZ	1:M:177:LEU:HD21	2.50	0.42
1:O:117:PRO:O	1:O:119:LYS:N	2.53	0.42
2:P:184:THR:HA	2:P:248:VAL:O	2.19	0.42
2:P:222:GLY:C	2:P:257:ALA:HB3	2.40	0.42
2:D:221:VAL:HG12	2:D:222:GLY:N	2.35	0.42
2:D:215:PHE:HD1	2:D:267:ASN:OD1	2.03	0.42
1:I:188:ARG:NH1	1:I:199:LYS:N	2.67	0.42
1:I:31:TYR:O	1:I:56:ALA:HA	2.20	0.42
1:I:41:ASP:C	1:I:43:VAL:H	2.22	0.42
2:L:58:LEU:H	2:L:90:THR:HG21	1.78	0.42
2:L:96:ASN:HD22	2:L:96:ASN:N	2.10	0.42
2:N:169:THR:OG1	2:N:181:ILE:HG23	2.20	0.42
1:M:108:ILE:HB	2:N:275:THR:HG23	2.02	0.42
2:N:41:GLN:C	2:N:42:ILE:HG13	2.40	0.42
1:O:77:GLN:HA	1:O:77:GLN:NE2	2.35	0.42
2:P:14:GLY:HA2	2:P:142:PHE:CZ	2.55	0.42
2:P:95:TYR:OH	2:P:103:TRP:CA	2.66	0.42
1:A:94:ASP:OD1	2:B:168:VAL:HG11	2.20	0.42
1:C:122:LEU:HD12	1:C:123:PRO:N	2.35	0.42
1:C:94:ASP:OD1	2:D:168:VAL:HG11	2.20	0.42
2:F:111:PRO:HB3	2:F:156:VAL:HG21	2.02	0.42
2:F:221:VAL:HG12	2:F:222:GLY:N	2.35	0.42
2:J:207:SER:HB3	2:J:233:PRO:HB3	2.01	0.42
1:K:134:ARG:HD2	1:K:141:THR:OG1	2.20	0.42
2:L:207:SER:HB3	2:L:233:PRO:HB3	2.01	0.42
2:L:223:VAL:CG1	2:L:224:GLN:N	2.82	0.42
1:O:136:SER:C	1:O:177:LEU:HD23	2.39	0.42
1:O:13:ALA:CB	1:O:117:PRO:HA	2.50	0.42
1:O:142:LEU:HD22	1:O:142:LEU:N	2.35	0.42
1:O:149:TYR:CG	1:O:169:PRO:HD3	2.54	0.42
1:O:156:ASN:C	1:O:158:GLY:N	2.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:THR:O	1:A:73:ASN:N	2.51	0.41
2:B:226:THR:HG22	2:B:255:ASN:HD21	1.84	0.41
1:C:142:LEU:N	1:C:142:LEU:HD22	2.34	0.41
1:C:67:ILE:N	1:C:67:ILE:HD12	2.34	0.41
2:D:90:THR:HG23	2:D:91:PRO:N	2.34	0.41
1:E:132:ARG:C	1:E:133:PHE:CD1	2.93	0.41
1:E:67:ILE:HD12	1:E:67:ILE:N	2.34	0.41
2:F:38:LEU:C	2:F:40:THR:H	2.22	0.41
1:I:77:GLN:HA	1:I:77:GLN:NE2	2.35	0.41
2:J:136:ASN:HD22	2:J:136:ASN:N	2.18	0.41
2:J:163:VAL:HA	2:J:185:VAL:CG2	2.36	0.41
1:K:28:ASN:O	1:K:29:SER:CB	2.68	0.41
2:L:122:ALA:N	2:L:153:ASP:OD1	2.53	0.41
2:L:14:GLY:HA2	2:L:142:PHE:CZ	2.54	0.41
2:L:64:TYR:CE1	2:L:128:VAL:HG23	2.55	0.41
1:M:156:ASN:C	1:M:158:GLY:N	2.73	0.41
2:N:184:THR:HA	2:N:248:VAL:O	2.20	0.41
2:P:8:GLY:O	2:P:9:THR:C	2.57	0.41
2:B:201:THR:CB	2:B:206:ASN:ND2	2.83	0.41
2:D:136:ASN:HD22	2:D:136:ASN:N	2.16	0.41
1:E:117:PRO:O	1:E:120:LEU:HG	2.20	0.41
2:F:170:VAL:C	2:F:172:LEU:N	2.73	0.41
1:I:134:ARG:HD2	1:I:141:THR:OG1	2.20	0.41
2:J:140:ASP:OD1	3:J:1605:MAN:O3	2.31	0.41
2:J:126:ILE:HD11	2:J:150:ALA:HB2	2.02	0.41
2:J:116:GLY:O	2:J:156:VAL:O	2.38	0.41
2:J:165:ALA:O	2:J:166:ARG:C	2.59	0.41
2:J:53:THR:H	2:J:136:ASN:HD21	1.68	0.41
1:K:122:LEU:CD1	1:K:126:GLN:HB3	2.50	0.41
1:K:12:PRO:HD2	1:K:15:GLN:HG3	2.00	0.41
1:M:122:LEU:CD1	1:M:126:GLN:HB3	2.50	0.41
1:M:136:SER:C	1:M:177:LEU:HD23	2.40	0.41
2:N:14:GLY:HA2	2:N:142:PHE:CZ	2.55	0.41
2:P:116:GLY:O	2:P:156:VAL:O	2.38	0.41
2:P:19:ASN:OD1	2:P:147:ASN:HB2	2.20	0.41
2:P:30:VAL:HG12	2:P:31:GLY:N	2.34	0.41
2:B:192:ASN:HA	2:B:241:GLY:O	2.20	0.41
1:C:181:ALA:HB1	1:C:182:GLY:H	1.53	0.41
2:D:201:THR:HB	2:D:206:ASN:ND2	2.36	0.41
1:E:12:PRO:CB	1:E:15:GLN:HG3	2.48	0.41
1:G:142:LEU:HD22	1:G:142:LEU:N	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:156:ASN:C	1:I:158:GLY:N	2.73	0.41
1:I:135:ARG:HH12	1:I:177:LEU:HD11	1.82	0.41
1:I:179:SER:C	1:I:181:ALA:H	2.20	0.41
2:J:227:ARG:HG2	2:J:232:ILE:HD11	2.02	0.41
1:K:77:GLN:NE2	1:K:77:GLN:HA	2.35	0.41
2:L:116:GLY:O	2:L:156:VAL:O	2.38	0.41
2:L:44:CYS:O	2:L:101:LYS:N	2.50	0.41
1:M:185:ILE:O	1:M:202:GLY:N	2.35	0.41
1:M:188:ARG:NH1	1:M:199:LYS:H	2.17	0.41
2:N:165:ALA:O	2:N:166:ARG:C	2.59	0.41
2:N:1:PHE:CD1	2:N:133:GLN:HG3	2.54	0.41
2:N:207:SER:HB3	2:N:233:PRO:HB3	2.01	0.41
1:O:122:LEU:CD1	1:O:126:GLN:HB3	2.50	0.41
1:O:28:ASN:O	1:O:29:SER:CB	2.68	0.41
2:B:170:VAL:C	2:B:172:LEU:N	2.74	0.41
1:C:38:GLU:OE1	1:C:110:ARG:NH2	2.46	0.41
2:D:136:ASN:H	2:D:136:ASN:ND2	2.17	0.41
2:F:126:ILE:CD1	2:F:150:ALA:HB2	2.25	0.41
2:F:162:ASP:HB3	2:F:186:TYR:CZ	2.55	0.41
1:G:186:THR:CG2	1:G:199:LYS:HZ2	2.33	0.41
1:I:13:ALA:CB	1:I:117:PRO:HA	2.50	0.41
2:J:19:ASN:OD1	2:J:147:ASN:HB2	2.20	0.41
2:J:250:LEU:CB	2:J:252:LEU:HG	2.50	0.41
1:K:135:ARG:CZ	1:K:177:LEU:HD21	2.50	0.41
1:K:31:TYR:O	1:K:56:ALA:HA	2.19	0.41
1:O:135:ARG:CZ	1:O:177:LEU:HD21	2.50	0.41
2:P:227:ARG:HG2	2:P:232:ILE:HD11	2.03	0.41
2:P:53:THR:H	2:P:136:ASN:HD21	1.66	0.41
2:F:138:ASN:HD22	2:F:138:ASN:C	2.23	0.41
2:F:201:THR:HB	2:F:206:ASN:ND2	2.35	0.41
1:I:140:LEU:C	1:I:140:LEU:HD23	2.41	0.41
1:K:117:PRO:O	1:K:119:LYS:N	2.53	0.41
1:K:188:ARG:NH1	1:K:199:LYS:H	2.18	0.41
2:L:169:THR:OG1	2:L:181:ILE:HG23	2.20	0.41
2:L:184:THR:HA	2:L:248:VAL:O	2.20	0.41
2:L:197:LEU:CD1	2:L:225:LEU:HD12	2.43	0.41
2:L:227:ARG:HG2	2:L:232:ILE:HD11	2.03	0.41
1:O:39:ASN:HD21	1:O:43:VAL:CG1	2.18	0.41
1:O:108:ILE:HB	2:P:275:THR:HG23	2.03	0.41
2:B:5:THR:HG22	2:B:9:THR:N	2.35	0.41
1:C:178:PRO:O	1:C:179:SER:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:136:ASN:ND2	2:H:136:ASN:H	2.18	0.41
2:J:29:ASN:OD1	2:J:157:PRO:HD2	2.20	0.41
2:J:169:THR:OG1	2:J:181:ILE:HG23	2.20	0.41
1:K:99:THR:C	1:K:100:GLU:HG3	2.41	0.41
1:K:140:LEU:HD23	1:K:140:LEU:C	2.41	0.41
2:L:222:GLY:C	2:L:257:ALA:HB3	2.41	0.41
1:M:80:GLU:HG3	1:M:148:TYR:HA	2.02	0.41
2:N:116:GLY:O	2:N:156:VAL:O	2.37	0.41
2:P:44:CYS:O	2:P:101:LYS:N	2.51	0.41
1:A:178:PRO:O	1:A:179:SER:HB3	2.21	0.41
2:L:20:VAL:CG1	2:L:22:VAL:HG13	2.50	0.41
1:M:135:ARG:HH12	1:M:177:LEU:HD11	1.82	0.41
2:N:19:ASN:OD1	2:N:147:ASN:HB2	2.21	0.41
2:N:20:VAL:CG1	2:N:22:VAL:HG13	2.50	0.41
2:N:22:VAL:HG12	2:N:41:GLN:HG3	2.02	0.41
2:N:90:THR:HG23	2:N:91:PRO:O	2.21	0.41
1:O:140:LEU:HD23	1:O:140:LEU:C	2.41	0.41
1:A:51:THR:HA	1:A:52:PRO:C	2.41	0.41
2:B:207:SER:HB3	2:B:233:PRO:HB3	2.02	0.41
2:B:215:PHE:HD1	2:B:267:ASN:OD1	2.04	0.41
1:C:183:SER:C	1:C:185:ILE:N	2.74	0.41
2:D:1:PHE:CG	2:D:133:GLN:HG3	2.56	0.41
1:E:94:ASP:OD1	2:F:168:VAL:HG11	2.20	0.41
1:G:107:ILE:HG12	4:G:216:HOH:O	2.21	0.41
1:G:183:SER:C	1:G:185:ILE:N	2.74	0.41
2:H:215:PHE:HD1	2:H:267:ASN:OD1	2.03	0.41
1:I:133:PHE:HB3	1:I:134:ARG:H	1.70	0.41
1:I:24:ASN:HB2	1:I:57:MET:HE3	2.01	0.41
2:L:136:ASN:HD22	2:L:136:ASN:N	2.17	0.41
1:M:99:THR:C	1:M:100:GLU:HG3	2.41	0.41
1:M:13:ALA:CB	1:M:117:PRO:HA	2.50	0.41
