



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:34 PM GMT

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
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

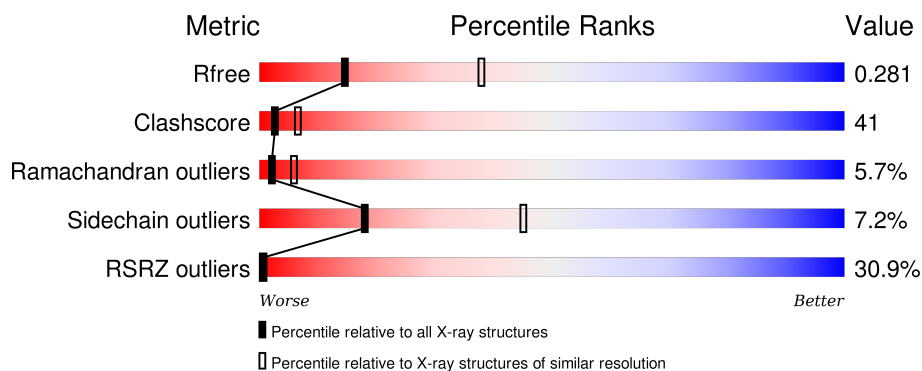
1 Overall quality at a glance

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}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (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. 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>45%</div> <div>47%</div> <div>8%</div> </div>
1	C	205	<div> <div>6%</div> <div>45%</div> <div>46%</div> <div>8%</div> </div>
1	E	205	<div> <div>2%</div> <div>46%</div> <div>46%</div> <div>8%</div> </div>
1	G	205	<div> <div>9%</div> <div>43%</div> <div>49%</div> <div>8%</div> </div>
1	I	205	<div> <div>72%</div> <div>38%</div> <div>55%</div> <div>6%</div> </div>

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Mol	Chain	Length	Quality of chain
1	K	205	
1	M	205	
1	O	205	
2	B	279	
2	D	279	
2	F	279	
2	H	279	
2	J	279	
2	L	279	
2	N	279	
2	P	279	

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			

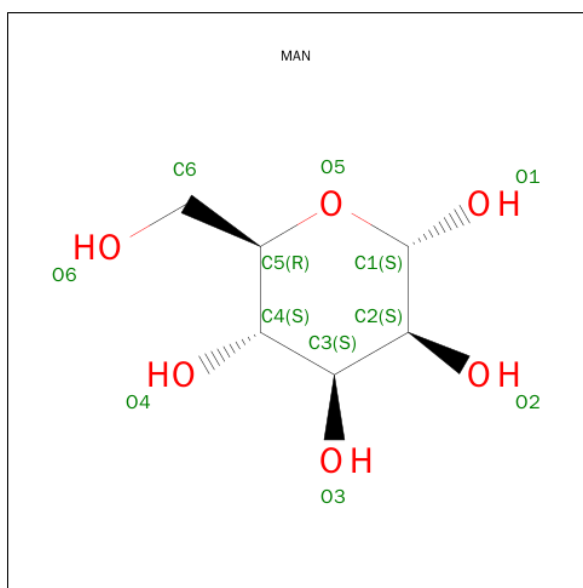
There are 8 discrepancies between the modelled and reference sequences:

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 SUGAR (ALPHA-D-MANNOSE) (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	L	1	Total	C	O	0	0
			12	6	6		
3	J	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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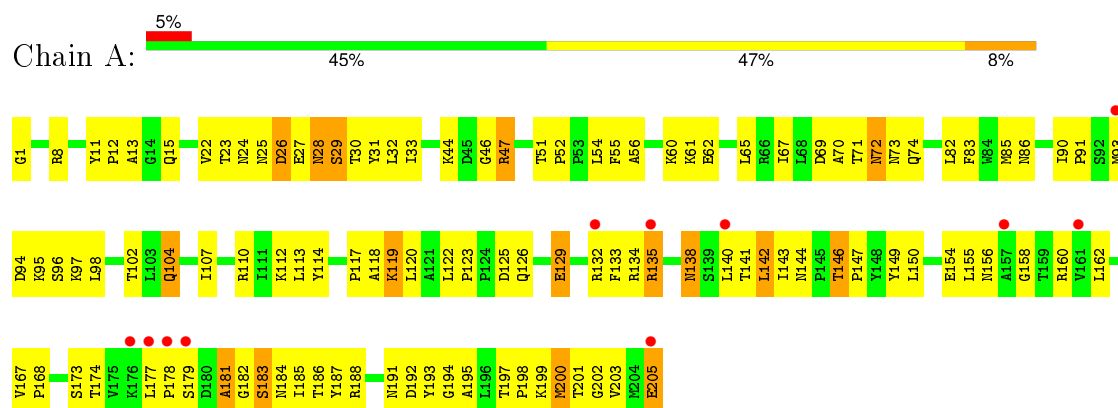
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	P	7	Total	O	0	0
			7	7		

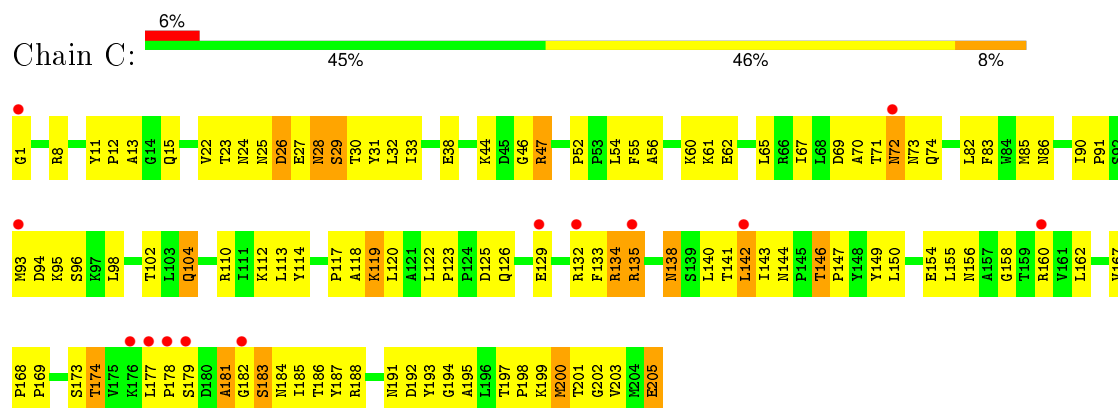
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($\text{RSRZ} > 2$). 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.

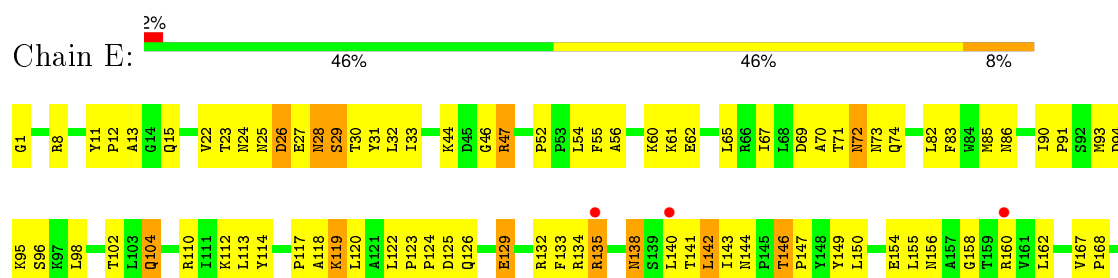
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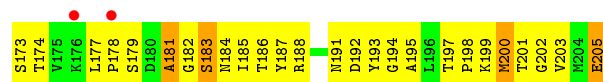


• Molecule 1: CHAPERONE PROTEIN FIMC

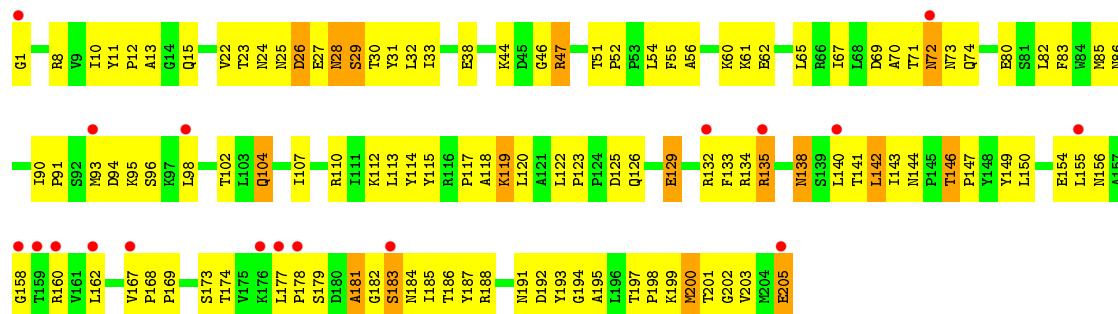


• Molecule 1: CHAPERONE PROTEIN FIMC

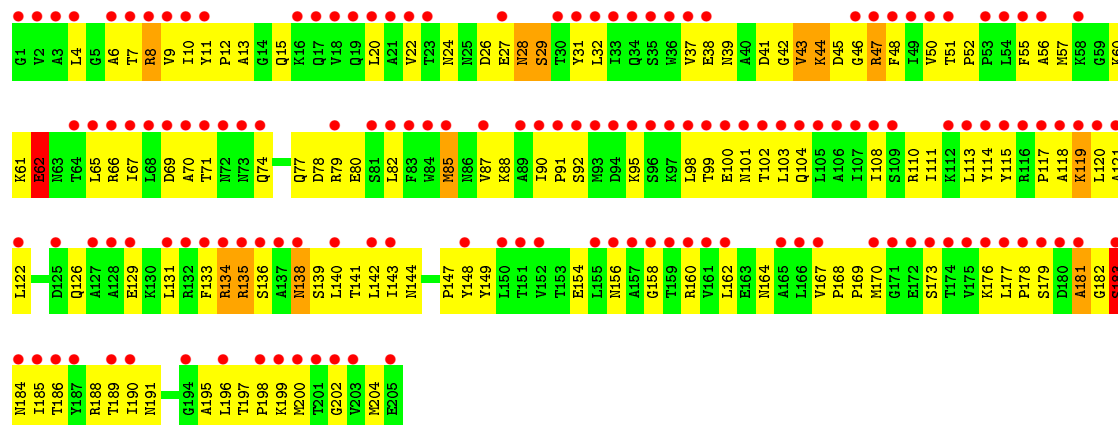




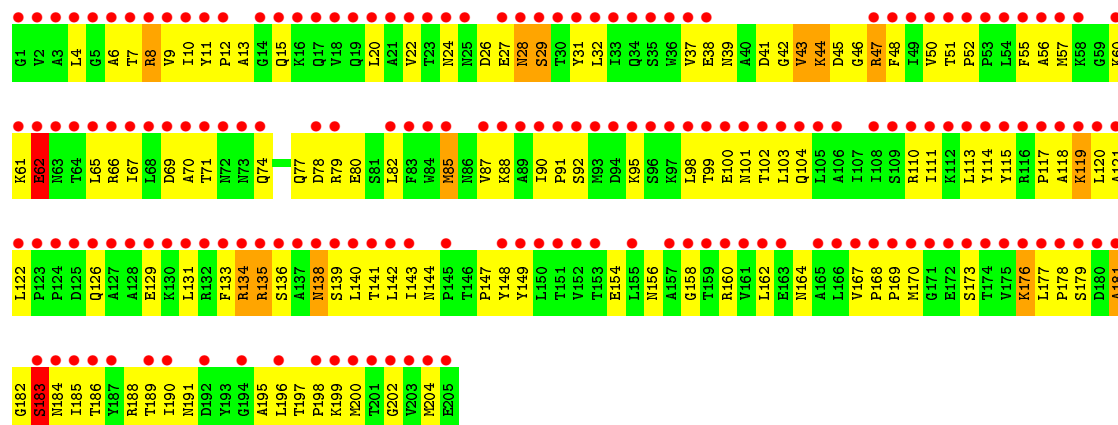
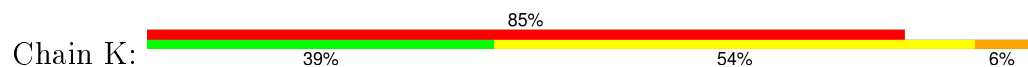
• Molecule 1: CHAPERONE PROTEIN FIMC