2:N:227:ARG:HG2	2:N:232:ILE:HD11	2.03	0.41
2:N:53:THR:H	2:N:136:ASN:HD21	1.67	0.41
2:P:67:VAL:CG2	2:P:126:ILE:HG23	2.36	0.41
2:P:165:ALA:O	2:P:166:ARG:C	2.59	0.41
2:P:250:LEU:CB	2:P:252:LEU:HG	2.50	0.41
2:P:46:ASN:HD22	2:P:96:ASN:HA	1.85	0.41
1:A:174:THR:CG2	1:A:174:THR:O	2.68	0.41
2:B:33:ASN:HA	2:B:33:ASN:HD22	1.60	0.41
2:D:116:GLY:HA2	2:D:189:LYS:CE	2.47	0.41
1:E:198:PRO:O	1:E:200:MET:HG2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:92:ARG:NH1	2:F:92:ARG:CG	2.83	0.41
1:G:71:THR:O	1:G:73:ASN:N	2.51	0.41
2:J:20:VAL:CG2	2:J:42:ILE:HD11	2.50	0.41
2:L:262:GLN:HA	2:L:262:GLN:HE21	1.85	0.41
1:M:133:PHE:HB3	1:M:134:ARG:H	1.71	0.41
1:M:13:ALA:HB3	1:M:118:ALA:H	1.84	0.41
2:N:64:TYR:CE1	2:N:128:VAL:HG23	2.56	0.41
1:O:135:ARG:HH12	1:O:177:LEU:HD11	1.83	0.41
2:P:20:VAL:CG1	2:P:22:VAL:HG13	2.51	0.41
2:P:262:GLN:HE21	2:P:262:GLN:HA	1.86	0.41
1:A:129:GLU:H	1:A:129:GLU:HG3	1.51	0.41
1:A:181:ALA:HB1	1:A:182:GLY:H	1.53	0.41
1:A:198:PRO:O	1:A:200:MET:HG2	2.21	0.41
2:B:226:THR:CG2	2:B:255:ASN:HD21	2.33	0.41
2:F:168:VAL:HG22	2:F:168:VAL:O	2.21	0.41
1:G:140:LEU:CD2	1:G:140:LEU:C	2.89	0.41
2:H:201:THR:CB	2:H:206:ASN:HD22	2.34	0.41
2:H:212:THR:O	2:H:269:GLN:HB2	2.20	0.41
2:J:222:GLY:C	2:J:257:ALA:HB3	2.41	0.41
1:K:126:GLN:O	1:K:126:GLN:HG2	2.21	0.41
1:M:117:PRO:O	1:M:119:LYS:N	2.53	0.41
2:N:136:ASN:N	2:N:136:ASN:HD22	2.18	0.41
2:N:222:GLY:C	2:N:257:ALA:HB3	2.41	0.41
2:N:262:GLN:HA	2:N:262:GLN:HE21	1.85	0.41
2:N:67:VAL:HG21	2:N:126:ILE:CG2	2.36	0.41
1:A:27:GLU:CG	1:A:60:LYS:HD2	2.49	0.41
1:C:198:PRO:O	1:C:200:MET:HG2	2.21	0.41
2:D:5:THR:N	2:D:9:THR:O	2.51	0.41
1:E:167:VAL:HA	1:E:168:PRO:HD2	1.75	0.41
2:F:135:ASN:HD21	2:F:138:ASN:HD21	1.67	0.41
1:G:80:GLU:HA	1:G:115:TYR:O	2.21	0.41
1:I:99:THR:C	1:I:100:GLU:HG3	2.41	0.41
1:K:80:GLU:HG3	1:K:148:TYR:HA	2.03	0.41
2:L:165:ALA:O	2:L:166:ARG:C	2.59	0.41
1:M:140:LEU:HD23	1:M:140:LEU:C	2.41	0.41
1:M:142:LEU:N	1:M:142:LEU:HD22	2.35	0.41
2:P:120:ILE:O	2:P:153:ASP:HA	2.21	0.41
2:P:175:TYR:CZ	2:P:263:VAL:HB	2.56	0.41
1:C:168:PRO:HA	1:C:169:PRO:HD3	1.87	0.40
2:D:138:ASN:C	2:D:138:ASN:HD22	2.24	0.40
2:F:90:THR:HG23	2:F:91:PRO:N	2.35	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:188:ARG:HG2	1:G:199:LYS:HA	2.04	0.40
2:H:162:ASP:HB3	2:H:186:TYR:CZ	2.56	0.40
1:I:142:LEU:HD22	1:I:142:LEU:N	2.36	0.40
2:L:19:ASN:OD1	2:L:147:ASN:HB2	2.21	0.40
2:L:175:TYR:CZ	2:L:263:VAL:HB	2.57	0.40
1:M:126:GLN:O	1:M:126:GLN:HG2	2.21	0.40
2:N:128:VAL:HG12	2:N:128:VAL:O	2.21	0.40
2:N:202:ALA:HB2	2:N:210:THR:CG2	2.34	0.40
2:N:46:ASN:HD22	2:N:96:ASN:HA	1.86	0.40
1:O:182:GLY:O	1:O:183:SER:CB	2.65	0.40
1:O:185:ILE:O	1:O:202:GLY:N	2.35	0.40
2:P:52:ILE:HD12	3:P:1607:MAN:H61	2.04	0.40
2:B:138:ASN:HD22	2:B:138:ASN:C	2.24	0.40
2:B:90:THR:HG23	2:B:91:PRO:N	2.36	0.40
1:C:191:ASN:ND2	1:C:195:ALA:HB3	2.34	0.40
2:D:111:PRO:HB3	2:D:156:VAL:HG21	2.02	0.40
2:D:168:VAL:HG22	2:D:168:VAL:O	2.20	0.40
2:D:59:GLN:HG2	2:D:132:ARG:CD	2.43	0.40
1:G:198:PRO:O	1:G:200:MET:HG2	2.21	0.40
1:G:51:THR:HA	1:G:52:PRO:C	2.41	0.40
2:H:168:VAL:HG22	2:H:168:VAL:O	2.22	0.40
2:H:170:VAL:C	2:H:172:LEU:N	2.74	0.40
2:H:228:ASN:HD22	2:H:228:ASN:N	2.19	0.40
1:I:80:GLU:HG3	1:I:148:TYR:HA	2.03	0.40
1:I:108:ILE:HB	2:J:275:THR:HG23	2.02	0.40
2:L:41:GLN:C	2:L:42:ILE:HG13	2.40	0.40
1:M:101:ASN:ND2	2:N:268:VAL:N	2.69	0.40
2:N:175:TYR:CZ	2:N:263:VAL:HB	2.56	0.40
1:O:99:THR:C	1:O:100:GLU:HG3	2.42	0.40
1:A:167:VAL:HA	1:A:168:PRO:HD2	1.76	0.40
1:A:82:LEU:HD12	1:A:83:PHE:H	1.84	0.40
1:C:188:ARG:HG2	1:C:199:LYS:HA	2.03	0.40
2:D:218:ALA:HB2	2:D:266:GLY:CA	2.51	0.40
1:G:167:VAL:HA	1:G:168:PRO:HD2	1.76	0.40
2:P:128:VAL:HG12	2:P:128:VAL:O	2.21	0.40
1:O:193:TYR:HB3	2:P:157:PRO:HG3	2.03	0.40
1:A:155:LEU:HA	1:A:186:THR:O	2.22	0.40
2:B:136:ASN:N	2:B:136:ASN:HD22	2.18	0.40
1:E:129:GLU:HG3	1:E:129:GLU:H	1.52	0.40
1:E:155:LEU:HA	1:E:186:THR:O	2.22	0.40
1:G:178:PRO:O	1:G:179:SER:HB3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:191:ASN:O	1:G:194:GLY:N	2.46	0.40
2:H:1:PHE:CG	2:H:133:GLN:HG3	2.57	0.40
2:J:22:VAL:HG12	2:J:41:GLN:HG3	2.03	0.40
2:J:46:ASN:HD22	2:J:96:ASN:HA	1.86	0.40
1:K:142:LEU:N	1:K:142:LEU:HD22	2.36	0.40
1:K:8:ARG:NH1	1:K:190:ILE:CG2	2.85	0.40
2:L:128:VAL:O	2:L:128:VAL:HG12	2.21	0.40
2:L:64:TYR:N	2:L:64:TYR:CD1	2.89	0.40
2:N:223:VAL:CG1	2:N:224:GLN:N	2.83	0.40
2:N:24:LEU:O	2:N:152:ASN:ND2	2.51	0.40
2:P:106:ALA:CB	2:P:108:TYR:HE1	2.35	0.40
2:P:11:ILE:HA	2:P:12:PRO:HD2	1.89	0.40
1:O:103:LEU:HD23	2:P:181:ILE:HD11	2.03	0.40
1:A:140:LEU:C	1:A:140:LEU:CD2	2.90	0.40
2:B:118:VAL:HG12	2:B:118:VAL:O	2.20	0.40
2:B:262:GLN:CA	2:B:262:GLN:HE21	2.25	0.40
1:E:47:ARG:NH2	1:E:74:GLN:NE2	2.55	0.40
2:F:116:GLY:HA2	2:F:189:LYS:CE	2.47	0.40
1:I:78:ASP:O	1:I:170:MET:HE1	2.20	0.40
2:J:120:ILE:O	2:J:153:ASP:HA	2.21	0.40
2:L:22:VAL:HG12	2:L:41:GLN:HG3	2.02	0.40
2:L:231:ILE:CG2	2:L:232:ILE:N	2.84	0.40
2:L:90:THR:HG23	2:L:91:PRO:O	2.22	0.40
1:M:193:TYR:HB3	2:N:157:PRO:HG3	2.04	0.40
2:N:209:PHE:CE2	2:N:272:ILE:HG23	2.57	0.40
2:N:231:ILE:CG2	2:N:232:ILE:N	2.85	0.40
1:O:101:ASN:ND2	2:P:268:VAL:N	2.69	0.40
1:O:126:GLN:O	1:O:126:GLN:HG2	2.21	0.40
2:P:162:ASP:O	2:P:185:VAL:HA	2.22	0.40
2:P:22:VAL:HG12	2:P:41:GLN:HG3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	203/205 (99%)	163 (80%)	29 (14%)	11 (5%)	2	5
1	C	203/205 (99%)	164 (81%)	28 (14%)	11 (5%)	2	5
1	E	203/205 (99%)	163 (80%)	29 (14%)	11 (5%)	2	5
1	G	203/205 (99%)	164 (81%)	28 (14%)	11 (5%)	2	5
1	I	203/205 (99%)	162 (80%)	29 (14%)	12 (6%)	1	4
1	K	203/205 (99%)	162 (80%)	29 (14%)	12 (6%)	1	4
1	M	203/205 (99%)	162 (80%)	29 (14%)	12 (6%)	1	4
1	O	203/205 (99%)	163 (80%)	28 (14%)	12 (6%)	1	4
2	B	277/279 (99%)	244 (88%)	24 (9%)	9 (3%)	4	13
2	D	277/279 (99%)	243 (88%)	24 (9%)	10 (4%)	3	11
2	F	277/279 (99%)	244 (88%)	23 (8%)	10 (4%)	3	11
2	H	277/279 (99%)	243 (88%)	24 (9%)	10 (4%)	3	11
2	J	277/279 (99%)	195 (70%)	60 (22%)	22 (8%)	1	2
2	L	277/279 (99%)	195 (70%)	60 (22%)	22 (8%)	1	2
2	N	277/279 (99%)	195 (70%)	60 (22%)	22 (8%)	1	2
2	P	277/279 (99%)	196 (71%)	59 (21%)	22 (8%)	1	2
All	All	3840/3872 (99%)	3058 (80%)	563 (15%)	219 (6%)	1	5

All (219) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	29	SER
1	A	119	LYS
1	A	181	ALA
1	A	183	SER
2	B	175	TYR
2	B	218	ALA
1	C	29	SER
1	C	119	LYS
1	C	181	ALA
1	C	183	SER
2	D	175	TYR
2	D	218	ALA
1	E	29	SER
1	E	119	LYS

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Mol	Chain	Res	Type
1	E	181	ALA
1	E	183	SER
2	F	175	TYR
2	F	218	ALA
1	G	29	SER
1	G	119	LYS
1	G	181	ALA
1	G	183	SER
2	H	175	TYR
2	H	218	ALA
1	I	29	SER
1	I	119	LYS
1	I	181	ALA
1	I	183	SER
1	K	29	SER
1	K	119	LYS
1	K	181	ALA
1	K	183	SER
2	L	264	THR
1	M	29	SER
1	M	119	LYS
1	M	181	ALA
1	M	183	SER
2	N	264	THR
1	O	29	SER
1	O	119	LYS
1	O	181	ALA
1	O	183	SER
2	P	264	THR
1	A	26	ASP
1	A	192	ASP
2	B	116	GLY
2	B	167	ASP
2	B	173	PRO
2	B	174	ASP
2	B	215	PHE
2	B	221	VAL
1	C	26	ASP
1	C	192	ASP
2	D	116	GLY
2	D	167	ASP
2	D	173	PRO

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Mol	Chain	Res	Type
2	D	174	ASP
2	D	215	PHE
2	D	221	VAL
1	E	26	ASP
1	E	192	ASP
2	F	116	GLY
2	F	167	ASP
2	F	173	PRO
2	F	174	ASP
2	F	215	PHE
2	F	221	VAL
1	G	26	ASP
1	G	192	ASP
2	H	116	GLY
2	H	167	ASP
2	H	173	PRO
2	H	174	ASP
2	H	215	PHE
2	H	221	VAL
1	I	62	GLU
2	J	9	THR
2	J	22	VAL
2	J	32	GLN
2	J	116	GLY
2	J	157	PRO
2	J	168	VAL
2	J	190	SER
2	J	247	ALA
2	J	264	THR
1	K	62	GLU
2	L	9	THR
2	L	22	VAL
2	L	32	GLN
2	L	116	GLY
2	L	157	PRO
2	L	168	VAL
2	L	190	SER
2	L	247	ALA
1	M	62	GLU
2	N	9	THR
2	N	22	VAL
2	N	116	GLY

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Mol	Chain	Res	Type
2	N	157	PRO
2	N	168	VAL
2	N	190	SER
2	N	247	ALA
1	O	62	GLU
2	P	9	THR
2	P	22	VAL
2	P	32	GLN
2	P	116	GLY
2	P	157	PRO
2	P	168	VAL
2	P	190	SER
2	P	247	ALA
1	A	134	ARG
1	A	138	ASN
1	C	134	ARG
1	C	138	ASN
1	E	134	ARG
1	E	138	ASN
1	G	134	ARG
1	G	138	ASN
1	I	26	ASP
2	J	97	SER
2	J	173	PRO
2	J	206	ASN
2	J	235	ASN
2	J	242	ALA
1	K	26	ASP
2	L	97	SER
2	L	173	PRO
2	L	206	ASN
2	L	235	ASN
2	L	242	ALA
1	M	26	ASP
2	N	32	GLN
2	N	97	SER
2	N	173	PRO
2	N	206	ASN
2	N	235	ASN
2	N	242	ALA
1	O	26	ASP
2	P	97	SER

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Mol	Chain	Res	Type
2	P	173	PRO
2	P	206	ASN
2	P	235	ASN
2	P	242	ALA
1	A	72	ASN
1	A	91	PRO
1	C	72	ASN
1	C	91	PRO
1	E	72	ASN
1	G	72	ASN
1	G	91	PRO
1	I	91	PRO
1	I	121	ALA
1	I	134	ARG
1	I	138	ASN
2	J	166	ARG
2	J	261	GLY
1	K	91	PRO
1	K	121	ALA
1	K	134	ARG
1	K	138	ASN
2	L	166	ARG
2	L	261	GLY
1	M	91	PRO
1	M	121	ALA
1	M	134	ARG
1	M	138	ASN
2	N	166	ARG
2	N	261	GLY
1	O	91	PRO
1	O	121	ALA
1	O	134	ARG
1	O	138	ASN
2	P	166	ARG
2	P	261	GLY
1	E	91	PRO
1	I	164	ASN
2	J	40	THR
2	J	100	ASP
1	K	164	ASN
2	L	40	THR
2	L	100	ASP

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Mol	Chain	Res	Type
1	M	164	ASN
2	N	40	THR
2	N	100	ASP
2	N	217	PRO
1	O	164	ASN
2	P	40	THR
2	P	100	ASP
1	A	147	PRO
1	C	147	PRO
2	D	260	GLY
1	E	147	PRO
2	F	260	GLY
1	G	147	PRO
2	H	260	GLY
2	J	217	PRO
2	L	217	PRO
2	P	217	PRO
2	B	260	GLY
2	J	26	PRO
1	I	42	GLY
2	J	273	GLY
2	J	274	VAL
1	K	42	GLY
2	L	26	PRO
2	L	273	GLY
2	L	274	VAL
1	M	42	GLY
2	N	26	PRO
2	N	273	GLY
1	O	42	GLY
2	P	26	PRO
2	P	273	GLY
2	P	274	VAL
2	N	274	VAL
2	D	104	PRO
2	F	104	PRO
2	H	104	PRO

5.3.2 Protein sidechains ⓘ

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

resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	176/176 (100%)	160 (91%)	16 (9%)	9	27
1	C	176/176 (100%)	159 (90%)	17 (10%)	8	24
1	E	176/176 (100%)	160 (91%)	16 (9%)	9	27
1	G	176/176 (100%)	160 (91%)	16 (9%)	9	27
1	I	176/176 (100%)	165 (94%)	11 (6%)	18	46
1	K	176/176 (100%)	164 (93%)	12 (7%)	16	42
1	M	176/176 (100%)	165 (94%)	11 (6%)	18	46
1	O	176/176 (100%)	165 (94%)	11 (6%)	18	46
2	B	226/226 (100%)	208 (92%)	18 (8%)	12	34
2	D	226/226 (100%)	208 (92%)	18 (8%)	12	34
2	F	226/226 (100%)	207 (92%)	19 (8%)	11	31
2	H	226/226 (100%)	207 (92%)	19 (8%)	11	31
2	J	226/226 (100%)	214 (95%)	12 (5%)	22	54
2	L	226/226 (100%)	214 (95%)	12 (5%)	22	54
2	N	226/226 (100%)	214 (95%)	12 (5%)	22	54
2	P	226/226 (100%)	213 (94%)	13 (6%)	20	50
All	All	3216/3216 (100%)	2983 (93%)	233 (7%)	14	38

All (233) 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	44	LYS
1	A	47	ARG
1	A	61	LYS
1	A	62	GLU
1	A	104	GLN
1	A	129	GLU
1	A	135	ARG
1	A	142	LEU
1	A	143	ILE

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Mol	Chain	Res	Type
1	A	146	THR
1	A	173	SER
1	A	200	MET
1	A	205	GLU
2	B	4	LYS
2	B	5	THR
2	B	33	ASN
2	B	40	THR
2	B	57	THR
2	B	59	GLN
2	B	81	SER
2	B	90	THR
2	B	96	ASN
2	B	107	LEU
2	B	126	ILE
2	B	136	ASN
2	B	138	ASN
2	B	190	SER
2	B	201	THR
2	B	211	ASN
2	B	262	GLN
2	B	271	ILE
1	C	8	ARG
1	C	23	THR
1	C	28	ASN
1	C	44	LYS
1	C	47	ARG
1	C	61	LYS
1	C	62	GLU
1	C	104	GLN
1	C	129	GLU
1	C	135	ARG
1	C	142	LEU
1	C	143	ILE
1	C	146	THR
1	C	173	SER
1	C	174	THR
1	C	200	MET
1	C	205	GLU
2	D	4	LYS
2	D	5	THR
2	D	33	ASN