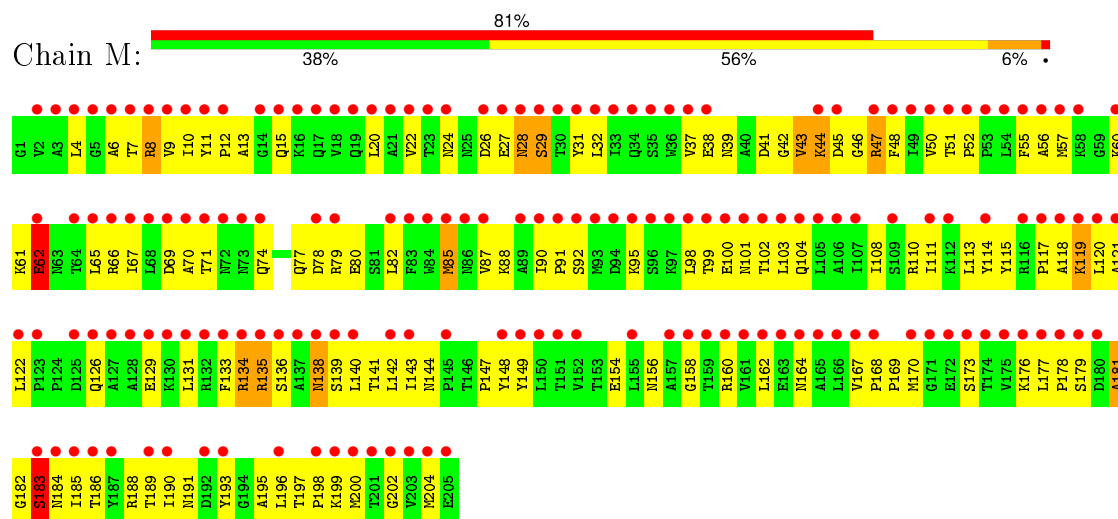
• Molecule 1: CHAPERONE PROTEIN FIMC



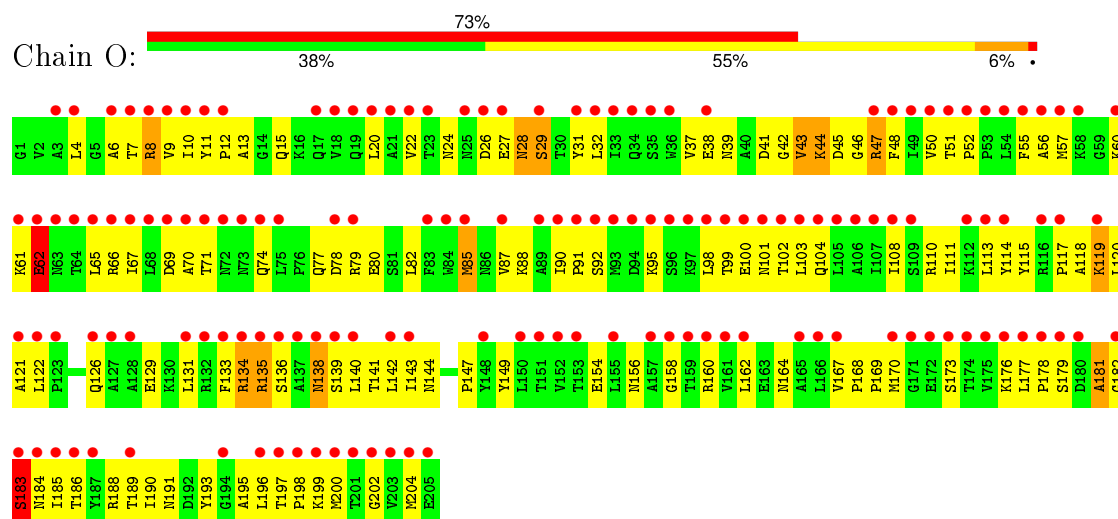
• Molecule 1: CHAPERONE PROTEIN FIMC



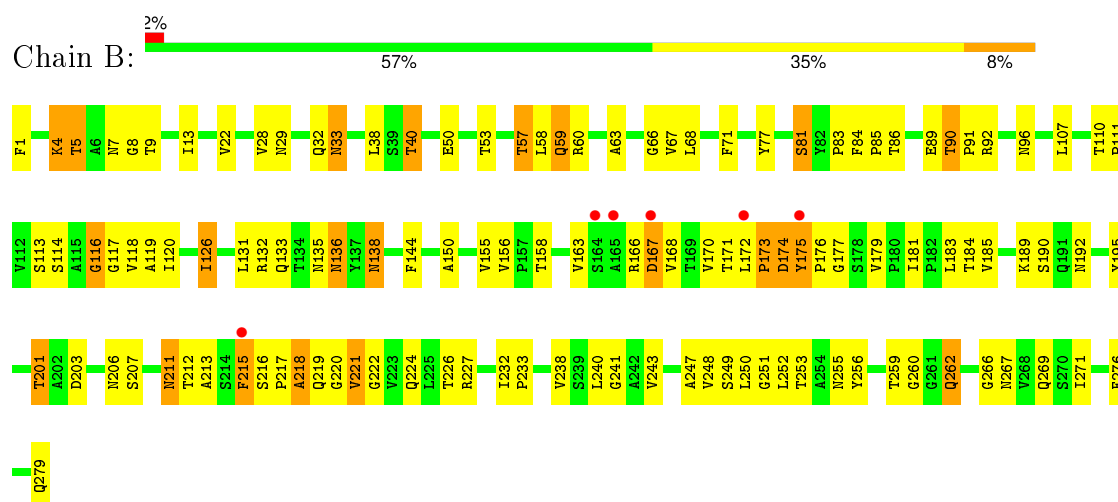
- Molecule 1: CHAPERONE PROTEIN FIMC



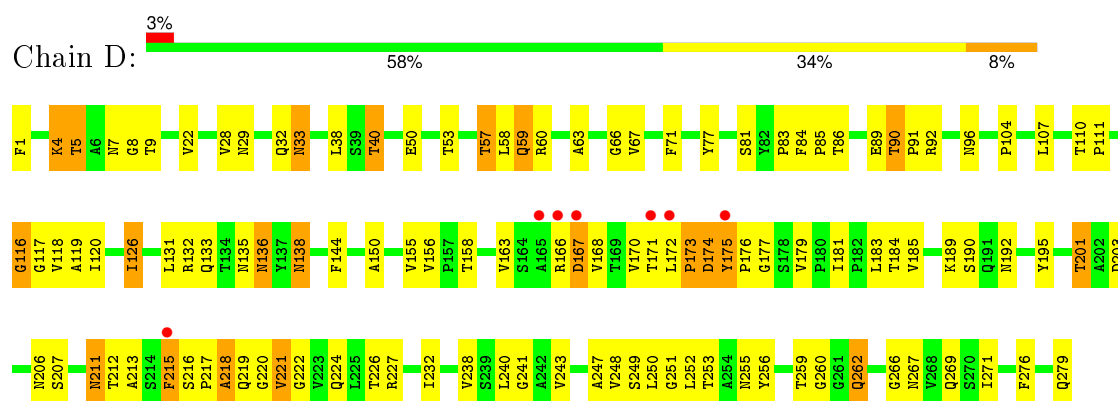
- Molecule 1: CHAPERONE PROTEIN FIMC



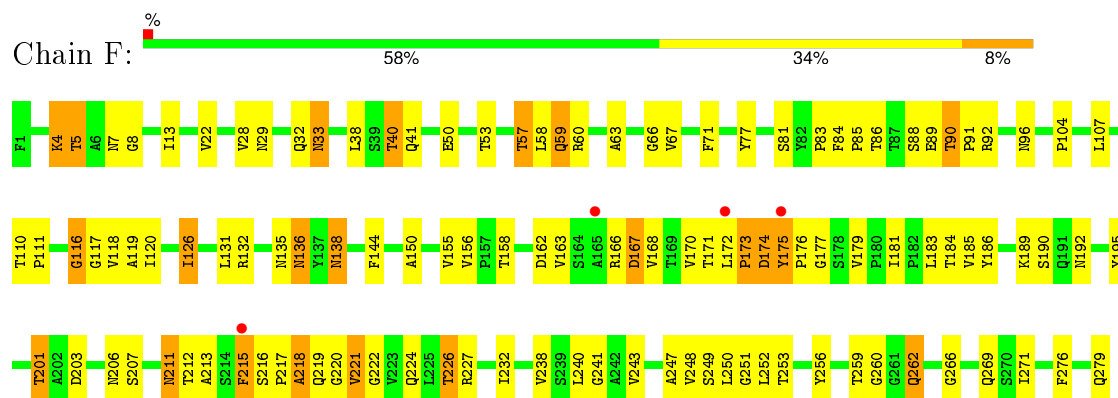
- Molecule 2: FIMH PROTEIN



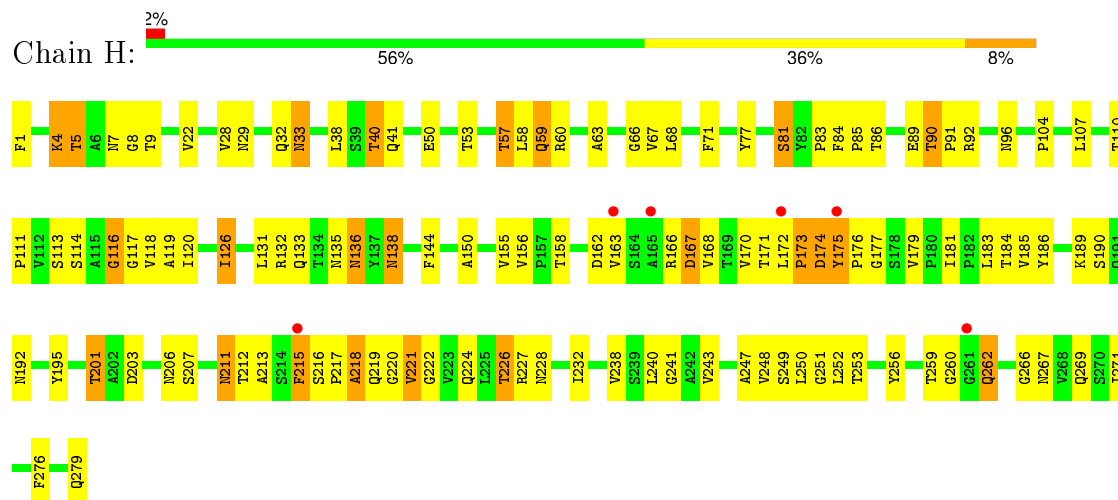
- Molecule 2: FIMH PROTEIN



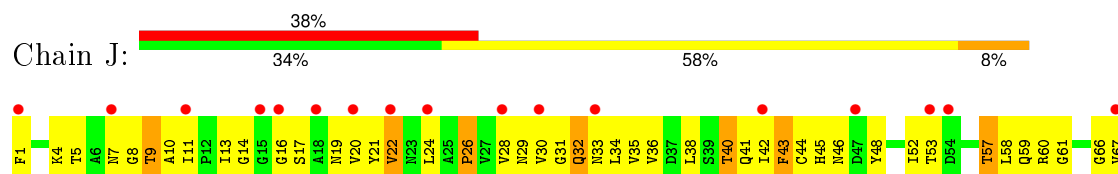
- Molecule 2: FIMH PROTEIN

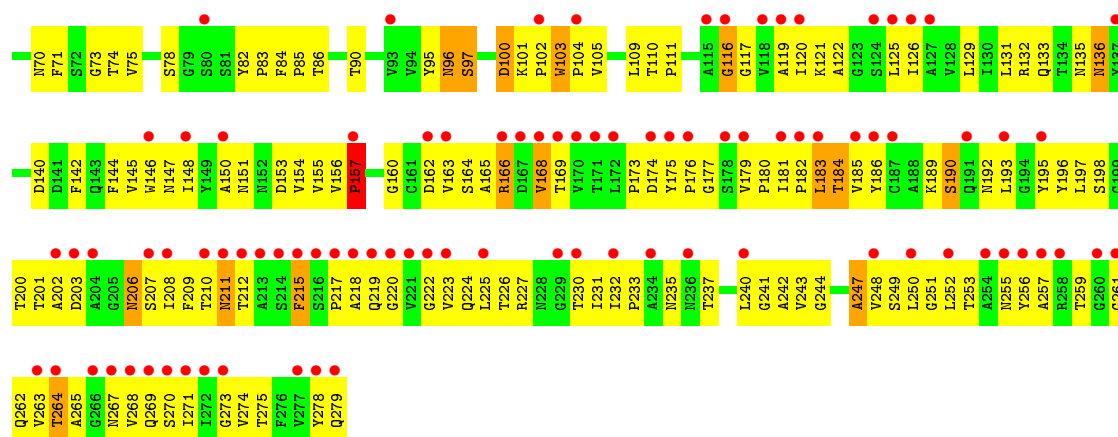


- Molecule 2: FIMH PROTEIN

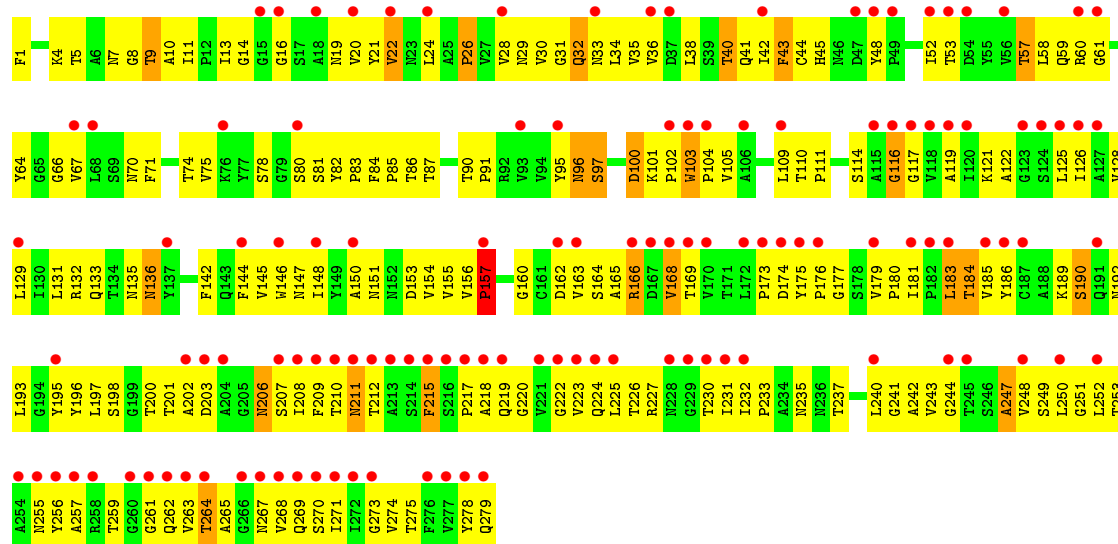


- Molecule 2: FIMH PROTEIN

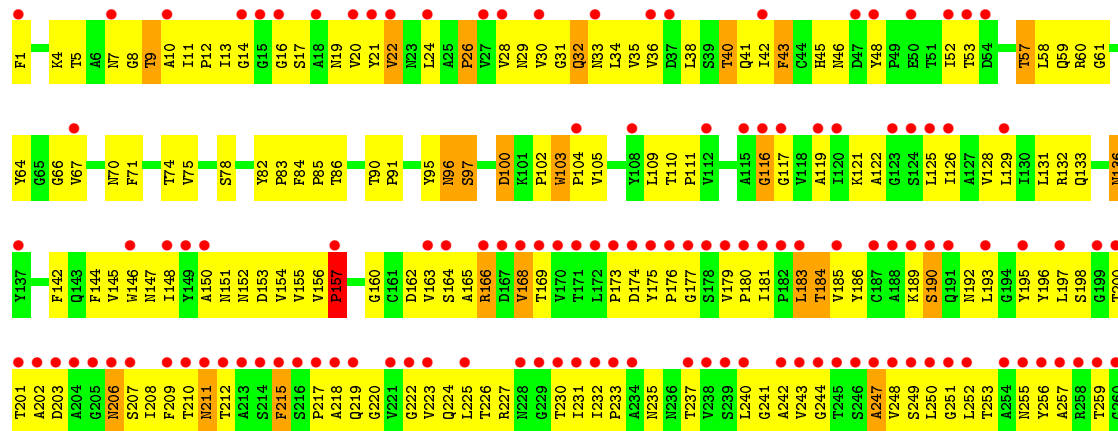


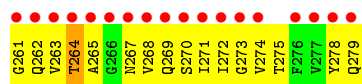


• Molecule 2: FIMH PROTEIN

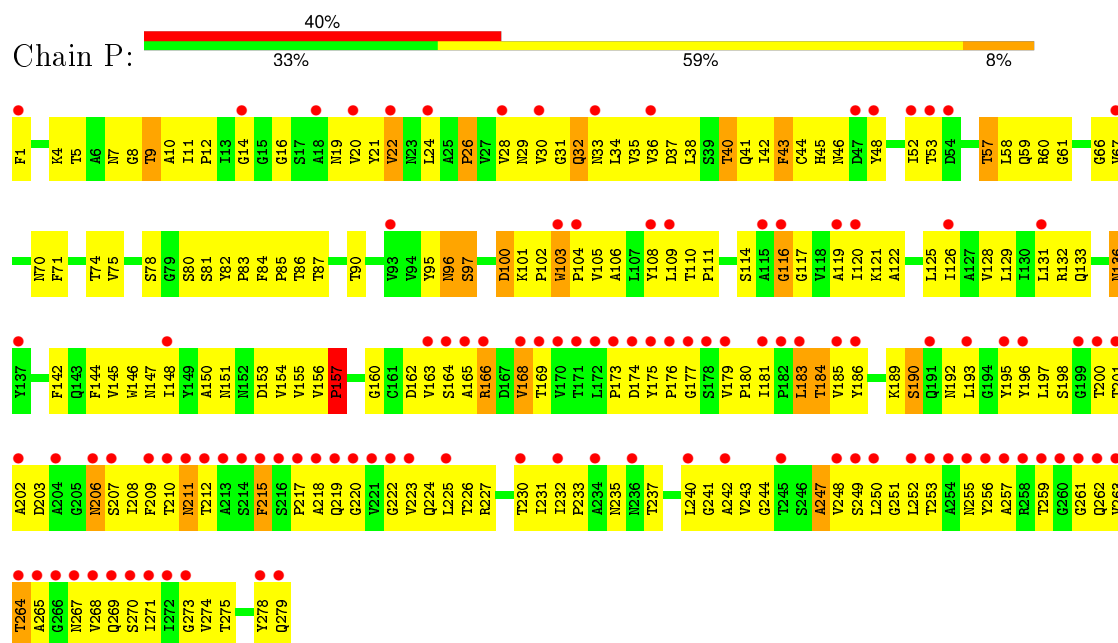


• Molecule 2: FIMH PROTEIN





● 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 0.242 , 0.281	Depositor DCC
R_{free} test set	9936 reflections (11.14%)	DCC
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
Estimated twinning fraction	0.477 for k,h,-l 0.476 for -k,-h,-l 0.477 for -h,-k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	1 of 99135 reflections (0.001%)	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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:P:224:GLN:HE21	2:P:231:ILE:HG21	1.16	1.10
2:F:126:ILE:HD12	2:F:150:ALA:HB2	1.33	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:N:57:THR:HG23	2:N:132:ARG:HB3	1.48	0.92
2:J:57:THR:HG23	2:J:132:ARG:HB3	1.49	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
2:H:120:ILE:HG21	2:H:126:ILE:HD11	1.49	0.92
1:G:47:ARG:HH22	1:G:74:GLN:HE21	0.98	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
1:M:39:ASN:HD21	1:M:43:VAL:HG13	1.35	0.91
2:L:67:VAL:HG21	2:L:126:ILE:HG23	1.51	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:G:179:SER:C	1:G:181:ALA:H	1.74	0.91
1:A:135:ARG:HH12	1:A:181:ALA:HB1	1.34	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:N:264:THR:HG22	2:N:265:ALA:H	1.36	0.89
2:B:57:THR:HG21	2:B:89:GLU:OE2	1.73	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:O:135:ARG:NH1	1:O:181:ALA:HB1	1.89	0.87
1:I:27:GLU:HG2	1:I:60:LYS:HD2	1.55	0.87
1:C:133:PHE:HD2	1:C:140:LEU:HD21	1.39	0.87
2:B:57:THR:HG22	2:B:132:ARG:HB3	1.57	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:M:27:GLU:HG2	1:M:60:LYS:HD2	1.55	0.86
1:I:134:ARG:HB3	1:I:141:THR:HB	1.56	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
1:G:133:PHE:HD2	1:G:140:LEU:HD21	1.39	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:K:27:GLU:HG2	1:K:60:LYS:HD2	1.55	0.86
2:J:58:LEU:H	2:J:90:THR:CG2	1.89	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
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:D:92:ARG:HH11	2:D:92:ARG:HG3	1.41	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:J:5:THR:HG22	2:J:7:ASN:H	1.42	0.84
2:B:92:ARG:HG3	2:B:92:ARG:HH11	1.40	0.84
1:O:176:LYS:H	1:O:176:LYS:HD2	1.38	0.84
2:P:196:TYR:CE1	2:P:198:SER:HB3	2.11	0.84
2:L:11:ILE:HG23	2:L:16:GLY:HA3	1.56	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
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
2:F:167:ASP:CG	2:F:168:VAL:H	1.76	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
1:I:135:ARG:HH12	1:I:181:ALA:CB	1.91	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
2:L:196:TYR:CE1	2:L:198:SER:HB3	2.11	0.83
1:A:135:ARG:HH12	1:A:181:ALA:CB	1.90	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
1:E:47:ARG:NH2	1:E:74:GLN:HE21	1.76	0.82
2:D:192:ASN:HD22	2:D:279:GLN:HE22	1.26	0.82
2:L:226:THR:HB	2:L:231:ILE:HG12	1.62	0.82
2:F:92:ARG:HH11	2:F:92:ARG:HG3	1.44	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:P:226:THR:HB	2:P:231:ILE:HG12	1.62	0.82
2:N:58:LEU:H	2:N:90:THR:HG22	1.42	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
1:G:47:ARG:NH2	1:G:74:GLN:HE21	1.76	0.82
2:F:59:GLN:HG2	2:F:132:ARG:HD2	1.60	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:J:253:THR:HG22	2:J:255:ASN:HD21	1.44	0.81
2:P:34:LEU:HD12	2:P:35:VAL:H	1.44	0.81
2:B:192:ASN:HD22	2:B:279:GLN:HE22	1.26	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
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: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
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
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:B:53:THR:H	2:B:136:ASN:HD21	1.26	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
1:I:39:ASN:ND2	1:I:43:VAL:HG13	1.96	0.80
2:D:218:ALA:HB2	2:D:266:GLY:C	2.02	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
1:M:8:ARG:HH21	1:M:8:ARG:HB3	1.47	0.80
2:L:208:ILE:HG23	2:L:257:ALA:HB1	1.63	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: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
2:B:218:ALA:HB2	2:B:266:GLY:C	2.02	0.79
2:N:226:THR:HB	2:N:231:ILE:HG12	1.62	0.79
1:K:47:ARG:NH2	1:K:74:GLN:HE21	1.81	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
1:O:47:ARG:NH2	1:O:74:GLN:HE21	1.81	0.79
2:F:192:ASN:HD22	2:F:279:GLN:HE22	1.31	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:224:GLN:NE2	2:L:231:ILE:HG21	1.95	0.79
1:K:32:LEU:HB2	1:K:90:ILE:HB	1.64	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
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:G:188:ARG:HH11	1:G:199:LYS:HB2	1.49	0.78
1:G:47:ARG:HG3	1:G:71:THR:HB	1.65	0.78
1:A:188:ARG:HH11	1:A:199:LYS:HB2	1.48	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:K:38:GLU:HG2	1:K:44:LYS:HG3	1.65	0.77
1:C:52:PRO:HG2	1:C:55:PHE:CD2	2.19	0.77
1:C:134:ARG:HD2	1:C:141:THR:CG2	2.14	0.77
2:P:226:THR:HG23	2:P:253:THR:HB	1.67	0.77
2:N:226:THR:HG23	2:N:253:THR:HB	1.66	0.77
1:M:47:ARG:NH2	1:M:74:GLN:HE21	1.81	0.77
1:O:38:GLU:HG2	1:O:44:LYS:HG3	1.65	0.77
2:J:226:THR:HG23	2:J:253:THR:HB	1.66	0.77
1:C:47:ARG:HG3	1:C:71:THR:HB	1.65	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:L:226:THR:HG23	2:L:253:THR:HB	1.67	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
1:C:134:ARG:HD2	1:C:141:THR:HG21	1.67	0.76
2:L:59:GLN:HG3	2:L:132:ARG:HB2	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: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:O:176:LYS:HD2	1:O:176:LYS:N	2.00	0.76
1:K:52:PRO:HG2	1:K:55:PHE:CD2	2.20	0.76
2:P:197:LEU:HD13	2:P:225:LEU:HD12	1.67	0.76
2:B:172:LEU:O	2:B:174:ASP:N	2.18	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:59:GLN:HG3	2:P:132:ARG:HB2	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: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:52:PRO:HG2	1:A:55:PHE:CD2	2.21	0.75
2:L:197:LEU:HD13	2:L:225:LEU:HD12	1.68	0.75
2:B:173:PRO:HG3	2:B:179:VAL:HG13	1.69	0.75
1:A:47:ARG:HH22	1:A:74:GLN:NE2	1.80	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:P:180:PRO:HA	2:P:253:THR:HA	1.70	0.74
2:J:197:LEU:HD13	2:J:225:LEU:HD12	1.67	0.74
2:N:197:LEU:HD13	2:N:225:LEU:HD12	1.68	0.74
1:I:185:ILE:HB	1:I:202:GLY:HA3	1.68	0.74
1:M:185:ILE:HB	1:M:202:GLY:HA3	1.68	0.74