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Mol	Chain	Res	Type
2	D	40	THR
2	D	57	THR
2	D	59	GLN
2	D	81	SER
2	D	90	THR
2	D	96	ASN
2	D	107	LEU
2	D	126	ILE
2	D	136	ASN
2	D	138	ASN
2	D	190	SER
2	D	201	THR
2	D	211	ASN
2	D	262	GLN
2	D	271	ILE
1	E	8	ARG
1	E	23	THR
1	E	28	ASN
1	E	44	LYS
1	E	47	ARG
1	E	61	LYS
1	E	62	GLU
1	E	104	GLN
1	E	129	GLU
1	E	135	ARG
1	E	142	LEU
1	E	143	ILE
1	E	146	THR
1	E	173	SER
1	E	200	MET
1	E	205	GLU
2	F	4	LYS
2	F	5	THR
2	F	33	ASN
2	F	40	THR
2	F	57	THR
2	F	59	GLN
2	F	81	SER
2	F	90	THR
2	F	96	ASN
2	F	107	LEU
2	F	126	ILE

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Mol	Chain	Res	Type
2	F	136	ASN
2	F	138	ASN
2	F	190	SER
2	F	201	THR
2	F	211	ASN
2	F	226	THR
2	F	262	GLN
2	F	271	ILE
1	G	8	ARG
1	G	23	THR
1	G	28	ASN
1	G	44	LYS
1	G	47	ARG
1	G	61	LYS
1	G	62	GLU
1	G	104	GLN
1	G	129	GLU
1	G	135	ARG
1	G	142	LEU
1	G	143	ILE
1	G	146	THR
1	G	173	SER
1	G	200	MET
1	G	205	GLU
2	H	4	LYS
2	H	5	THR
2	H	33	ASN
2	H	40	THR
2	H	57	THR
2	H	59	GLN
2	H	81	SER
2	H	90	THR
2	H	96	ASN
2	H	107	LEU
2	H	126	ILE
2	H	136	ASN
2	H	138	ASN
2	H	190	SER
2	H	201	THR
2	H	211	ASN
2	H	226	THR
2	H	262	GLN

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Mol	Chain	Res	Type
2	H	271	ILE
1	I	8	ARG
1	I	28	ASN
1	I	43	VAL
1	I	44	LYS
1	I	47	ARG
1	I	62	GLU
1	I	85	MET
1	I	92	SER
1	I	135	ARG
1	I	183	SER
1	I	200	MET
2	J	33	ASN
2	J	43	PHE
2	J	57	THR
2	J	96	ASN
2	J	103	TRP
2	J	121	LYS
2	J	136	ASN
2	J	157	PRO
2	J	183	LEU
2	J	184	THR
2	J	211	ASN
2	J	215	PHE
1	K	8	ARG
1	K	28	ASN
1	K	43	VAL
1	K	44	LYS
1	K	47	ARG
1	K	62	GLU
1	K	85	MET
1	K	92	SER
1	K	135	ARG
1	K	176	LYS
1	K	183	SER
1	K	200	MET
2	L	33	ASN
2	L	43	PHE
2	L	57	THR
2	L	96	ASN
2	L	103	TRP
2	L	121	LYS

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Mol	Chain	Res	Type
2	L	136	ASN
2	L	157	PRO
2	L	183	LEU
2	L	184	THR
2	L	211	ASN
2	L	215	PHE
1	M	8	ARG
1	M	28	ASN
1	M	43	VAL
1	M	44	LYS
1	M	47	ARG
1	M	62	GLU
1	M	85	MET
1	M	92	SER
1	M	135	ARG
1	M	183	SER
1	M	200	MET
2	N	33	ASN
2	N	43	PHE
2	N	57	THR
2	N	96	ASN
2	N	103	TRP
2	N	121	LYS
2	N	136	ASN
2	N	157	PRO
2	N	183	LEU
2	N	184	THR
2	N	211	ASN
2	N	215	PHE
1	O	8	ARG
1	O	28	ASN
1	O	43	VAL
1	O	44	LYS
1	O	47	ARG
1	O	62	GLU
1	O	85	MET
1	O	92	SER
1	O	135	ARG
1	O	183	SER
1	O	200	MET
2	P	33	ASN
2	P	37	ASP

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Mol	Chain	Res	Type
2	P	43	PHE
2	P	57	THR
2	P	96	ASN
2	P	103	TRP
2	P	121	LYS
2	P	136	ASN
2	P	157	PRO
2	P	183	LEU
2	P	184	THR
2	P	211	ASN
2	P	215	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (181) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	28	ASN
1	A	72	ASN
1	A	74	GLN
1	A	86	ASN
1	A	126	GLN
1	A	184	ASN
2	B	32	GLN
2	B	33	ASN
2	B	41	GLN
2	B	70	ASN
2	B	136	ASN
2	B	138	ASN
2	B	206	ASN
2	B	211	ASN
2	B	219	GLN
2	B	224	GLN
2	B	228	ASN
2	B	255	ASN
2	B	262	GLN
2	B	279	GLN
1	C	15	GLN
1	C	28	ASN
1	C	72	ASN
1	C	74	GLN
1	C	86	ASN
1	C	126	GLN

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Mol	Chain	Res	Type
1	C	184	ASN
2	D	23	ASN
2	D	32	GLN
2	D	33	ASN
2	D	41	GLN
2	D	136	ASN
2	D	138	ASN
2	D	206	ASN
2	D	211	ASN
2	D	219	GLN
2	D	224	GLN
2	D	228	ASN
2	D	255	ASN
2	D	262	GLN
2	D	279	GLN
1	E	15	GLN
1	E	28	ASN
1	E	72	ASN
1	E	74	GLN
1	E	86	ASN
1	E	126	GLN
1	E	184	ASN
2	F	23	ASN
2	F	32	GLN
2	F	33	ASN
2	F	41	GLN
2	F	70	ASN
2	F	136	ASN
2	F	138	ASN
2	F	206	ASN
2	F	211	ASN
2	F	219	GLN
2	F	228	ASN
2	F	255	ASN
2	F	262	GLN
2	F	279	GLN
1	G	15	GLN
1	G	28	ASN
1	G	72	ASN
1	G	74	GLN
1	G	77	GLN
1	G	86	ASN

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Mol	Chain	Res	Type
1	G	126	GLN
1	G	184	ASN
2	H	32	GLN
2	H	33	ASN
2	H	41	GLN
2	H	136	ASN
2	H	138	ASN
2	H	206	ASN
2	H	211	ASN
2	H	219	GLN
2	H	224	GLN
2	H	228	ASN
2	H	255	ASN
2	H	262	GLN
2	H	279	GLN
1	I	28	ASN
1	I	72	ASN
1	I	74	GLN
1	I	77	GLN
1	I	86	ASN
1	I	101	ASN
1	I	104	GLN
1	I	126	GLN
1	I	184	ASN
2	J	19	ASN
2	J	33	ASN
2	J	70	ASN
2	J	96	ASN
2	J	136	ASN
2	J	138	ASN
2	J	151	ASN
2	J	191	GLN
2	J	211	ASN
2	J	224	GLN
2	J	228	ASN
2	J	255	ASN
2	J	262	GLN
2	J	269	GLN
2	J	279	GLN
1	K	28	ASN
1	K	72	ASN
1	K	74	GLN

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Mol	Chain	Res	Type
1	K	77	GLN
1	K	86	ASN
1	K	101	ASN
1	K	104	GLN
1	K	126	GLN
1	K	184	ASN
2	L	33	ASN
2	L	70	ASN
2	L	96	ASN
2	L	136	ASN
2	L	138	ASN
2	L	143	GLN
2	L	151	ASN
2	L	191	GLN
2	L	211	ASN
2	L	219	GLN
2	L	224	GLN
2	L	228	ASN
2	L	255	ASN
2	L	262	GLN
2	L	269	GLN
2	L	279	GLN
1	M	28	ASN
1	M	72	ASN
1	M	74	GLN
1	M	77	GLN
1	M	86	ASN
1	M	101	ASN
1	M	104	GLN
1	M	126	GLN
1	M	184	ASN
2	N	19	ASN
2	N	33	ASN
2	N	70	ASN
2	N	96	ASN
2	N	136	ASN
2	N	138	ASN
2	N	151	ASN
2	N	191	GLN
2	N	211	ASN
2	N	224	GLN
2	N	228	ASN

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Mol	Chain	Res	Type
2	N	255	ASN
2	N	262	GLN
2	N	269	GLN
2	N	279	GLN
1	O	28	ASN
1	O	72	ASN
1	O	74	GLN
1	O	77	GLN
1	O	86	ASN
1	O	101	ASN
1	O	104	GLN
1	O	126	GLN
1	O	184	ASN
2	P	33	ASN
2	P	70	ASN
2	P	96	ASN
2	P	136	ASN
2	P	138	ASN
2	P	151	ASN
2	P	191	GLN
2	P	211	ASN
2	P	219	GLN
2	P	224	GLN
2	P	228	ASN
2	P	255	ASN
2	P	262	GLN
2	P	269	GLN
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 monosaccharides 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	MAN	L	1504	-	12,12,12	0.30	0	17,17,17	0.44	0
3	MAN	F	1502	-	12,12,12	0.38	0	17,17,17	0.53	0
3	MAN	J	1605	-	12,12,12	0.30	0	17,17,17	0.35	0
3	MAN	N	1506	-	12,12,12	0.26	0	17,17,17	0.44	0
3	MAN	D	1601	-	12,12,12	0.35	0	17,17,17	0.49	0
3	MAN	P	1607	-	12,12,12	0.29	0	17,17,17	0.39	0
3	MAN	B	1500	-	12,12,12	0.39	0	17,17,17	0.37	0
3	MAN	H	1603	-	12,12,12	0.41	0	17,17,17	0.47	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	MAN	L	1504	-	-	0/2/22/22	0/1/1/1
3	MAN	F	1502	-	-	1/2/22/22	0/1/1/1
3	MAN	J	1605	-	-	0/2/22/22	0/1/1/1
3	MAN	N	1506	-	-	0/2/22/22	0/1/1/1
3	MAN	D	1601	-	-	1/2/22/22	0/1/1/1
3	MAN	P	1607	-	-	0/2/22/22	0/1/1/1
3	MAN	B	1500	-	-	2/2/22/22	0/1/1/1
3	MAN	H	1603	-	-	2/2/22/22	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	H	1603	MAN	C4-C5-C6-O6
3	B	1500	MAN	C4-C5-C6-O6
3	B	1500	MAN	O5-C5-C6-O6
3	H	1603	MAN	O5-C5-C6-O6
3	D	1601	MAN	C4-C5-C6-O6
3	F	1502	MAN	C4-C5-C6-O6

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L	1504	MAN	2	0
3	J	1605	MAN	4	0
3	N	1506	MAN	1	0
3	P	1607	MAN	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	205/205 (100%)	0.51	10 (4%)	29 20	20, 55, 108, 132	0
1	C	205/205 (100%)	0.48	12 (5%)	22 14	20, 57, 108, 130	0
1	E	205/205 (100%)	0.41	3 (1%)	73 68	20, 59, 108, 129	0
1	G	205/205 (100%)	0.47	16 (7%)	13 7	19, 58, 110, 132	0
1	I	205/205 (100%)	3.93	145 (70%)	0 0	20, 168, 190, 196	0
1	K	205/205 (100%)	4.77	171 (83%)	0 0	20, 171, 195, 198	0
1	M	205/205 (100%)	4.55	165 (80%)	0 0	20, 170, 193, 198	0
1	O	205/205 (100%)	3.98	148 (72%)	0 0	20, 168, 193, 198	0
2	B	279/279 (100%)	0.30	5 (1%)	68 61	17, 40, 79, 114	0
2	D	279/279 (100%)	0.30	7 (2%)	57 47	18, 41, 80, 116	0
2	F	279/279 (100%)	0.23	4 (1%)	75 70	18, 41, 83, 112	0
2	H	279/279 (100%)	0.28	5 (1%)	68 61	17, 42, 83, 114	0
2	J	279/279 (100%)	2.04	105 (37%)	0 0	51, 112, 192, 200	0
2	L	279/279 (100%)	2.36	124 (44%)	0 0	56, 113, 190, 200	0
2	N	279/279 (100%)	2.60	143 (51%)	0 0	53, 115, 193, 200	0
2	P	279/279 (100%)	2.14	109 (39%)	0 0	50, 112, 191, 200	0
All	All	3872/3872 (100%)	1.75	1172 (30%)	0 0	17, 85, 186, 200	0

All (1172) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	48	PHE	17.8
1	I	102	THR	16.6
1	M	102	THR	15.5
2	L	270	SER	15.4
1	K	95	LYS	15.0

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Mol	Chain	Res	Type	RSRZ
1	M	150	LEU	14.4
1	K	102	THR	14.1
1	K	65	LEU	13.8
1	M	183	SER	13.8
1	K	205	GLU	13.7
1	M	95	LYS	13.2
1	O	103	LEU	13.1
1	M	133	PHE	12.7
1	O	48	PHE	12.6
1	M	71	THR	12.5
1	K	127	ALA	12.5
1	K	69	ASP	12.5
1	O	71	THR	12.4
1	O	162	LEU	12.4
1	K	101	ASN	12.4
1	M	179	SER	12.1
2	L	202	ALA	12.0
2	N	179	VAL	11.9
2	J	256	TYR	11.9
1	I	127	ALA	11.9
1	I	95	LYS	11.8
1	O	67	ILE	11.7
1	I	205	GLU	11.7
1	K	174	THR	11.7
2	P	256	TYR	11.7
1	O	105	LEU	11.6
1	K	98	LEU	11.6
1	K	104	GLN	11.5
2	L	271	ILE	11.5
1	M	18	VAL	11.4
1	K	184	ASN	11.4
1	O	95	LYS	11.3
1	M	93	MET	11.3
1	K	48	PHE	11.3
1	K	170	MET	11.2
1	I	174	THR	11.1
2	P	215	PHE	10.9
1	O	184	ASN	10.8
1	M	105	LEU	10.8
2	P	218	ALA	10.7
1	K	150	LEU	10.7
2	N	168	VAL	10.7

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Mol	Chain	Res	Type	RSRZ
1	M	184	ASN	10.6
1	M	162	LEU	10.5
1	K	183	SER	10.5
1	K	18	VAL	10.4
1	M	55	PHE	10.4
1	K	135	ARG	10.3
1	M	201	THR	10.1
1	M	65	LEU	10.0
2	N	218	ALA	10.0
2	P	214	SER	9.9
2	J	268	VAL	9.8
2	J	215	PHE	9.8
1	O	201	THR	9.8
1	M	104	GLN	9.8
1	O	96	SER	9.8
1	O	104	GLN	9.7
2	P	263	VAL	9.7
1	K	93	MET	9.6
1	M	205	GLU	9.6
2	L	256	TYR	9.6
1	K	71	THR	9.5
1	M	135	ARG	9.4
2	L	168	VAL	9.4
2	J	217	PRO	9.4
1	I	67	ILE	9.4
2	N	271	ILE	9.4
1	M	174	THR	9.4
2	P	272	ILE	9.4
1	I	135	ARG	9.3
2	N	181	ILE	9.3
1	K	133	PHE	9.2
1	O	150	LEU	9.2
1	I	65	LEU	9.2
1	I	133	PHE	9.2
1	O	65	LEU	9.1
1	K	67	ILE	9.0
1	K	137	ALA	9.0
1	I	150	LEU	8.9
1	I	184	ASN	8.9
2	N	267	ASN	8.9
1	K	103	LEU	8.9
2	J	179	VAL	8.9

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Mol	Chain	Res	Type	RSRZ
1	I	69	ASP	8.8
1	M	101	ASN	8.8
1	K	94	ASP	8.8
2	J	213	ALA	8.8
1	O	94	ASP	8.8
2	N	175	TYR	8.8
1	K	185	ILE	8.7
1	M	47	ARG	8.7
1	K	55	PHE	8.7
2	P	217	PRO	8.6
1	K	201	THR	8.6
2	N	207	SER	8.6
2	P	179	VAL	8.6
2	P	202	ALA	8.6
1	K	20	LEU	8.6
2	L	268	VAL	8.5
1	I	101	ASN	8.5
1	K	106	ALA	8.5
2	L	223	VAL	8.5
2	N	268	VAL	8.5
1	I	131	LEU	8.4
1	K	128	ALA	8.4
1	O	102	THR	8.4
1	M	116	ARG	8.4
1	O	20	LEU	8.3
2	L	116	GLY	8.3
1	I	94	ASP	8.3
1	M	148	TYR	8.2
1	K	34	GLN	8.2
1	I	170	MET	8.2
1	M	185	ILE	8.1
1	O	174	THR	8.1
1	O	177	LEU	8.1
2	J	212	THR	8.0
1	I	128	ALA	8.0
2	P	211	ASN	8.0
1	I	162	LEU	8.0
1	K	162	LEU	8.0
1	M	137	ALA	8.0
1	I	48	PHE	8.0
1	O	127	ALA	7.9
1	K	157	ALA	7.9

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Mol	Chain	Res	Type	RSRZ
2	J	204	ALA	7.9
2	N	211	ASN	7.9
1	M	98	LEU	7.9
2	N	174	ASP	7.9
1	M	151	THR	7.9
2	N	272	ILE	7.9
1	O	183	SER	7.9
2	N	172	LEU	7.8
1	M	128	ALA	7.8
1	O	18	VAL	7.8
1	I	20	LEU	7.8
1	I	183	SER	7.7
1	K	173	SER	7.7
1	M	70	ALA	7.7
2	N	219	GLN	7.7
1	I	186	THR	7.7
2	N	270	SER	7.7
1	K	138	ASN	7.7
2	N	214	SER	7.6
1	K	37	VAL	7.6
2	P	271	ILE	7.6
1	O	55	PHE	7.6
2	N	260	GLY	7.6
1	M	67	ILE	7.5
2	N	256	TYR	7.5
1	K	19	GLN	7.5
1	M	87	VAL	7.5
2	P	213	ALA	7.5
1	M	155	LEU	7.5
1	I	201	THR	7.5
1	I	93	MET	7.4
1	K	68	LEU	7.4
1	M	178	PRO	7.4
1	O	69	ASP	7.4
1	O	136	SER	7.4
1	M	127	ALA	7.4
1	O	205	GLU	7.4
1	O	135	ARG	7.4
2	N	202	ALA	7.4
1	M	152	VAL	7.4
1	I	35	SER	7.3
1	K	200	MET	7.3

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Mol	Chain	Res	Type	RSRZ
1	K	105	LEU	7.3
1	M	94	ASP	7.3
2	N	261	GLY	7.3
1	I	98	LEU	7.3
2	P	212	THR	7.2
2	P	261	GLY	7.2
1	O	87	VAL	7.2
1	M	100	GLU	7.2
1	O	133	PHE	7.2
2	J	175	TYR	7.2
1	I	117	PRO	7.2
2	P	270	SER	7.1
1	K	92	SER	7.1
1	I	4	LEU	7.1
1	I	33	ILE	7.1
1	K	36	TRP	7.1
1	I	151	THR	7.1
2	L	222	GLY	7.0
1	M	52	PRO	7.0
1	O	35	SER	7.0
2	J	225	LEU	7.0
1	K	35	SER	7.0
1	I	157	ALA	7.0
1	M	91	PRO	6.9
1	M	11	TYR	6.9
2	L	182	PRO	6.9
1	K	74	GLN	6.9
1	O	98	LEU	6.8
2	P	268	VAL	6.8
1	M	51	THR	6.8
1	I	142	LEU	6.8
1	M	203	VAL	6.8
2	J	271	ILE	6.8
2	L	272	ILE	6.8
1	I	55	PHE	6.8
2	L	181	ILE	6.8
1	O	21	ALA	6.7
2	J	257	ALA	6.7
1	K	96	SER	6.7
2	N	20	VAL	6.7
2	P	216	SER	6.7
1	O	91	PRO	6.7

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Mol	Chain	Res	Type	RSRZ
1	K	9	VAL	6.6
1	O	50	VAL	6.6
1	I	148	TYR	6.6
1	K	4	LEU	6.6
1	O	7	THR	6.6
1	I	18	VAL	6.6
2	P	219	GLN	6.6
1	O	84	TRP	6.6
1	I	21	ALA	6.6
1	K	181	ALA	6.6
2	N	222	GLY	6.6
1	M	69	ASP	6.6
1	O	47	ARG	6.5
1	M	177	LEU	6.5
1	I	83	PHE	6.5
2	L	219	GLN	6.5
1	O	93	MET	6.5
1	I	104	GLN	6.5
2	N	215	PHE	6.4
2	N	266	GLY	6.4
2	P	225	LEU	6.4
1	O	128	ALA	6.4
2	L	232	ILE	6.4
2	J	223	VAL	6.4
2	J	218	ALA	6.4
2	P	221	VAL	6.4
1	O	179	SER	6.4
1	O	185	ILE	6.4
2	P	222	GLY	6.4
2	N	170	VAL	6.3
2	J	202	ALA	6.3
1	I	68	LEU	6.3
2	N	178	SER	6.3
2	J	22	VAL	6.3
2	L	213	ALA	6.3
1	O	52	PRO	6.3
1	I	136	SER	6.3
1	K	87	VAL	6.3
2	N	248	VAL	6.3
1	I	158	GLY	6.3
1	K	83	PHE	6.3
1	I	7	THR	6.3