1:G:32:LEU:HB2	1:G:90:ILE:HB	1.69	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
2:H:171:THR:C	2:H:173:PRO:HD2	2.08	0.74
1:E:32:LEU:HB2	1:E:90:ILE:HB	1.70	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:L:180:PRO:HA	2:L:253:THR:HA	1.70	0.73
2:H:173:PRO:HG3	2:H:179:VAL:HG13	1.70	0.73
2:L:180:PRO:HB3	2:L:253:THR:HG23	1.71	0.73
2:F:171:THR:C	2:F:173:PRO:HD2	2.08	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:L:186:TYR:HB3	2:L:247:ALA:HA	1.71	0.73
2:D:29:ASN:HD22	2:D:32:GLN:HE22	1.37	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:N:19:ASN:HD21	2:P:219:GLN:NE2	1.85	0.73
2:H:29:ASN:HD22	2:H:32:GLN:HE22	1.36	0.73
1:M:111:ILE:HG22	2:N:278:TYR:HB2	1.72	0.72
2:J:19:ASN:HD21	2:L:219:GLN:NE2	1.87	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:J:180:PRO:HB3	2:J:253:THR:HG23	1.72	0.72
2:D:201:THR:HG21	2:D:206:ASN:HD22	1.55	0.72
2:H:57:THR:CG2	2:H:132:ARG:HB3	2.19	0.72
2:H:29:ASN:HD22	2:H:32:GLN:NE2	1.88	0.72
1:M:101:ASN:HD22	2:N:268:VAL:HG23	1.55	0.72
2:B:29:ASN:HD22	2:B:32:GLN:HE22	1.37	0.72
1:C:141:THR:HB	1:C:174:THR:HG23	1.72	0.72
1:A:112:LYS:HG3	4:A:208:HOH:O	1.90	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
2:D:171:THR:C	2:D:173:PRO:HD2	2.10	0.71
1:C:47:ARG:HH22	1:C:74:GLN:NE2	1.83	0.71
2:F:57:THR:CG2	2:F:132:ARG:HB3	2.21	0.71
2:D:32:GLN:O	2:D:110:THR:HG23	1.91	0.71
2:J:48:TYR:HB2	2:J:52:ILE:HD12	1.73	0.71
1:I:111:ILE:HG22	2:J:278:TYR:HB2	1.72	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:N:48:TYR:HB2	2:N:52:ILE:HD12	1.74	0.69
2:F:262:GLN:HA	2:F:262:GLN:HE21	1.56	0.69
2:D:57:THR:CG2	2:D:132:ARG:HB3	2.22	0.69
1:I:12:PRO:HB2	1:I:15:GLN:HG2	1.73	0.69
1:E:12:PRO:HG2	1:E:15:GLN:HE21	1.57	0.69
2:B:173:PRO:HB2	2:B:177:GLY:HA3	1.74	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:B:81:SER:O	2:P:114:SER:HB2	1.92	0.69
1:O:162:LEU:HD21	1:O:178:PRO:HD3	1.75	0.69
1:K:162:LEU:HD21	1:K:178:PRO:HD3	1.75	0.69
1:K:12:PRO:HB2	1:K:15:GLN:HG2	1.73	0.69
1:O:12:PRO:HB2	1:O:15:GLN:HG2	1.73	0.69
2:H:58:LEU:H	2:H:90:THR:HG22	1.57	0.69
2:F:172:LEU:N	2:F:173:PRO:HD2	2.07	0.69
1:I:162:LEU:HD21	1:I:178:PRO:HD3	1.75	0.69
1:G:25:ASN:O	1:G:60:LYS:HG2	1.93	0.69
2:L:48:TYR:HB2	2:L:52:ILE:HD12	1.73	0.69
2:D:262:GLN:HE21	2:D:262:GLN:HA	1.57	0.69
2:D:172:LEU:N	2:D:173:PRO:HD2	2.08	0.69
2:H:173:PRO:HB2	2:H:177:GLY:HA3	1.74	0.69
2:H:172:LEU:N	2:H:173:PRO:HD2	2.06	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:J:155:VAL:HG12	2:J:157:PRO:HD3	1.73	0.69
1:I:182:GLY:O	1:I:183:SER:HB2	1.93	0.69
2:L:155:VAL:HG12	2:L:157:PRO:HD3	1.73	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: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:I:82:LEU:HD13	1:I:114:TYR:CE2	2.28	0.69
1:C:12:PRO:HB2	1:C:15:GLN:CG	2.23	0.69
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:J:164:SER:HB2	2:J:184:THR:HG23	1.74	0.68
1:A:12:PRO:HB2	1:A:15:GLN:CG	2.22	0.68
1:C:182:GLY:O	1:C:183:SER:HB2	1.92	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
2:H:81:SER:O	2:L:114:SER:HB2	1.93	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
1:A:12:PRO:HG2	1:A:15:GLN:HE21	1.58	0.68
2:B:57:THR:CG2	2:B:132:ARG:HB3	2.24	0.68
2:B:218:ALA:HB2	2:B:266:GLY:O	1.94	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
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
2:H:53:THR:HB	2:H:136:ASN:OD1	1.93	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
1:O:135:ARG:NH1	1:O:181:ALA:CB	2.53	0.68
1:G:27:GLU:HG3	1:G:60:LYS:HD2	1.74	0.68
2:F:173:PRO:HB2	2:F:177:GLY:HA3	1.74	0.68
1:E:182:GLY:O	1:E:183:SER:HB2	1.93	0.68
1:K:79:ARG:HB3	1:K:170:MET:CE	2.24	0.68
1:M:138:ASN:HA	1:M:177:LEU:O	1.94	0.68
1:K:135:ARG:NH1	1:K:181:ALA:CB	2.53	0.68
2:B:116:GLY:HA2	2:B:189:LYS:HE2	1.76	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:K:88:LYS:HE2	1:K:90:ILE:HG12	1.76	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: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)
2:B:53:THR:H	2:B:136:ASN:ND2	1.92	0.67
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
1:K:138:ASN:HA	1:K:177:LEU:O	1.94	0.67
1:I:138:ASN:HA	1:I:177:LEU:O	1.94	0.67
2:F:58:LEU:H	2:F:90:THR:HG22	1.59	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:P:24:LEU:HD22	2:P:36:VAL:HG22	1.77	0.67
1:E:25:ASN:O	1:E:60:LYS:HG2	1.93	0.67
2:B:58:LEU:H	2:B:90:THR:HG22	1.58	0.67
2:B:226:THR:HG23	4:B:1508:HOH:O	1.94	0.67
1:O:138:ASN:HA	1:O:177:LEU:O	1.94	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:12:PRO:HB2	1:O:15:GLN:CG	2.25	0.67
2:B:217:PRO:O	2:B:219:GLN:N	2.28	0.67
2:D:221:VAL:O	2:D:259:THR:HG23	1.95	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
2:H:211:ASN:HD22	2:H:212:THR:N	1.92	0.67
2:D:53:THR:H	2:D:136:ASN:ND2	1.93	0.67
1:E:27:GLU:HG3	1:E:60:LYS:HD2	1.74	0.67
1:C:86:ASN:HD21	1:C:110:ARG:HE	1.42	0.67
2:D:116:GLY:HA2	2:D:189:LYS:HE2	1.77	0.67
1:O:182:GLY:O	1:O:183:SER:HB2	1.93	0.67
2:H:218:ALA:HB2	2:H:266:GLY:O	1.93	0.67
1:A:12:PRO:HB2	1:A:15:GLN:HG3	1.77	0.67
1:C:188:ARG:NH1	1:C:199:LYS:H	1.92	0.67
1:A:188:ARG:NH1	1:A:199:LYS:H	1.93	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
2:N:24:LEU:HD22	2:N:36:VAL:HG22	1.77	0.66
1:M:135:ARG:CZ	1:M:181:ALA:HB1	2.25	0.66
1:C:27:GLU:HG3	1:C:60:LYS:HD2	1.75	0.66
1:A:27:GLU:HG3	1:A:60:LYS:HD2	1.76	0.66
1:E:188:ARG:NH1	1:E:199:LYS:H	1.94	0.66
2:P:219:GLN:OE1	2:P:262:GLN:HG2	1.95	0.66
2:N:186:TYR:HB2	2:N:244:GLY:O	1.95	0.66
1:C:12:PRO:HB2	1:C:15:GLN:HG3	1.77	0.66
2:H:84:PHE:HA	2:H:85:PRO:C	2.15	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:264:THR:HG22	2:P:265:ALA:N	2.07	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:H:217:PRO:O	2:H:219:GLN:N	2.28	0.66
1:M:12:PRO:HB2	1:M:15:GLN:CG	2.25	0.66
2:H:77:TYR:CD2	2:H:90:THR:HG21	2.30	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:N:264:THR:HG22	2:N:265:ALA:N	2.08	0.66
2:L:219:GLN:OE1	2:L:262:GLN:HG2	1.94	0.66
2:P:186:TYR:HB2	2:P:244:GLY:O	1.96	0.66
2:L:24:LEU:HD22	2:L:36:VAL:HG22	1.76	0.66
2:F:211:ASN:HD22	2:F:212:THR:N	1.93	0.66
1:O:135:ARG:CZ	1:O:181:ALA:HB1	2.25	0.66
1:I:102:THR:O	2:J:269:GLN:HA	1.96	0.66
2:D:217:PRO:O	2:D:219:GLN:N	2.29	0.66
1:I:10:ILE:O	1:I:12:PRO:HD3	1.96	0.66
1:K:103:LEU:HD12	2:L:270:SER:O	1.96	0.66
2:J:219:GLN:OE1	2:J:262:GLN:HG2	1.94	0.66
2:B:221:VAL:O	2:B:259:THR:HG23	1.96	0.66
2:F:116:GLY:HA2	2:F:189:LYS:HE2	1.77	0.66
1:M:135:ARG:NH1	1:M:181:ALA:CB	2.53	0.66
1:I:12:PRO:HB2	1:I:15:GLN:CG	2.25	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:K:126:GLN:HA	1:K:129:GLU:OE1	1.95	0.66
2:L:43:PHE:CD2	2:L:102:PRO:HB3	2.31	0.66
2:H:53:THR:H	2:H:136:ASN:ND2	1.94	0.65
2:D:58:LEU:H	2:D:90:THR:HG22	1.60	0.65
2:N:43:PHE:CD2	2:N:102:PRO:HB3	2.31	0.65
1:G:12:PRO:HB2	1:G:15:GLN:HG3	1.78	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
1:A:122:LEU:HD11	1:A:126:GLN:O	1.96	0.65
1:M:102:THR:O	2:N:269:GLN:HA	1.96	0.65
1:I:103:LEU:HD12	2:J:270:SER:O	1.96	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:135:ARG:CZ	1:K:181:ALA:HB1	2.25	0.65
1:K:12:PRO:HB2	1:K:15:GLN:CG	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