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Mol	Chain	Res	Type	RSRZ
1	K	172	GLU	6.2
1	I	103	LEU	6.2
2	P	207	SER	6.2
2	P	181	ILE	6.2
1	M	12	PRO	6.2
1	O	158	GLY	6.2
1	O	33	ILE	6.2
1	I	85	MET	6.2
1	M	85	MET	6.2
1	M	167	VAL	6.2
1	O	11	TYR	6.1
2	N	264	THR	6.1
1	K	179	SER	6.1
1	M	106	ALA	6.1
2	L	267	ASN	6.1
1	M	33	ILE	6.1
1	I	56	ALA	6.1
1	K	152	VAL	6.1
1	O	198	PRO	6.1
1	I	172	GLU	6.1
2	N	169	THR	6.1
2	J	181	ILE	6.1
2	N	166	ARG	6.1
1	I	96	SER	6.0
1	C	178	PRO	6.0
1	K	38	GLU	6.0
1	I	71	THR	6.0
1	K	10	ILE	6.0
2	L	266	GLY	6.0
2	N	263	VAL	6.0
2	L	207	SER	6.0
2	L	119	ALA	6.0
1	I	70	ALA	5.9
2	L	225	LEU	5.9
2	L	230	THR	5.9
1	M	140	LEU	5.9
2	N	22	VAL	5.9
1	O	70	ALA	5.9
1	O	106	ALA	5.9
2	J	20	VAL	5.9
1	K	33	ILE	5.9
2	L	215	PHE	5.9

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Mol	Chain	Res	Type	RSRZ
1	O	85	MET	5.8
2	N	182	PRO	5.8
2	P	20	VAL	5.8
1	O	4	LEU	5.8
2	N	223	VAL	5.8
1	O	143	ILE	5.8
2	L	166	ARG	5.8
1	K	54	LEU	5.8
2	L	269	GLN	5.8
1	K	194	GLY	5.8
1	K	11	TYR	5.8
1	M	143	ILE	5.8
1	O	140	LEU	5.8
1	M	165	ALA	5.8
1	O	137	ALA	5.8
1	I	87	VAL	5.8
1	M	34	GLN	5.7
1	M	90	ILE	5.7
1	K	136	SER	5.7
2	L	67	VAL	5.7
1	K	177	LEU	5.7
1	I	19	GLN	5.7
1	M	66	ARG	5.7
1	I	84	TRP	5.7
2	J	261	GLY	5.7
2	L	120	ILE	5.7
2	J	214	SER	5.7
2	L	126	ILE	5.7
1	I	181	ALA	5.6
1	K	85	MET	5.6
1	K	70	ALA	5.6
1	K	142	LEU	5.6
1	M	160	ARG	5.6
1	O	142	LEU	5.6
1	M	29	SER	5.6
1	M	136	SER	5.6
1	M	103	LEU	5.6
1	O	178	PRO	5.6
1	I	11	TYR	5.6
2	N	213	ALA	5.6
1	K	114	TYR	5.5
1	K	90	ILE	5.5

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Mol	Chain	Res	Type	RSRZ
2	P	223	VAL	5.5
2	L	229	GLY	5.5
2	P	262	GLN	5.5
2	J	222	GLY	5.5
2	L	211	ASN	5.5
1	O	83	PHE	5.5
2	N	116	GLY	5.5
1	M	7	THR	5.5
2	N	212	THR	5.5
1	K	176	LYS	5.5
1	I	167	VAL	5.4
2	N	188	ALA	5.4
2	J	273	GLY	5.4
1	K	7	THR	5.4
2	L	210	THR	5.4
1	K	155	LEU	5.4
2	L	214	SER	5.4
2	P	166	ARG	5.4
2	P	210	THR	5.4
1	K	53	PRO	5.4
1	O	203	VAL	5.4
1	K	21	ALA	5.4
2	L	170	VAL	5.4
1	I	179	SER	5.3
2	L	53	THR	5.3
1	O	176	LYS	5.3
1	K	166	LEU	5.3
1	M	180	ASP	5.3
1	K	167	VAL	5.3
1	K	203	VAL	5.3
1	M	170	MET	5.3
1	O	34	GLN	5.3
2	L	260	GLY	5.3
1	I	177	LEU	5.3
2	L	273	GLY	5.3
2	P	170	VAL	5.3
1	M	200	MET	5.3
2	N	225	LEU	5.3
2	P	53	THR	5.2
1	O	92	SER	5.2
2	J	210	THR	5.2
1	K	16	LYS	5.2

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Mol	Chain	Res	Type	RSRZ
1	K	148	TYR	5.2
2	L	124	SER	5.2
2	J	260	GLY	5.2
1	I	200	MET	5.2
2	J	272	ILE	5.2
1	M	5	GLY	5.2
1	K	6	ALA	5.1
2	P	260	GLY	5.1
2	N	230	THR	5.1
1	K	116	ARG	5.1
1	I	198	PRO	5.1
1	O	9	VAL	5.1
1	K	29	SER	5.1
1	K	132	ARG	5.1
1	M	74	GLN	5.1
2	J	211	ASN	5.1
2	L	20	VAL	5.1
2	N	242	ALA	5.1
2	P	267	ASN	5.1
2	J	207	SER	5.1
1	K	186	THR	5.1
1	M	68	LEU	5.0
1	O	167	VAL	5.0
1	M	138	ASN	5.0
1	K	47	ARG	5.0
1	M	4	LEU	5.0
1	I	106	ALA	5.0
1	I	165	ALA	5.0
1	I	116	ARG	5.0
1	O	74	GLN	5.0
2	J	115	ALA	4.9
2	L	257	ALA	4.9
1	M	53	PRO	4.9
2	N	199	GLY	4.9
1	I	47	ARG	4.9
2	L	175	TYR	4.9
1	K	64	THR	4.9
1	O	131	LEU	4.9
2	P	174	ASP	4.9
1	M	171	GLY	4.9
2	P	266	GLY	4.9
1	O	148	TYR	4.9

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Mol	Chain	Res	Type	RSRZ
1	K	196	LEU	4.9
1	O	101	ASN	4.9
1	I	105	LEU	4.9
1	K	151	THR	4.9
1	O	152	VAL	4.8
1	K	31	TYR	4.8
2	J	148	ILE	4.8
2	J	15	GLY	4.8
1	O	53	PRO	4.8
1	I	54	LEU	4.8
1	M	96	SER	4.8
2	N	18	ALA	4.8
2	L	252	LEU	4.8
2	N	269	GLN	4.8
2	P	104	PRO	4.8
1	I	176	LYS	4.7
1	I	137	ALA	4.7
1	K	160	ARG	4.7
1	M	35	SER	4.7
2	P	22	VAL	4.7
2	N	233	PRO	4.7
1	M	172	GLU	4.7
1	K	117	PRO	4.7
1	K	120	LEU	4.7
2	P	28	VAL	4.7
1	M	129	GLU	4.6
2	N	24	LEU	4.6
1	I	10	ILE	4.6
2	L	148	ILE	4.6
2	N	177	GLY	4.6
1	K	100	GLU	4.6
1	M	92	SER	4.6
1	O	19	GLN	4.6
1	O	116	ARG	4.6
2	N	209	PHE	4.6
2	N	148	ILE	4.5
2	P	273	GLY	4.5
2	P	169	THR	4.5
1	M	117	PRO	4.5
1	K	99	THR	4.5
1	I	203	VAL	4.5
1	K	91	PRO	4.5

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Mol	Chain	Res	Type	RSRZ
1	O	97	LYS	4.5
2	N	257	ALA	4.5
1	K	126	GLN	4.5
2	J	124	SER	4.5
1	I	6	ALA	4.5
1	I	36	TRP	4.5
2	P	264	THR	4.5
1	K	158	GLY	4.5
1	M	173	SER	4.4
1	M	84	TRP	4.4
1	I	50	VAL	4.4
2	N	221	VAL	4.4
1	M	54	LEU	4.4
1	I	9	VAL	4.4
1	I	99	THR	4.4
2	L	218	ALA	4.4
2	L	191	GLN	4.4
1	K	109	SER	4.4
2	J	267	ASN	4.4
1	I	160	ARG	4.4
1	O	99	THR	4.4
1	M	9	VAL	4.4
1	O	187	TYR	4.4
2	P	115	ALA	4.4
2	J	219	GLN	4.4
1	K	66	ARG	4.4
1	K	178	PRO	4.4
1	O	180	ASP	4.4
1	M	83	PHE	4.4
1	K	57	MET	4.3
1	K	140	LEU	4.3
1	I	185	ILE	4.3
1	O	49	ILE	4.3
2	N	259	THR	4.3
1	M	145	PRO	4.3
2	N	53	THR	4.3
2	N	258	ARG	4.3
2	J	216	SER	4.3
1	M	17	GLN	4.3
2	P	168	VAL	4.3
1	M	157	ALA	4.3
2	L	18	ALA	4.3

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Mol	Chain	Res	Type	RSRZ
2	N	201	THR	4.3
2	L	185	VAL	4.3
1	M	99	THR	4.3
2	J	166	ARG	4.3
1	I	34	GLN	4.3
1	K	119	LYS	4.3
1	O	200	MET	4.3
1	M	79	ARG	4.3
1	G	178	PRO	4.3
1	O	170	MET	4.3
1	O	114	TYR	4.3
1	O	151	THR	4.3
2	L	150	ALA	4.3
1	K	58	LYS	4.3
2	N	228	ASN	4.3
2	N	197	LEU	4.2
1	M	45	ASP	4.2
1	G	177	LEU	4.2
1	I	132	ARG	4.2
2	L	250	LEU	4.2
1	K	159	THR	4.2
2	P	148	ILE	4.2
1	I	122	LEU	4.2
1	K	171	GLY	4.2
1	M	36	TRP	4.2
1	K	121	ALA	4.2
2	L	115	ALA	4.2
1	I	143	ILE	4.2
2	L	33	ASN	4.2
1	M	121	ALA	4.2
1	O	122	LEU	4.1
1	O	172	GLU	4.1
2	L	104	PRO	4.1
2	L	217	PRO	4.1
2	P	191	GLN	4.1
2	L	212	THR	4.1
2	N	217	PRO	4.1
1	K	122	LEU	4.1
2	N	234	ALA	4.1
2	L	278	TYR	4.1
1	K	202	GLY	4.1
1	I	120	LEU	4.1