1:G:73:ASN:HA	4:G:222:HOH:O	1.97	0.65
2:F:53:THR:HB	2:F:136:ASN:OD1	1.95	0.65
2:B:77:TYR:CD2	2:B:90:THR:HG21	2.31	0.65
1:G:144:ASN:ND2	1:G:150:LEU:HG	2.12	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:N:116:GLY:HA3	2:N:189:LYS:HG3	1.79	0.65
2:L:105:VAL:HG11	2:L:129:LEU:HD13	1.77	0.65
1:E:122:LEU:HD11	1:E:126:GLN:O	1.97	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
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
2:F:217:PRO:O	2:F:219:GLN:N	2.30	0.65
2:L:186:TYR:HB2	2:L:244:GLY:O	1.95	0.65
1:E:12:PRO:HB2	1:E:15:GLN:CG	2.26	0.65
2:F:221:VAL:O	2:F:259:THR:HG23	1.96	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
1:E:144:ASN:ND2	1:E:150:LEU:HG	2.11	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:D:84:PHE:HA	2:D:85:PRO:C	2.17	0.65
2:B:90:THR:HG23	2:B:91:PRO:O	1.96	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:J:38:LEU:C	2:J:40:THR:H	2.00	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
1:M:10:ILE:O	1:M:12:PRO:HD3	1.96	0.64
2:D:90:THR:HG23	2:D:91:PRO:O	1.97	0.64
2:J:43:PHE:CD2	2:J:102:PRO:HB3	2.32	0.64
2:J:116:GLY:HA3	2:J:189:LYS:HG3	1.79	0.64
2:F:84:PHE:HA	2:F:85:PRO:C	2.17	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:58:LEU:N	2:P:90:THR:HG22	2.12	0.64
2:B:192:ASN:ND2	2:B:279:GLN:HE22	1.95	0.64
2:J:43:PHE:HA	2:J:102:PRO:HA	1.80	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
1:M:27:GLU:HA	1:M:60:LYS:HG3	1.79	0.64
2:J:95:TYR:OH	2:J:103:TRP:HA	1.97	0.64
2:H:116:GLY:HA2	2:H:189:LYS:HE2	1.79	0.64
1:C:134:ARG:CD	1:C:141:THR:HG21	2.28	0.64
2:N:95:TYR:OH	2:N:103:TRP:HA	1.97	0.64
2:L:43:PHE:HA	2:L:102:PRO:HA	1.79	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
1:A:97:LYS:HE3	4:B:1573:HOH:O	1.96	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:G:102:THR:CA	2:H:171:THR:HG22	2.28	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
1:O:135:ARG:NH1	1:O:177:LEU:HD11	2.13	0.63
2:D:167:ASP:CG	2:D:168:VAL:N	2.50	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
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
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:D:92:ARG:NH1	2:D:92:ARG:HG3	2.10	0.63
2:P:84:PHE:HA	2:P:85:PRO:C	2.17	0.63
1:G:140:LEU:HD23	1:G:141:THR:N	2.14	0.63
2:B:92:ARG:HG3	2:B:92:ARG:NH1	2.09	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:134:ARG:CZ	1:C:141:THR:HG21	2.29	0.63
1:C:11:TYR:HB2	1:C:113:LEU:HD11	1.81	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
2:F:67:VAL:HG23	2:F:126:ILE:HG12	1.81	0.63
1:A:102:THR:CA	2:B:171:THR:HG22	2.28	0.63
1:G:94:ASP:HB3	1:G:96:SER:OG	1.98	0.63
1:O:162:LEU:HD21	1:O:178:PRO:CD	2.29	0.63
2:J:32:GLN:O	2:J:110:THR:HG23	1.99	0.63
1:G:179:SER:C	1:G:181:ALA:N	2.50	0.62
1:M:135:ARG:NH1	1:M:177:LEU:HD11	2.13	0.62
1:I:27:GLU:HA	1:I:60:LYS:HG3	1.80	0.62
1:O:27:GLU:HA	1:O:60:LYS:HG3	1.80	0.62
2:H:90:THR:HG23	2:H:91:PRO:O	1.98	0.62
1:I:4:LEU:HD21	1:I:87:VAL:HG21	1.80	0.62
2:N:38:LEU:C	2:N:40:THR:H	2.01	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: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
1:A:185:ILE:HB	1:A:202:GLY:HA3	1.82	0.62
1:I:135:ARG:NH1	1:I:177:LEU:HD11	2.13	0.62
2:D:192:ASN:ND2	2:D:279:GLN:HE22	1.94	0.62
1:G:185:ILE:HB	1:G:202:GLY:HA3	1.81	0.62
1:E:12:PRO:HB2	1:E:15:GLN:HG3	1.82	0.62
2:D:172:LEU:O	2:D:172:LEU:HD23	1.99	0.62
2:N:59:GLN:CG	2:N:132:ARG:HB2	2.28	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
1:E:156:ASN:HB2	1:E:186:THR:OG1	2.00	0.62
2:B:59:GLN:CG	2:B:132:ARG:HD2	2.30	0.62
1:G:156:ASN:HB2	1:G:186:THR:OG1	2.00	0.62
2:P:59:GLN:CG	2:P:132:ARG:HB2	2.29	0.62
2:P:43:PHE:HA	2:P:102:PRO:HA	1.79	0.62
2:N:32:GLN:O	2:N:110:THR:HG23	2.00	0.62
1:G:191:ASN:HD21	1:G:195:ALA:HB3	1.64	0.62
2:J:59:GLN:CG	2:J:132:ARG:HB2	2.29	0.62
2:P:67:VAL:HG13	2:P:109:LEU:HD13	1.80	0.62
1:A:94:ASP:HB3	1:A:96:SER:OG	2.00	0.62
1:K:162:LEU:HD21	1:K:178:PRO:CD	2.29	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
1:C:156:ASN:HB2	1:C:186:THR:OG1	2.00	0.62
2:B:170:VAL:CG1	2:B:172:LEU:HB2	2.27	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:59:GLN:CG	2:L:132:ARG:HB2	2.29	0.62
2:J:67:VAL:HG13	2:J:109:LEU:HD13	1.80	0.62
2:L:184:THR:HA	2:L:249:SER:HA	1.81	0.62
1:K:79:ARG:HB3	1:K:170:MET:HE1	1.80	0.62
2:B:172:LEU:HD23	2:B:172:LEU:O	2.00	0.62
1:A:135:ARG:HH22	1:A:181:ALA:CB	2.13	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
2:F:59:GLN:CG	2:F:132:ARG:HD2	2.30	0.61
1:E:104:GLN:HG3	2:F:168:VAL:HG23	1.82	0.61
2:J:201:THR:CG2	2:J:206:ASN:HA	2.24	0.61
2:H:172:LEU:O	2:H:172:LEU:HD23	2.00	0.61
1:E:135:ARG:HH22	1:E:181:ALA:CB	2.14	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: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
2:L:32:GLN:O	2:L:110:THR:HG23	1.99	0.61
1:E:185:ILE:HB	1:E:202:GLY:HA3	1.82	0.61
1:E:191:ASN:HD21	1:E:195:ALA:HB3	1.63	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
2:H:59:GLN:CG	2:H:132:ARG:HD2	2.30	0.61
1:E:140:LEU:HD23	1:E:141:THR:N	2.15	0.61
2:N:19:ASN:HD21	2:P:219:GLN:HE22	1.46	0.61
2:J:184:THR:HA	2:J:249:SER:HA	1.81	0.61
1:I:7:THR:O	1:I:111:ILE:HB	2.01	0.61
1:G:11:TYR:HB2	1:G:113:LEU:HD11	1.81	0.61
2:F:170:VAL:CG1	2:F:172:LEU:HB2	2.26	0.61
1:A:104:GLN:HG3	2:B:168:VAL:HG23	1.82	0.61
2:L:20:VAL:HG21	2:L:42:ILE:HD11	1.82	0.61
1:I:4:LEU:O	2:J:160:GLY:N	2.33	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:P:184:THR:HA	2:P:249:SER:HA	1.81	0.61
2:N:175:TYR:N	2:N:176:PRO:HD2	2.16	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:P:20:VAL:HG21	2:P:42:ILE:HD11	1.81	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:D:175:TYR:O	2:D:256:TYR:CD1	2.54	0.60
1:O:27:GLU:CG	1:O:60:LYS:HD2	2.29	0.60
1:M:7:THR:O	1:M:111:ILE:HB	2.01	0.60
2:L:193:LEU:HB3	2:L:240:LEU:HD12	1.82	0.60
1:E:188:ARG:NH1	1:E:199:LYS:HB2	2.17	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
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:N:20:VAL:HG21	2:N:42:ILE:HD11	1.82	0.60
1:K:7:THR:O	1:K:111:ILE:HB	2.00	0.60
2:J:74:THR:HG22	2:J:83:PRO:HA	1.82	0.60
2:H:192:ASN:ND2	2:H:279:GLN:HE22	1.96	0.60
2:P:21:TYR:HB3	2:P:151:ASN:ND2	2.15	0.60
2:L:14:GLY:HA2	2:L:142:PHE:CE1	2.37	0.60
2:P:74:THR:HG22	2:P:83:PRO:HA	1.82	0.60
1:A:11:TYR:HB2	1:A:113:LEU:HD11	1.83	0.60
2:J:175:TYR:OH	2:J:263:VAL:HB	2.01	0.60
2:L:125:LEU:HD12	2:L:148:ILE:O	2.02	0.60
2:J:175:TYR:N	2:J:176:PRO:HD2	2.16	0.60
2:L:201:THR:CG2	2:L:206:ASN:HA	2.24	0.60
1:A:177:LEU:HD12	1:A:178:PRO:HD2	1.83	0.60
1:C:104:GLN:HG3	2:D:168:VAL:HG23	1.84	0.60
1:O:117:PRO:O	1:O:120:LEU:HG	2.02	0.60
1:A:191:ASN:HD21	1:A:195:ALA:HB3	1.66	0.60
2:L:175:TYR:N	2:L:176:PRO:HD2	2.16	0.60
2:F:227:ARG:HB3	2:F:232:ILE:HD11	1.84	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:B:167:ASP:OD2	2:B:168:VAL:N	2.35	0.60
2:J:193:LEU:HB3	2:J:240:LEU:HD12	1.83	0.60
2:B:184:THR:HG22	2:B:249:SER:HA	1.82	0.60
2:B:174:ASP:O	2:B:176:PRO:N	2.35	0.60
2:F:174:ASP:O	2:F: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:175:TYR:N	2:P:176:PRO:HD2	2.16	0.60