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Mol	Chain	Res	Type	RSRZ
2	N	195	TYR	4.1
2	J	30	VAL	4.1
1	M	186	THR	4.1
2	N	176	PRO	4.1
1	K	56	ALA	4.1
2	L	129	LEU	4.0
1	I	31	TYR	4.0
2	J	150	ALA	4.0
2	N	229	GLY	4.0
1	I	152	VAL	4.0
1	M	6	ALA	4.0
1	M	120	LEU	4.0
2	L	221	VAL	4.0
1	M	31	TYR	4.0
2	N	42	ILE	4.0
1	O	165	ALA	4.0
1	M	158	GLY	4.0
2	L	28	VAL	4.0
2	J	279	GLN	4.0
2	P	230	THR	4.0
1	I	121	ALA	4.0
1	I	114	TYR	4.0
2	L	15	GLY	4.0
1	K	180	ASP	4.0
2	N	124	SER	4.0
1	K	198	PRO	4.0
2	P	177	GLY	3.9
2	P	172	LEU	3.9
2	J	232	ILE	3.9
1	I	166	LEU	3.9
1	I	8	ARG	3.9
1	K	189	THR	3.9
2	B	172	LEU	3.9
1	K	84	TRP	3.9
1	K	143	ILE	3.9
1	I	173	SER	3.9
1	M	109	SER	3.9
1	O	186	THR	3.9
2	L	245	THR	3.9
1	I	187	TYR	3.9
2	N	262	GLN	3.9
1	O	90	ILE	3.9

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Mol	Chain	Res	Type	RSRZ
2	H	215	PHE	3.9
1	K	22	VAL	3.9
1	K	82	LEU	3.9
1	K	79	ARG	3.9
2	N	278	TYR	3.9
1	I	37	VAL	3.9
2	N	210	THR	3.9
2	L	174	ASP	3.9
2	P	257	ALA	3.8
1	K	187	TYR	3.8
1	O	72	ASN	3.8
1	I	22	VAL	3.8
2	F	172	LEU	3.8
2	J	240	LEU	3.8
2	N	243	VAL	3.8
1	K	192	ASP	3.8
2	J	258	ARG	3.8
1	K	49	ILE	3.8
1	K	199	LYS	3.8
1	M	166	LEU	3.8
2	J	270	SER	3.8
1	I	161	VAL	3.8
2	P	36	VAL	3.8
1	M	199	LYS	3.8
2	P	175	TYR	3.8
2	N	191	GLN	3.8
2	N	254	ALA	3.8
1	M	37	VAL	3.8
1	M	189	THR	3.8
1	O	121	ALA	3.8
2	L	24	LEU	3.8
2	L	93	VAL	3.8
1	K	123	PRO	3.8
1	O	57	MET	3.8
2	L	42	ILE	3.7
2	J	169	THR	3.7
2	N	239	SER	3.7
2	J	263	VAL	3.7
1	M	168	PRO	3.7
1	M	176	LYS	3.7
2	J	137	TYR	3.7
2	N	232	ILE	3.7

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Mol	Chain	Res	Type	RSRZ
2	N	36	VAL	3.7
2	N	249	SER	3.7
2	J	255	ASN	3.7
2	N	112	VAL	3.7
2	N	216	SER	3.7
1	O	8	ARG	3.7
1	O	22	VAL	3.7
2	J	53	THR	3.7
1	K	24	ASN	3.7
2	N	137	TYR	3.7
1	O	58	LYS	3.7
1	I	100	GLU	3.7
2	N	255	ASN	3.7
1	M	187	TYR	3.7
1	K	129	GLU	3.7
2	N	115	ALA	3.6
1	A	161	VAL	3.6
1	M	10	ILE	3.6
2	N	200	THR	3.6
2	L	224	GLN	3.6
1	M	132	ARG	3.6
2	N	250	LEU	3.6
1	I	138	ASN	3.6
2	J	254	ALA	3.6
2	L	146	TRP	3.6
1	I	74	GLN	3.6
1	M	131	LEU	3.6
1	M	21	ALA	3.6
1	O	51	THR	3.6
1	M	27	GLU	3.6
2	J	67	VAL	3.6
1	O	109	SER	3.6
2	P	196	TYR	3.6
1	K	190	ILE	3.6
1	I	115	TYR	3.6
1	M	122	LEU	3.6
2	J	252	LEU	3.6
2	P	193	LEU	3.6
2	P	255	ASN	3.6
2	J	118	VAL	3.6
2	P	204	ALA	3.5
1	O	64	THR	3.5

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Mol	Chain	Res	Type	RSRZ
2	L	244	GLY	3.5
2	F	215	PHE	3.5
1	A	93	MET	3.5
1	O	27	GLU	3.5
1	O	100	GLU	3.5
1	I	16	LYS	3.5
1	M	16	LYS	3.5
2	P	242	ALA	3.5
1	M	2	VAL	3.5
1	M	49	ILE	3.5
2	P	120	ILE	3.5
2	N	33	ASN	3.5
1	M	20	LEU	3.5
2	J	174	ASP	3.5
1	O	23	THR	3.5
2	P	33	ASN	3.5
1	K	17	GLN	3.5
2	L	106	ALA	3.5
1	K	88	LYS	3.5
2	N	16	GLY	3.5
2	N	203	ASP	3.5
2	P	232	ILE	3.5
1	O	66	ARG	3.5
2	J	278	TYR	3.5
2	N	189	LYS	3.5
2	D	165	ALA	3.5
1	M	130	LYS	3.4
1	I	159	THR	3.4
1	O	155	LEU	3.4
2	D	172	LEU	3.4
1	M	64	THR	3.4
1	K	73	ASN	3.4
2	L	255	ASN	3.4
1	I	129	GLU	3.4
1	M	190	ILE	3.4
1	O	38	GLU	3.4
1	I	64	THR	3.4
2	J	168	VAL	3.4
2	P	250	LEU	3.4
1	I	38	GLU	3.4
1	M	164	ASN	3.4
1	O	6	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
2	J	157	PRO	3.4
1	K	112	LYS	3.4
2	J	191	GLN	3.4
1	O	89	ALA	3.4
2	P	186	TYR	3.4
1	M	196	LEU	3.4
2	H	172	LEU	3.4
1	O	189	THR	3.4
2	N	244	GLY	3.4
1	O	199	LYS	3.4
1	I	32	LEU	3.4
2	N	245	THR	3.3
1	I	125	ASP	3.3
2	L	54	ASP	3.3
1	O	166	LEU	3.3
1	M	192	ASP	3.3
2	N	231	ILE	3.3
1	O	160	ARG	3.3
1	K	161	VAL	3.3
2	L	167	ASP	3.3
1	O	68	LEU	3.3
2	P	195	TYR	3.3
1	I	180	ASP	3.3
1	M	163	GLU	3.3
2	J	120	ILE	3.3
1	O	157	ALA	3.3
2	N	15	GLY	3.3
1	A	178	PRO	3.3
1	O	32	LEU	3.3
2	J	178	SER	3.3
2	L	80	SER	3.3
2	L	248	VAL	3.3
1	A	177	LEU	3.3
1	I	23	THR	3.3
1	I	109	SER	3.3
2	L	179	VAL	3.3
2	N	237	THR	3.3
2	N	123	GLY	3.3
2	P	258	ARG	3.3
2	L	22	VAL	3.2
1	K	169	PRO	3.2
1	O	138	ASN	3.2

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Mol	Chain	Res	Type	RSRZ
2	J	104	PRO	3.2
1	K	78	ASP	3.2
2	L	264	THR	3.2
1	M	198	PRO	3.2
1	I	30	THR	3.2
1	M	50	VAL	3.2
1	M	119	LYS	3.2
2	L	204	ALA	3.2
1	I	79	ARG	3.2
1	I	199	LYS	3.2
1	O	17	GLN	3.2
1	I	2	VAL	3.2
2	J	28	VAL	3.2
1	I	196	LEU	3.2
1	K	139	SER	3.2
1	O	119	LYS	3.2
1	M	125	ASP	3.1
1	O	107	ILE	3.1
2	P	137	TYR	3.1
1	I	92	SER	3.1
2	J	116	GLY	3.1
1	O	54	LEU	3.1
1	I	189	THR	3.1
2	N	180	PRO	3.1
1	K	8	ARG	3.1
2	J	170	VAL	3.1
2	L	187	CYS	3.1
1	O	194	GLY	3.1
1	M	112	LYS	3.1
2	L	183	LEU	3.1
2	J	186	TYR	3.1
1	M	38	GLU	3.1
2	N	265	ALA	3.1
2	N	167	ASP	3.1
1	K	134	ARG	3.1
2	N	205	GLY	3.1
2	N	277	VAL	3.1
2	H	165	ALA	3.1
2	N	187	CYS	3.1
2	L	137	TYR	3.1
2	P	116	GLY	3.1
1	K	2	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
2	J	24	LEU	3.1
2	N	183	LEU	3.1
1	K	168	PRO	3.1
1	M	15	GLN	3.1
2	N	146	TRP	3.0
1	C	72	ASN	3.0
2	J	236	ASN	3.0
2	L	263	VAL	3.0
2	P	109	LEU	3.0
1	I	156	ASN	3.0
2	J	230	THR	3.0
1	K	113	LEU	3.0
2	N	279	GLN	3.0
2	N	104	PRO	3.0
1	I	66	ARG	3.0
1	M	175	VAL	3.0
2	P	234	ALA	3.0
1	M	202	GLY	3.0
2	J	126	ILE	3.0
2	N	108	TYR	3.0
2	P	54	ASP	3.0
1	I	178	PRO	3.0
1	M	8	ARG	3.0
2	L	144	PHE	3.0
1	M	30	THR	3.0
2	N	163	VAL	3.0
1	E	178	PRO	3.0
2	N	52	ILE	3.0
2	N	120	ILE	3.0
1	C	160	ARG	3.0
1	O	196	LEU	3.0
1	M	114	TYR	3.0
2	P	178	SER	3.0
2	P	30	VAL	3.0
1	I	81	SER	2.9
2	D	215	PHE	2.9
2	L	216	SER	2.9
2	L	276	PHE	2.9
2	J	250	LEU	2.9
2	L	163	VAL	2.9
2	N	193	LEU	2.9
1	I	53	PRO	2.9