2:L:175:TYR:OH	2:L:263:VAL:HB	2.01	0.60
2:L:21:TYR:HB3	2:L:151:ASN:ND2	2.16	0.59
1:K:4:LEU:O	2:L:160:GLY:N	2.33	0.59
2:N:175:TYR:OH	2:N:263:VAL:HB	2.00	0.59
2:P:193:LEU:HB3	2:P:240:LEU:HD12	1.82	0.59
2:N:74:THR:HG22	2:N:83:PRO:HA	1.82	0.59
2:P:125:LEU:HD12	2:P:148:ILE:O	2.02	0.59
1:I:101:ASN:ND2	2:J:268:VAL:HG23	2.17	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:M:117:PRO:O	1:M:120:LEU:HG	2.02	0.59
1:A:102:THR:HA	2:B:171:THR:HG22	1.82	0.59
2:H:175:TYR:O	2:H:256:TYR:CD1	2.55	0.59
1:I:27:GLU:CG	1:I:60:LYS:HD2	2.29	0.59
1:C:82:LEU:HD12	1:C:83:PHE:N	2.17	0.59
2:H:163:VAL:HG22	2:H:185:VAL:HG12	1.84	0.59
2:H:167:ASP:OD2	2:H:168:VAL:N	2.36	0.59
1:K:101:ASN:ND2	2:L:268:VAL:HG23	2.17	0.59
2:L:177:GLY:HA3	2:L:256:TYR:CE1	2.38	0.59
1:I:117:PRO:O	1:I:120:LEU:HG	2.02	0.59
1:M:188:ARG:HH11	1:M:199:LYS:HB2	1.67	0.59
1:E:118:ALA:O	1:E:119:LYS:HB2	2.02	0.59
2:J:14:GLY:HA2	2:J:142:PHE:CE1	2.38	0.59
2:D:67:VAL:HG23	2:D:126:ILE:HG12	1.85	0.59
2:D:174:ASP:O	2:D:176:PRO:N	2.35	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:E:11:TYR:HB2	1:E:113:LEU:HD11	1.83	0.59
1:G:177:LEU:HD12	1:G:178:PRO:HD2	1.84	0.59
1:A:135:ARG:HH22	1:A:181:ALA:HB1	1.68	0.59
1:O:7:THR:O	1:O:111:ILE:HB	2.01	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: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:D:184:THR:HG22	2:D:249:SER:HA	1.85	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)
2:F:175:TYR:O	2:F:256:TYR:CD1	2.55	0.59
1:M:4:LEU:O	2:N:160:GLY:N	2.33	0.59
2:F:13:ILE:HG13	4:F:1539:HOH:O	2.03	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:G:118:ALA:O	1:G:119:LYS:HB2	2.02	0.59
1:A:82:LEU:HD12	1:A:83:PHE:N	2.18	0.59
1:C:179:SER:C	1:C:181:ALA:N	2.51	0.59
2:N:24:LEU:HD11	2:N:126:ILE:HD11	1.84	0.59
2:F:167:ASP:OD2	2:F:168:VAL:N	2.36	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
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:I:188:ARG:HH11	1:I:199:LYS:HB2	1.68	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:G:47:ARG:HH22	1:G:74:GLN:HB2	1.69	0.58
1:K:27:GLU:CG	1:K:60:LYS:HD2	2.30	0.58
1:C:27:GLU:HA	1:C:60:LYS:HG3	1.85	0.58
1:I:103:LEU:O	2:J:168:VAL:HG23	2.03	0.58
2:F:5:THR:HG22	2:F:8:GLY:H	1.67	0.58
1:A:118:ALA:O	1:A:119:LYS:HB2	2.01	0.58
1:A:138:ASN:C	1:A:177:LEU:HB3	2.24	0.58
2:J:24:LEU:HD11	2:J:126:ILE:HD11	1.85	0.58
2:D:59:GLN:CG	2:D:132:ARG:HD2	2.31	0.58
1:K:188:ARG:HH11	1:K:199:LYS:HB2	1.68	0.58
2:B:227:ARG:HB3	2:B:232:ILE:HD11	1.86	0.58
2:H:114:SER:HB3	2:L:80:SER:HB3	1.85	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
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
1:I:11:TYR:HB2	1:I:113:LEU:HD11	1.85	0.58
2:B:179:VAL:O	2:B:253:THR:HG23	2.03	0.58
1:M:101:ASN:ND2	2:N:268:VAL:HG23	2.17	0.58
2:B:58:LEU:H	2:B:90:THR:CG2	2.16	0.58
1:C:188:ARG:HH12	1:C:199:LYS:H	1.50	0.58
1:G:135:ARG:NH2	1:G:181:ALA:HB1	2.19	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:92:ARG:HG3	2:F:92:ARG:NH1	2.12	0.58
1:G:188:ARG:HH12	1:G:199:LYS:H	1.51	0.58
1:O:103:LEU:O	2:P:168:VAL:HG23	2.04	0.58
2:N:84:PHE:CD1	2:N:85:PRO:HA	2.39	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
1:O:11:TYR:HB2	1:O:113:LEU:HD11	1.85	0.58
2:N:201:THR:CG2	2:N:206:ASN:HA	2.24	0.58
2:H:170:VAL:CG1	2:H:172:LEU:HB2	2.27	0.58
1:G:135:ARG:HH22	1:G:181:ALA:HB1	1.68	0.58
2:F:192:ASN:ND2	2:F:279:GLN:HE22	1.99	0.58
2:H:58:LEU:H	2:H:90:THR:CG2	2.16	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: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
1:G:1:GLY:H1	1:G:26:ASP:CG	2.07	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
2:P:201:THR:CG2	2:P:206:ASN:HA	2.24	0.57
2:B:167:ASP:CG	2:B:168:VAL:N	2.50	0.57
1:E:138:ASN:C	1:E:177:LEU:HB3	2.24	0.57
2:D:167:ASP:OD2	2:D:168:VAL:N	2.35	0.57
1:A:27:GLU:HA	1:A:60:LYS:HG3	1.86	0.57
2:F:58:LEU:H	2:F:90:THR:CG2	2.16	0.57
1:O:4:LEU:O	2:P:160:GLY:N	2.33	0.57
1:K:6:ALA:HB3	1:K:20:LEU:HD11	1.86	0.57
2:B:68:LEU:O	2:P:87:THR:HG21	2.03	0.57
2:J:177:GLY:HA3	2:J:256:TYR:CE1	2.38	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:G:135:ARG:CZ	1:G:181:ALA:HB1	2.34	0.57
1:I:27:GLU:HG2	1:I:60:LYS:CD	2.32	0.57
1:G:158:GLY:HA2	1:G:184:ASN:HD22	1.69	0.57
1:K:79:ARG:HA	1:K:147:PRO:HB2	1.85	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:I:122:LEU:HD11	1:I:126:GLN:O	2.04	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)
1:O:101:ASN:ND2	2:P:268:VAL:HG23	2.17	0.57
1:O:188:ARG:HH11	1:O:199:LYS:HB2	1.68	0.57
2:L:131:LEU:HB3	2:L:144:PHE:HB2	1.87	0.57
1:C:135:ARG:NH2	1:C:181:ALA:HB1	2.19	0.57
2:B:120:ILE:CG2	2:B:126:ILE:HD11	2.31	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
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:M:156:ASN:C	1:M:158:GLY:H	2.06	0.57
2:D:5:THR:HG22	2:D:8:GLY:H	1.69	0.57
1:K:156:ASN:C	1:K:158:GLY:H	2.07	0.57
1:C:158:GLY:HA2	1:C:184:ASN:HD22	1.69	0.57
1:C:135:ARG:CZ	1:C:181:ALA:HB1	2.34	0.57
2:F:179:VAL:O	2:F:253:THR:HG23	2.03	0.57
2:L:24:LEU:HD11	2:L:126:ILE:HD11	1.84	0.57
1:A:135:ARG:NH2	1:A:181:ALA:HB1	2.19	0.57
1:K:103:LEU:O	2:L:168:VAL:HG23	2.04	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
1:E:197:THR:HB	1:E:198:PRO:HD2	1.87	0.57
2:B:114:SER:HB3	2:P:80:SER:HB3	1.85	0.57
1:I:79:ARG:HA	1:I:147:PRO:HB2	1.85	0.57
2:J:71:PHE:CE2	2:J:111:PRO:HG3	2.40	0.57
2:F:163:VAL:HG22	2:F:185:VAL:HG12	1.86	0.57
2:L:96:ASN:HD22	2:L:96:ASN:H	1.53	0.57
2:N:66:GLY:O	2:N:70:ASN:HB2	2.05	0.57
1:M:6:ALA:HB3	1:M:20:LEU:HD11	1.87	0.57
1:M:197:THR:HB	1:M:198:PRO:HD2	1.86	0.57
2:J:131:LEU:HB3	2:J:144:PHE:HB2	1.87	0.57
2:D:163:VAL:HG22	2:D:185:VAL:HG12	1.87	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:J:223:VAL:HG12	2:J:224:GLN:N	2.19	0.57
2:N:224:GLN:HG2	2:N:231:ILE:CG2	2.35	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:B:5:THR:HG22	2:B:8:GLY:H	1.69	0.57
1:C:188:ARG:NH1	1:C:199:LYS:N	2.53	0.57
2:H:5:THR:HG22	2:H:8:GLY:H	1.70	0.57
1:A:135:ARG:CZ	1:A:181:ALA:HB1	2.34	0.57
1:E:135:ARG:HH22	1:E:181:ALA:HB1	1.68	0.57
1:M:122:LEU:HD11	1:M:126:GLN:O	2.04	0.57
2:J:84:PHE:CD1	2:J:85:PRO:HA	2.40	0.57
2:P:224:GLN:HG2	2:P:231:ILE:CG2	2.35	0.56
1:E:135:ARG:CZ	1:E:181:ALA:HB1	2.34	0.56
1:E:158:GLY:HA2	1:E:184:ASN:HD22	1.69	0.56
1:O:11:TYR:CE2	1:O:69:ASP:HB2	2.40	0.56
1:K:197:THR:HB	1:K:198:PRO:HD2	1.86	0.56
2:J:96:ASN:H	2:J:96:ASN:HD22	1.53	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:D:179:VAL:O	2:D:253:THR:HG23	2.05	0.56
1:A:158:GLY:HA2	1:A:184:ASN:HD22	1.69	0.56
2:L:11:ILE:HD12	2:L:146:TRP:CZ2	2.40	0.56
1:E:24:ASN:O	1:E:60:LYS:HA	2.05	0.56
2:B:219:GLN:HG2	2:B:220:GLY:N	2.20	0.56
2:H:219:GLN:HG2	2:H:220:GLY:N	2.20	0.56
2:D:219:GLN:HG2	2:D:220:GLY:N	2.19	0.56
2:P:267:ASN:HB3	2:P:269:GLN:HG3	1.87	0.56
1:G:193:TYR:O	2:H:158:THR:HG22	2.06	0.56
1:M:11:TYR:CE2	1:M:69:ASP:HB2	2.40	0.56
2:J:66:GLY:O	2:J:70:ASN:HB2	2.05	0.56
2:H:28:VAL:O	2:H:156:VAL:HA	2.06	0.56
2:J:250:LEU:HB2	2:J:252:LEU:HG	1.87	0.56
1:E:193:TYR:O	2:F:158:THR:HG22	2.06	0.56
2:N:227:ARG:HH22	2:N:230:THR:HG21	1.70	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:A:188:ARG:NH1	1:A:199:LYS:N	2.53	0.56