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Mol	Chain	Res	Type	RSRZ
2	L	279	GLN	2.9
1	C	132	ARG	2.9
2	P	199	GLY	2.9
1	M	161	VAL	2.9
2	N	173	PRO	2.9
1	K	111	ILE	2.9
1	G	176	LYS	2.9
1	K	5	GLY	2.9
1	M	19	GLN	2.9
2	L	169	THR	2.9
2	P	67	VAL	2.9
2	P	182	PRO	2.9
2	P	265	ALA	2.9
2	J	146	TRP	2.9
1	O	78	ASP	2.9
1	I	140	LEU	2.9
1	K	51	THR	2.9
1	M	22	VAL	2.9
1	I	58	LYS	2.9
2	J	33	ASN	2.9
1	M	111	ILE	2.9
2	H	261	GLY	2.9
2	N	14	GLY	2.9
2	N	276	PHE	2.9
1	I	119	LYS	2.9
2	L	102	PRO	2.9
1	O	173	SER	2.9
1	K	141	THR	2.9
2	P	236	ASN	2.9
2	J	47	ASP	2.8
2	J	119	ALA	2.8
1	M	149	TYR	2.8
2	L	68	LEU	2.8
2	D	171	THR	2.8
2	L	123	GLY	2.8
1	A	140	LEU	2.8
1	M	126	GLN	2.8
1	O	197	THR	2.8
2	L	277	VAL	2.8
2	P	163	VAL	2.8
2	D	175	TYR	2.8
2	J	80	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	O	79	ARG	2.8
1	A	176	LYS	2.8
1	I	82	LEU	2.8
2	P	259	THR	2.8
2	L	186	TYR	2.8
2	L	262	GLN	2.8
1	K	30	THR	2.8
2	N	157	PRO	2.8
1	M	62	GLU	2.8
1	M	32	LEU	2.8
2	B	215	PHE	2.8
2	P	126	ILE	2.8
2	L	258	ARG	2.8
2	J	195	TYR	2.8
2	H	175	TYR	2.7
1	G	135	ARG	2.7
1	M	73	ASN	2.7
1	O	63	ASN	2.7
2	L	61	GLY	2.7
2	J	93	VAL	2.7
1	M	97	LYS	2.7
1	G	158	GLY	2.7
1	O	202	GLY	2.7
2	N	1	PHE	2.7
2	L	208	ILE	2.7
1	O	60	LYS	2.7
1	K	145	PRO	2.7
1	O	175	VAL	2.7
1	K	14	GLY	2.7
2	N	171	THR	2.7
1	O	26	ASP	2.7
2	P	18	ALA	2.7
2	N	206	ASN	2.7
2	P	24	LEU	2.7
1	O	31	TYR	2.7
2	L	47	ASP	2.7
2	J	221	VAL	2.7
1	I	72	ASN	2.7
1	I	113	LEU	2.7
2	J	183	LEU	2.7
1	K	175	VAL	2.7
2	L	36	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
2	N	251	GLY	2.7
2	N	252	LEU	2.7
2	F	175	TYR	2.7
2	N	126	ILE	2.7
2	J	220	GLY	2.6
1	I	27	GLU	2.6
1	E	176	LYS	2.6
1	O	29	SER	2.6
1	I	171	GLY	2.6
2	N	238	VAL	2.6
1	O	112	LYS	2.6
2	L	172	LEU	2.6
1	K	12	PRO	2.6
1	M	159	THR	2.6
2	L	195	TYR	2.6
1	O	10	ILE	2.6
1	O	73	ASN	2.6
2	J	163	VAL	2.6
2	N	185	VAL	2.6
2	P	93	VAL	2.6
2	L	209	PHE	2.6
2	N	54	ASP	2.6
1	I	107	ILE	2.6
1	C	1	GLY	2.6
1	M	58	LYS	2.6
2	J	266	GLY	2.6
2	N	21	TYR	2.6
2	P	176	PRO	2.6
1	K	15	GLN	2.6
2	J	248	VAL	2.6
1	I	155	LEU	2.6
1	K	204	MET	2.6
2	L	52	ILE	2.6
2	N	204	ALA	2.6
2	P	269	GLN	2.6
1	I	134	ARG	2.6
2	L	228	ASN	2.5
2	N	149	TYR	2.5
1	M	142	LEU	2.5
2	L	261	GLY	2.5
1	K	63	ASN	2.5
1	I	90	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	I	46	GLY	2.5
2	P	240	LEU	2.5
1	A	132	ARG	2.5
2	J	182	PRO	2.5
1	M	56	ALA	2.5
1	I	89	ALA	2.5
1	M	23	THR	2.5
1	O	56	ALA	2.5
2	N	150	ALA	2.5
1	O	161	VAL	2.5
2	P	185	VAL	2.5
2	P	1	PHE	2.5
2	P	249	SER	2.5
1	K	61	LYS	2.5
1	M	134	ARG	2.5
2	L	157	PRO	2.5
1	G	140	LEU	2.5
1	K	149	TYR	2.5
1	I	97	LYS	2.5
1	O	132	ARG	2.5
1	I	194	GLY	2.5
2	J	42	ILE	2.5
2	L	95	TYR	2.5
1	K	23	THR	2.5
1	I	49	ILE	2.5
1	K	60	LYS	2.5
2	L	125	LEU	2.5
1	M	193	TYR	2.5
2	P	108	TYR	2.5
1	M	72	ASN	2.5
1	C	182	GLY	2.4
2	N	50	GLU	2.4
1	O	117	PRO	2.4
2	F	165	ALA	2.4
2	J	264	THR	2.4
1	G	155	LEU	2.4
1	I	1	GLY	2.4
2	N	7	ASN	2.4
2	P	47	ASP	2.4
1	M	57	MET	2.4
1	I	3	ALA	2.4
2	P	171	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	K	131	LEU	2.4
2	J	125	LEU	2.4
2	J	193	LEU	2.4
1	M	86	ASN	2.4
2	P	278	TYR	2.4
1	K	52	PRO	2.4
2	L	49	PRO	2.4
1	K	118	ALA	2.4
1	O	36	TRP	2.4
2	J	269	GLN	2.4
2	N	274	VAL	2.4
1	K	1	GLY	2.4
2	L	16	GLY	2.4
1	C	135	ARG	2.4
1	M	60	LYS	2.4
1	O	159	THR	2.4
1	M	107	ILE	2.4
2	J	7	ASN	2.4
2	P	248	VAL	2.4
1	O	62	GLU	2.4
1	I	91	PRO	2.4
2	J	102	PRO	2.4
2	J	18	ALA	2.4
2	N	10	ALA	2.4
2	P	164	SER	2.4
2	J	11	ILE	2.4
1	K	27	GLU	2.4
1	G	162	LEU	2.4
2	L	109	LEU	2.4
1	M	26	ASP	2.4
1	G	72	ASN	2.4
1	M	24	ASN	2.4
1	M	44	LYS	2.4
2	N	28	VAL	2.4
1	M	3	ALA	2.3
1	M	78	ASP	2.3
1	O	61	LYS	2.3
2	L	231	ILE	2.3
2	J	1	PHE	2.3
2	J	176	PRO	2.3
2	P	173	PRO	2.3
1	G	1	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
2	J	229	GLY	2.3
2	D	166	ARG	2.3
1	O	204	MET	2.3
2	J	167	ASP	2.3
1	M	82	LEU	2.3
2	N	240	LEU	2.3
1	I	175	VAL	2.3
1	K	50	VAL	2.3
1	K	25	ASN	2.3
1	K	97	LYS	2.3
2	L	127	ALA	2.3
2	P	119	ALA	2.3
1	K	163	GLU	2.3
2	L	118	VAL	2.3
1	K	130	LYS	2.3
1	G	167	VAL	2.3
1	O	126	GLN	2.2
2	N	190	SER	2.2
1	K	62	GLU	2.2
1	K	3	ALA	2.2
2	J	16	GLY	2.2
2	N	117	GLY	2.2
1	O	113	LEU	2.2
1	O	123	PRO	2.2
1	O	3	ALA	2.2
2	L	162	ASP	2.2
1	K	124	PRO	2.2
1	O	75	LEU	2.2
2	L	240	LEU	2.2
1	K	89	ALA	2.2
2	N	48	TYR	2.2
1	G	183	SER	2.2
2	L	176	PRO	2.2
2	P	183	LEU	2.2
2	N	119	ALA	2.2
1	I	51	THR	2.2
1	M	14	GLY	2.2
2	P	220	GLY	2.2
1	I	108	ILE	2.2
2	P	252	LEU	2.2
2	L	103	TRP	2.2
2	J	54	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
2	N	47	ASP	2.2
2	P	209	PHE	2.2
1	I	190	ILE	2.2
2	N	27	VAL	2.2
1	K	32	LEU	2.2
1	K	153	THR	2.2
2	P	245	THR	2.2
1	A	179	SER	2.2
2	B	164	SER	2.2
2	L	76	LYS	2.2
2	J	203	ASP	2.2
1	M	118	ALA	2.2
2	B	165	ALA	2.2
2	L	254	ALA	2.2
2	P	103	TRP	2.2
2	N	164	SER	2.1
2	N	246	SER	2.1
2	J	172	LEU	2.1
1	I	202	GLY	2.1
1	C	93	MET	2.1
1	G	205	GLU	2.1
2	P	206	ASN	2.1
1	I	17	GLN	2.1
2	J	185	VAL	2.1
2	J	208	ILE	2.1
2	N	30	VAL	2.1
1	C	176	LYS	2.1
2	B	175	TYR	2.1
1	G	98	LEU	2.1
2	P	131	LEU	2.1
2	J	171	THR	2.1
2	P	279	GLN	2.1
1	C	177	LEU	2.1
1	K	108	ILE	2.1
1	O	182	GLY	2.1
2	N	67	VAL	2.1
2	P	52	ILE	2.1
2	L	173	PRO	2.1
2	P	253	THR	2.1
1	C	179	SER	2.1
2	D	167	ASP	2.1
2	L	37	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
2	N	37	ASP	2.1
1	E	140	LEU	2.1
1	M	123	PRO	2.1
2	L	48	TYR	2.1
2	P	254	ALA	2.1
1	O	25	ASN	2.1
2	J	127	ALA	2.1
2	P	165	ALA	2.1
1	A	135	ARG	2.1
1	M	204	MET	2.1
1	O	153	THR	2.1
1	C	129	GLU	2.1
2	P	14	GLY	2.1
2	L	56	VAL	2.1
1	O	12	PRO	2.1
2	P	48	TYR	2.1
1	A	157	ALA	2.1
2	N	247	ALA	2.1
1	G	132	ARG	2.1
1	I	73	ASN	2.1
1	M	139	SER	2.1
2	N	125	LEU	2.0
1	K	110	ARG	2.0
1	O	134	ARG	2.0
1	G	159	THR	2.0
1	O	139	SER	2.0
2	N	129	LEU	2.0
1	K	72	ASN	2.0
2	L	117	GLY	2.0
2	L	60	ARG	2.0
2	J	162	ASP	2.0
2	J	234	ALA	2.0
2	L	203	ASP	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	MAN	L	1504	12/12	0.81	0.23	96,99,103,106	0
3	MAN	J	1605	12/12	0.88	0.25	96,100,105,106	0
3	MAN	P	1607	12/12	0.90	0.26	110,112,116,117	0
3	MAN	N	1506	12/12	0.91	0.18	90,94,100,101	0
3	MAN	F	1502	12/12	0.95	0.19	29,35,41,41	0
3	MAN	H	1603	12/12	0.96	0.17	28,34,39,39	0
3	MAN	B	1500	12/12	0.97	0.15	30,35,39,39	0
3	MAN	D	1601	12/12	0.98	0.19	28,36,41,41	0

6.5 Other polymers [i](#)

There are no such residues in this entry.