2:N:11:ILE:HD12	2:N:146:TRP:CZ2	2.40	0.56
1:I:11:TYR:CE2	1:I:69:ASP:HB2	2.40	0.56
1:O:154:GLU:OE2	1:O:188:ARG:HD3	2.06	0.56
2:H:120:ILE:HD13	2:H:126:ILE:HD11	1.87	0.56
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:G:188:ARG:NH1	1:G:199:LYS:N	2.54	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:30:VAL:HA	2:J:111:PRO:HB2	1.87	0.56
2:D:227:ARG:HB3	2:D:232:ILE:HD11	1.88	0.56
2:P:223:VAL:HG12	2:P:224:GLN:N	2.19	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:K:189:THR:O	1:K:196:LEU:HA	2.06	0.56
2:J:227:ARG:HH22	2:J:230:THR:HG21	1.70	0.56
1:O:189:THR:O	1:O:196:LEU:HA	2.06	0.56
1:I:6:ALA:HB3	1:I:20:LEU:HD11	1.86	0.56
2:J:224:GLN:HG2	2:J:231:ILE:CG2	2.35	0.56
2:L:224:GLN:HG2	2:L:231:ILE:CG2	2.35	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
1:K:80:GLU:HG3	1:K:147:PRO:O	2.05	0.56
2:N:267:ASN:HB3	2:N:269:GLN:HG3	1.87	0.56
1:C:193:TYR:O	2:D:158:THR:HG22	2.06	0.56
2:B:163:VAL:HG22	2:B:185:VAL:HG12	1.88	0.56
1:G:197:THR:HB	1:G:198:PRO:HD2	1.88	0.56
1:O:27:GLU:HG2	1:O:60:LYS:CD	2.32	0.56
2:J:11:ILE:HD12	2:J:146:TRP:CZ2	2.41	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
2:B:28:VAL:O	2:B:156:VAL:HA	2.05	0.56
1:M:22:VAL:CG2	1:M:65:LEU:HG	2.36	0.56
1:E:142:LEU:CD2	1:E:142:LEU:H	2.19	0.56
2:P:224:GLN:HG2	2:P:231:ILE:HG21	1.88	0.56
2:N:223:VAL:HG12	2:N:224:GLN:N	2.20	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:B:226:THR:HG22	2:B:253:THR:HB	1.88	0.56
1:A:188:ARG:HH12	1:A:199:LYS:H	1.51	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
2:F:28:VAL:O	2:F:156:VAL:HA	2.05	0.56
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
1:K:162:LEU:CD2	1:K:178:PRO:HD3	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: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)
2:P:30:VAL:HA	2:P:111:PRO:HB2	1.89	0.55
2:D:28:VAL:O	2:D:156:VAL:HA	2.07	0.55
1:K:22:VAL:CG2	1:K:65:LEU:HG	2.36	0.55
2:P:250:LEU:HB2	2:P:252:LEU:HG	1.87	0.55
1:A:197:THR:HB	1:A:198:PRO:HD2	1.88	0.55
2:H:207:SER:O	2:H:224:GLN:HG3	2.06	0.55
1:A:47:ARG:HH22	1:A:74:GLN:HB2	1.71	0.55
2:N:264:THR:CG2	2:N:265:ALA:H	2.16	0.55
1:I:154:GLU:OE2	1:I:188:ARG:HD3	2.06	0.55
2:F:71:PHE:CE2	2:F:111:PRO:HG3	2.41	0.55
2:D:120:ILE:HD13	2:D:126:ILE:HD11	1.87	0.55
2:H:226:THR:HG22	2:H:253:THR:HB	1.88	0.55
2:N:220:GLY:HA2	2:N:259:THR:OG1	2.07	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:O:22:VAL:CG2	1:O:65:LEU:HG	2.36	0.55
1:I:22:VAL:CG2	1:I:65:LEU:HG	2.37	0.55
2:B:207:SER:O	2:B:224:GLN:HG3	2.06	0.55
1:O:28:ASN:N	1:O:28:ASN:HD22	2.03	0.55
2:F:131:LEU:C	2:F:131:LEU:HD23	2.27	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: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: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: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:A:142:LEU:H	1:A:142:LEU:CD2	2.20	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
2:P:117:GLY:O	2:P:155:VAL:HA	2.06	0.55
2:L:30:VAL:HA	2:L:111:PRO:HB2	1.87	0.55
1:M:104:GLN:O	2:N:271:ILE:HA	2.07	0.55
1:I:28:ASN:N	1:I:28:ASN:HD22	2.03	0.55
2:B:136:ASN:C	2:B:136:ASN:HD22	2.09	0.55
2:J:28:VAL:O	2:J:156:VAL:HA	2.07	0.55
2:H:131:LEU:HD23	2:H:131:LEU:C	2.27	0.55
2:F:120:ILE:CG2	2:F:126:ILE:HD11	2.29	0.55
1:O:135:ARG:HH12	1:O:181:ALA:HB2	1.68	0.55
1:I:80:GLU:HG3	1:I:147:PRO:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:I:28:ASN:N	1:I:28:ASN:ND2	2.54	0.55
2:J:73:GLY:HA2	4:J:1611:HOH:O	2.06	0.55
2:N:250:LEU:HB2	2:N:252:LEU:HG	1.88	0.55
1:I:189:THR:O	1:I:196:LEU:HA	2.07	0.55
2:J:19:ASN:ND2	2:L:219:GLN:NE2	2.54	0.55
2:J:117:GLY:O	2:J:155:VAL:HA	2.07	0.55
1:M:28:ASN:H	1:M:28:ASN:HD22	1.54	0.55
2:L:4:LYS:HA	2:L:10:ALA:HA	1.89	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: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
1:M:28:ASN:N	1:M:28:ASN:ND2	2.54	0.55
2:L:250:LEU:HB2	2:L:252:LEU:HG	1.87	0.55
2:J:224:GLN:HG2	2:J:231:ILE:HG21	1.88	0.54
1:O:184:ASN:O	1:O:186:THR:HG23	2.08	0.54
1:K:28:ASN:HD22	1:K:28:ASN:H	1.54	0.54
2:H:71:PHE:CE2	2:H:111:PRO:HG3	2.42	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
1:M:115:TYR:O	1:M:117:PRO:HD3	2.08	0.54
2:J:4:LYS:HA	2:J:10:ALA:HA	1.89	0.54
2:L:200:THR:O	2:L:209:PHE:HA	2.07	0.54
2:P:200:THR:O	2:P:209:PHE:HA	2.07	0.54
2:P:28:VAL:O	2:P:156:VAL:HA	2.07	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
1:M:189:THR:O	1:M:196:LEU:HA	2.06	0.54
2:D:131:LEU:C	2:D:131:LEU:HD23	2.28	0.54
2:F:120:ILE:HD13	2:F:126:ILE:HD11	1.89	0.54
2:J:200:THR:O	2:J:209:PHE:HA	2.07	0.54
2:F:170:VAL:C	2:F:172:LEU:H	2.10	0.54
2:L:162:ASP:O	2:L:185:VAL:HG13	2.07	0.54
1:C:24:ASN:O	1:C:60:LYS:HA	2.06	0.54
1:K:104:GLN:O	2:L:271:ILE:HA	2.07	0.54
2:L:224:GLN:HG2	2:L:231:ILE:HG21	1.88	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:H:117:GLY:O	2:H:155:VAL:HA	2.07	0.54
2:N:200:THR:O	2:N:209:PHE:HA	2.08	0.54
2:F:172:LEU:O	2:F:173:PRO:C	2.46	0.54
1:O:162:LEU:CD2	1:O:178:PRO:HD3	2.36	0.54
1:I:185:ILE:HD12	1:I:204:MET:SD	2.48	0.54
2:N:60:ARG:HG3	2:N:61:GLY:N	2.22	0.54
2:D:71:PHE:CE2	2:D:111:PRO:HG3	2.42	0.54
2:J:201:THR:HA	2:J:209:PHE:HA	1.90	0.54
2:J:264:THR:CG2	2:J:265:ALA:H	2.16	0.54
2:L:264:THR:CG2	2:L:265:ALA:H	2.15	0.54
1:K:135:ARG:HH12	1:K:181:ALA:HB2	1.69	0.54
2:J:20:VAL:HG12	2:J:22:VAL:HG13	1.88	0.54
1:G:24:ASN:O	1:G:60:LYS:HA	2.07	0.54
2:L:74:THR:HB	2:L:82:TYR:O	2.07	0.54
1:I:115:TYR:O	1:I:117:PRO:HD3	2.07	0.54
2:F:5:THR:HG23	2:F:7:ASN:H	1.72	0.54
1:O:28:ASN:HD22	1:O:28:ASN:H	1.55	0.54
2:N:96:ASN:H	2:N:96:ASN:HD22	1.55	0.54
2:P:162:ASP:O	2:P:185:VAL:HG13	2.07	0.54
2:N:117:GLY:O	2:N:155:VAL:HA	2.07	0.54
1:K:154:GLU:OE2	1:K:188:ARG:HD3	2.06	0.54
1:I:28:ASN:H	1:I:28:ASN:HD22	1.54	0.54
2:L:201:THR:HA	2:L:209:PHE:HA	1.90	0.54
1:K:185:ILE:HD12	1:K:204:MET:SD	2.48	0.54
2:H:136:ASN:C	2:H:136:ASN:HD22	2.09	0.54
2:J:220:GLY:HA2	2:J:259:THR:OG1	2.07	0.54
2:N:28:VAL:O	2:N:156:VAL:HA	2.07	0.54
2:L:40:THR:O	2:L:40:THR:HG22	2.08	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
1:I:131:LEU:HD12	1:I:143:ILE:O	2.08	0.54
2:D:83:PRO:O	2:D:86:THR:HA	2.07	0.54
2:B:201:THR:CG2	2:B:206:ASN:HD22	2.20	0.54
2:H:201:THR:CG2	2:H:206:ASN:HA	2.29	0.54
1:E:183:SER:C	1:E:185:ILE:H	2.12	0.54
1:O:133:PHE:CE1	1:O:202:GLY:HA2	2.43	0.54
1:G:186:THR:HG21	1:G:199:LYS:HZ1	1.73	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
2:F:207:SER:O	2:F:224:GLN:HG3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:134:ARG:HD2	1:C:141:THR:HG22	1.91	0.53
1:G:140:LEU:HB2	1:G:177:LEU:HD22	1.90	0.53
1:G:133:PHE:CD2	1:G:140:LEU:HD21	2.31	0.53
1:M:185:ILE:HD12	1:M:204:MET:SD	2.48	0.53
2:P:71:PHE:HE2	2:P:111:PRO:HG3	1.74	0.53
1:A:193:TYR:O	2:B:158:THR:HG22	2.06	0.53
2:P:192:ASN:HB2	2:P:279:GLN:NE2	2.23	0.53
1:K:131:LEU:HD12	1:K:143:ILE:O	2.08	0.53
2:N:162:ASP:O	2:N:185:VAL:HG13	2.07	0.53
1:A:183:SER:C	1:A:185:ILE:H	2.12	0.53
1:O:185:ILE:HD12	1:O:204:MET:SD	2.48	0.53
1:G:183:SER:C	1:G:185:ILE:H	2.12	0.53
2:B:71:PHE:CE2	2:B:111:PRO:HG3	2.43	0.53
2:N:192:ASN:HB2	2:N:279:GLN:NE2	2.23	0.53
2:J:192:ASN:HB2	2:J:279:GLN:NE2	2.24	0.53
2:J:224:GLN:NE2	2:J:231:ILE:HD13	2.23	0.53
2:N:224:GLN:NE2	2:N:231:ILE:HD13	2.24	0.53
1:E:174:THR:O	1:E:174:THR:HG23	2.07	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:40:THR:HG22	2:N:40:THR:O	2.09	0.53
2:J:74:THR:HB	2:J:82:TYR:O	2.08	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:P:224:GLN:NE2	2:P:231:ILE:HD13	2.24	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
1:M:101:ASN:ND2	2:N:268:VAL:H	2.07	0.53
1:K:101:ASN:ND2	2:L:268:VAL:H	2.07	0.53
2:P:40:THR:O	2:P:40:THR:HG22	2.08	0.53
2:J:174:ASP:HB3	2:J:176:PRO:HD2	1.91	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
2:B:131:LEU:HD23	2:B:131:LEU:C	2.29	0.53
1:C:205:GLU:OXT	1:C:205:GLU:HG3	2.09	0.53
2:H:172:LEU:O	2:H:173:PRO:C	2.46	0.53
1:G:205:GLU:OXT	1:G:205:GLU:HG3	2.09	0.53
1:A:140:LEU:HB2	1:A:177:LEU:HD22	1.91	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)
1:K:133:PHE:CE1	1:K:202:GLY:HA2	2.44	0.53
1:I:133:PHE:CE1	1:I:202:GLY:HA2	2.43	0.53
2:P:20:VAL:HG12	2:P:22:VAL:HG13	1.89	0.53
2:N:71:PHE:HE2	2:N:111:PRO:HG3	1.73	0.53
2:H:83:PRO:O	2:H:86:THR:HA	2.08	0.53
2:P:4:LYS:HA	2:P:10:ALA:HA	1.90	0.53
1:C:186:THR:HG21	1:C:199:LYS:NZ	2.23	0.53
2:D:63:ALA:HB1	2:D:67:VAL:HG12	1.89	0.53
2:D:170:VAL:C	2:D:172:LEU:H	2.12	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
2:H:7:ASN:HB2	4:H:1661:HOH:O	2.09	0.53
2:D:211:ASN:C	2:D:211:ASN:HD22	2.12	0.53
2:L:220:GLY:HA2	2:L:259:THR:OG1	2.06	0.53
2:L:192:ASN:HB2	2:L:279:GLN:NE2	2.24	0.53
1:G:184:ASN:O	1:G:186:THR:HG23	2.08	0.53
1:I:101:ASN:ND2	2:J:268:VAL:H	2.07	0.53
1:C:197:THR:HB	1:C:198:PRO:HD2	1.90	0.53
1:M:191:ASN:HD21	1:M:195:ALA:HB3	1.74	0.53
2:N:201:THR:HA	2:N:209:PHE:HA	1.90	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:P:34:LEU:HD12	2:P:35:VAL:N	2.20	0.53
2:P:174:ASP:HB3	2:P:176:PRO:HD2	1.91	0.53
2:N:4:LYS:HA	2:N:10:ALA:HA	1.90	0.53
1:O:46:GLY:O	1:O:70:ALA:HB3	2.09	0.53
2:L:224:GLN:NE2	2:L:231:ILE:HD13	2.24	0.52
2:H:211:ASN:HD22	2:H:211:ASN:C	2.10	0.52
2:F:211:ASN:C	2:F:211:ASN:HD22	2.11	0.52
2:N:174:ASP:HB3	2:N:176:PRO:HD2	1.91	0.52
1:M:28:ASN:O	1:M:29:SER:HB3	2.09	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
1:C:183:SER:C	1:C:185:ILE:H	2.12	0.52
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:H:167:ASP:CG	2:H:168:VAL:N	2.50	0.52
2:B:185:VAL:HG23	2:B:243:VAL:HG11	1.90	0.52
1:E:22:VAL:CG2	1:E:65:LEU:HG	2.39	0.52
2:J:78:SER:H	2:J:104:PRO:HB2	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:120:ILE:HD13	2:B:126:ILE:HD11	1.90	0.52
2:L:208:ILE:HG21	2:L:259:THR:HG22	1.91	0.52
2:D:117:GLY:O	2:D:155:VAL:HA	2.08	0.52
1:A:184:ASN:O	1:A:186:THR:HG23	2.08	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
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
2:D:22:VAL:HG23	2:D:22:VAL:O	2.09	0.52
2:B:174:ASP:O	2:B:176:PRO:CD	2.58	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:I:140:LEU:HD23	1:I:141:THR:N	2.25	0.52
2:N:208:ILE:HG21	2:N:259:THR:HG22	1.92	0.52
1:G:186:THR:HG21	1:G:199:LYS:NZ	2.23	0.52
1:C:122:LEU:CD1	1:C:126:GLN:HB3	2.40	0.52
2:H:185:VAL:HG23	2:H:243:VAL:HG11	1.92	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
1:O:191:ASN:HD21	1:O:195:ALA:HB3	1.74	0.52
1:O:140:LEU:HD23	1:O:141:THR:N	2.25	0.52
2:N:14:GLY:HA2	2:N:142:PHE:CD1	2.45	0.52
1:M:131:LEU:HD12	1:M:143:ILE:O	2.08	0.52
2:B:83:PRO:O	2:B:86:THR:HA	2.08	0.52
2:H:174:ASP:O	2:H:176:PRO:CD	2.58	0.52
2:L:43:PHE:CD1	2:L:43:PHE:N	2.78	0.52
1:O:28:ASN:O	1:O:29:SER:HB3	2.09	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:B:211:ASN:C	2:B:211:ASN:HD22	2.12	0.52
1:K:140:LEU:HD23	1:K:141:THR:N	2.25	0.52
2:J:40:THR:O	2:J:40:THR:HG22	2.09	0.52
2:P:14:GLY:HA2	2:P:142:PHE:CD1	2.45	0.52
2:B:5:THR:HG23	2:B:7:ASN:H	1.73	0.52
1:C:186:THR:HG21	1:C:199:LYS:HZ1	1.75	0.51
2:B:173:PRO:HG3	2:B:179:VAL:CG1	2.39	0.51
1:E:205:GLU:HG3	1:E:205:GLU:OXT	2.09	0.51
2:N:164:SER:HB2	2:N:184:THR:O	2.10	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)
1:I:191:ASN:HD21	1:I:195:ALA:HB3	1.74	0.51
2:H:63:ALA:HB1	2:H:67:VAL:HG12	1.91	0.51
2:D:172:LEU:O	2:D:173:PRO:C	2.47	0.51
2:H:170:VAL:C	2:H:172:LEU:H	2.12	0.51
1:A:186:THR:HG21	1:A:199:LYS:NZ	2.25	0.51
1:O:160:ARG:CG	1:O:178:PRO:HG3	2.41	0.51
2:N:34:LEU:HD12	2:N:35:VAL:N	2.20	0.51
1:A:85:MET:O	1:A:110:ARG:HA	2.10	0.51
2:F:33:ASN:ND2	2:F:110:THR:OG1	2.44	0.51
1:C:144:ASN:OD1	1:C:146:THR:HG23	2.10	0.51
2:L:14:GLY:HA2	2:L:142:PHE:CD1	2.45	0.51
2:F:185:VAL:HG23	2:F:243:VAL:HG11	1.91	0.51
2:N:78:SER:H	2:N:104:PRO:HB2	1.75	0.51
1:A:133:PHE:CD2	1:A:140:LEU:HD21	2.30	0.51
1:M:160:ARG:CG	1:M:178:PRO:HG3	2.41	0.51
1:E:85:MET:O	1:E:110:ARG:HA	2.10	0.51
2:N:207:SER:O	2:N:224:GLN:HG3	2.10	0.51
2:H:211:ASN:ND2	2:H:269:GLN:H	2.09	0.51
2:P:208:ILE:HG21	2:P:259:THR:HG22	1.92	0.51
1:A:144:ASN:OD1	1:A:146:THR:HG23	2.10	0.51
1:G:144:ASN:OD1	1:G:146:THR:HG23	2.11	0.51
1:E:122:LEU:CD1	1:E:126:GLN:HB3	2.40	0.51
1:I:28:ASN:O	1:I:29:SER:HB3	2.09	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
2:L:215:PHE:CD2	2:L:215:PHE:C	2.84	0.51
2:D:211:ASN:HD21	2:D:269:GLN:H	1.58	0.51
1:A:1:GLY:H1	1:A:26:ASP:CG	2.14	0.51
2:H:50:GLU:CD	2:H:50:GLU:H	2.14	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:N	2:N:43:PHE:CD1	2.78	0.51
1:A:122:LEU:CD1	1:A:126:GLN:HB3	2.40	0.51
1:C:13:ALA:HB3	1:C:118:ALA:H	1.76	0.51
2:B:117:GLY:O	2:B:155:VAL:HA	2.09	0.51
2:H:120:ILE:CG2	2:H:126:ILE:HD11	2.31	0.51
2:J:67:VAL:HG21	2:J:126:ILE:CG2	2.35	0.51
2:J:208:ILE:HG21	2:J:259:THR:HG22	1.91	0.51
2:F:67:VAL:CG2	2:F:126:ILE:HG12	2.41	0.51
1:M:140:LEU:HD23	1:M:141:THR:N	2.25	0.51
2:P:190:SER:HA	2:P:244:GLY:HA2	1.93	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:A:22:VAL:CG2	1:A:65:LEU:HG	2.41	0.51
1:I:66:ARG:HH11	1:I:66:ARG:HG2	1.75	0.51
1:M:66:ARG:HH11	1:M:66:ARG:HG2	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
2:P:43:PHE:CD1	2:P:43:PHE:N	2.78	0.51
2:D:5:THR:HG23	2:D:7:ASN:H	1.76	0.51
1:C:22:VAL:CG2	1:C:65:LEU:HG	2.41	0.51
1:K:66:ARG:HH11	1:K:66:ARG:HG2	1.76	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:A:205:GLU:HG3	1:A:205:GLU:OXT	2.10	0.51
1:I:160:ARG:CG	1:I:178:PRO:HG3	2.41	0.51
2:P:164:SER:HB2	2:P:184:THR:O	2.11	0.51
1:O:67:ILE:N	1:O:67:ILE:HD12	2.26	0.51
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
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
2:B:163:VAL:CG1	2:B:183:LEU:HD21	2.41	0.50
2:N:96:ASN:N	2:N:96:ASN:ND2	2.60	0.50
2:D:226:THR:HG22	2:D:253:THR:HB	1.94	0.50
2:L:163:VAL:HA	2:L:185:VAL:CG2	2.35	0.50
2:B:227:ARG:HA	2:B:251:GLY:O	2.11	0.50
1:I:9:VAL:O	1:I:113:LEU:HA	2.11	0.50
2:B:131:LEU:HB3	2:B:144:PHE:HB2	1.93	0.50
2:B:174:ASP:O	2:B:176:PRO:HD2	2.11	0.50
2:L:202:ALA:HB2	2:L:210:THR:CG2	2.34	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
1:A:13:ALA:HB3	1:A:118:ALA:H	1.76	0.50
2:J:96:ASN:N	2:J:96:ASN:ND2	2.59	0.50
2:P:96:ASN:ND2	2:P:96:ASN:N	2.59	0.50
2:J:215:PHE:C	2:J:215:PHE:CD2	2.84	0.50
2:J:207:SER:O	2:J:224:GLN:HG3	2.10	0.50
1:K:47:ARG:HH22	1:K:74:GLN:HB2	1.76	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

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:211:ASN:ND2	2:B:269:GLN:H	2.10	0.49
1:O:149:TYR:CD2	1:O:168:PRO:HA	2.47	0.49
1:C:11:TYR:CE2	1:C:69:ASP:HB2	2.47	0.49
1:G:22:VAL:CG2	1:G:65:LEU:HG	2.42	0.49
2:L:190:SER:HA	2:L:244:GLY:HA2	1.93	0.49
1:K:79:ARG:HB3	1:K:170:MET:HE3	1.93	0.49
1:E:142:LEU:HD22	1:E:142:LEU:H	1.77	0.49
2:B:22:VAL:HG23	2:B:22:VAL:O	2.11	0.49
1:M:67:ILE:N	1:M:67:ILE:HD12	2.26	0.49
2:B:50:GLU:CD	2:B:50:GLU:H	2.14	0.49
2:J:225:LEU:O	2:J:231:ILE:HG23	2.12	0.49
1:I:47:ARG:HH22	1:I:74:GLN:HB2	1.76	0.49
1:G:94:ASP:CG	2:H:168:VAL:HG11	2.33	0.49
1:E:94:ASP:CG	2:F:168:VAL:HG11	2.32	0.49
1:I:149:TYR:CD2	1:I:168:PRO:HA	2.47	0.49
1:A:12:PRO:HD2	1:A:15:GLN:HG3	1.93	0.49
2:L:271:ILE:HD12	2:L:271:ILE:N	2.28	0.49
2:F:227:ARG:HA	2:F:251:GLY:O	2.12	0.49
2:B:163:VAL:HG13	2:B:183:LEU:HD21	1.95	0.49
1:C:186:THR:CG2	1:C:199:LYS:NZ	2.75	0.49
2:J:253:THR:HG22	2:J:255:ASN:ND2	2.21	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:J:145:VAL:HG12	2:J:146:TRP:N	2.27	0.49
2:N:208:ILE:HG23	2:N:257:ALA:CB	2.40	0.49
1:K:149:TYR:CD2	1:K:168:PRO:HA	2.47	0.49
2:P:271:ILE:N	2:P:271:ILE:HD12	2.28	0.49
1:K:11:TYR:CZ	1:K:69:ASP:HB2	2.47	0.49
2:J:75:VAL:HG13	2:J:75:VAL:O	2.11	0.49
2:N:225:LEU:O	2:N:231:ILE:HG23	2.12	0.49
1:K:41:ASP:HB2	1:K:43:VAL:HG12	1.94	0.49
1:O:41:ASP:HB2	1:O:43:VAL:HG12	1.94	0.49
1:A:156:ASN:C	1:A:158:GLY:H	2.16	0.49
2:L:21:TYR:CB	2:L:151:ASN:HD21	2.24	0.49
2:J:164:SER:HB2	2:J:184:THR:O	2.11	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
1:M:9:VAL:O	1:M:113:LEU:HA	2.11	0.49
1:A:132:ARG:HB3	1:A:205:GLU:HB3	1.93	0.49
2:N:145:VAL:HG12	2:N:146:TRP:N	2.27	0.49
1:M:140:LEU:HD22	1:M:142:LEU:HD22	1.95	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:I:11:TYR:CZ	1:I:69:ASP:HB2	2.47	0.49
1:O:11:TYR:CZ	1:O:69:ASP:HB2	2.47	0.49
2:D:163:VAL:CG1	2:D:183:LEU:HD21	2.43	0.49
2:P:227:ARG:HA	2:P:251:GLY:O	2.13	0.49
2:P:66:GLY:HA3	2:P:119:ALA:O	2.12	0.49
1:M:98:LEU:HD13	1:M:98:LEU:C	2.33	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:E:13:ALA:HB3	1:E:118:ALA:H	1.76	0.49
1:O:39:ASN:CG	1:O:43:VAL:HG13	2.33	0.49
2:J:126:ILE:HD12	2:J:148:ILE:HG22	1.94	0.49
1:K:140:LEU:HD22	1:K:142:LEU:HD22	1.95	0.49
1:O:140:LEU:HD22	1:O:142:LEU:HD22	1.95	0.49
1:A:12:PRO:HB2	1:A:15:GLN:HG2	1.93	0.49
2:N:271:ILE:HD12	2:N:271:ILE:N	2.27	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:45:HIS:HB3	2:J:100:ASP:HA	1.95	0.49
2:B:67:VAL:CG2	2:B:126:ILE:HG12	2.42	0.49
2:H:185:VAL:HG11	2:H:276:PHE:CE2	2.48	0.49
2:F:185:VAL:HG11	2:F:276:PHE:CE2	2.48	0.49
2:P:225:LEU:O	2:P:231:ILE:HG23	2.13	0.49
2:F:173:PRO:O	2:F:256:TYR:HE1	1.96	0.49
1:I:47:ARG:HH22	1:I:74:GLN:NE2	1.92	0.49
2:P:163:VAL:HA	2:P:185:VAL:CG2	2.35	0.49
1:G:156:ASN:C	1:G:158:GLY:H	2.16	0.49
2:L:270:SER:C	2:L:271:ILE:HD12	2.33	0.49
2:J:271:ILE:N	2:J:271:ILE:HD12	2.27	0.49
1:M:11:TYR:CZ	1:M:69:ASP:HB2	2.47	0.49
2:F:163:VAL:CG1	2:F:183:LEU:HD21	2.42	0.49
2:D:163:VAL:HG13	2:D:183:LEU:HD21	1.95	0.49
1:K:98:LEU:HD13	1:K:98:LEU:C	2.33	0.49
1:M:39:ASN:HB3	1:M:45:ASP:OD2	2.13	0.48
1:I:39:ASN:CG	1:I:43:VAL:HG13	2.32	0.48
2:H:211:ASN:ND2	2:H:211:ASN:C	2.66	0.48
1:I:27:GLU:HA	1:I:60:LYS:CG	2.43	0.48
1:I:140:LEU:HD22	1:I:142:LEU:HD22	1.95	0.48
2:J:34:LEU:HD12	2:J:35:VAL:N	2.21	0.48
1:C:12:PRO:HD2	1:C:15:GLN:HG3	1.94	0.48
2:N:267:ASN:HB3	2:N:269:GLN:HE21	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:270:SER:C	2:J:271:ILE:HD12	2.33	0.48
2:H:227:ARG:HA	2:H:251:GLY:O	2.13	0.48
2:L:131:LEU:HD23	2:L:131:LEU:C	2.33	0.48
2:F:66:GLY:HA3	2:F:119:ALA:O	2.13	0.48
1:K:39:ASN:HB3	1:K:45:ASP:OD2	2.13	0.48
2:J:202:ALA:HB2	2:J:210:THR:CG2	2.34	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
1:K:101:ASN:HD22	2:L:268:VAL:CG2	2.24	0.48
2:P:267:ASN:HB3	2:P:269:GLN:HE21	1.78	0.48
1:G:13:ALA:HB3	1:G:118:ALA:H	1.76	0.48
2:P:75:VAL:O	2:P:75:VAL:HG13	2.13	0.48
2:H:66:GLY:HA3	2:H:119:ALA:O	2.14	0.48
2:B:63:ALA:HB1	2:B:67:VAL:HG12	1.94	0.48
1:I:41:ASP:HB2	1:I:43:VAL:HG12	1.94	0.48
2:F:211:ASN:ND2	2:F:211:ASN:C	2.66	0.48
2:D:166:ARG:O	2:D:167:ASP:HB2	2.14	0.48
1:O:101:ASN:HD22	2:P:268:VAL:CG2	2.23	0.48
2:N:270:SER:C	2:N:271:ILE:HD12	2.33	0.48
2:P:270:SER:C	2:P:271:ILE:HD12	2.33	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
1:A:142:LEU:H	1:A:142:LEU:HD22	1.78	0.48
1:G:93:MET:CE	1:G:98:LEU:HD23	2.43	0.48
1:I:39:ASN:HB3	1:I:45:ASP:OD2	2.13	0.48
2:B:166:ARG:O	2:B:167:ASP:HB2	2.13	0.48
2:L:145:VAL:HG12	2:L:146:TRP:N	2.28	0.48
1:E:11:TYR:CE2	1:E:69:ASP:HB2	2.49	0.48
2:J:96:ASN:N	2:J:96:ASN:HD22	2.10	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
2:P:215:PHE:CD2	2:P:215:PHE:C	2.84	0.48
1:M:39:ASN:CG	1:M:43:VAL:HG13	2.33	0.48
2:H:172:LEU:N	2:H:173:PRO:CD	2.75	0.48
2:D:33:ASN:ND2	2:D:110:THR:OG1	2.46	0.48
2:P:38:LEU:C	2:P:40:THR:N	2.67	0.48
2:P:45:HIS:HB3	2:P:100:ASP:HA	1.96	0.48
2:D:66:GLY:HA3	2:D:119:ALA:O	2.13	0.48
2:P:253:THR:HG22	2:P:255:ASN:ND2	2.22	0.48
1:O:39:ASN:HB3	1:O:45:ASP:OD2	2.13	0.48
1:A:71:THR:HG23	1:A:71:THR:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:136:ASN:C	2:D:136:ASN:ND2	2.67	0.48
2:J:17:SER:HB2	2:L:262:GLN:OE1	2.13	0.48
2:B:33:ASN:ND2	2:B:110:THR:OG1	2.46	0.48
1:G:11:TYR:CE2	1:G:69:ASP:HB2	2.48	0.48
2:N:131:LEU:C	2:N:131:LEU:HD23	2.34	0.48
1:K:6:ALA:HB3	1:K:20:LEU:CD1	2.43	0.48
2:B:181:ILE:HB	2:B:252:LEU:HB2	1.95	0.48
1:O:98:LEU:HD13	1:O:98:LEU:C	2.33	0.48
2:B:66:GLY:HA3	2:B:119:ALA:O	2.13	0.48
1:C:140:LEU:H	1:C:177:LEU:HB2	1.79	0.48
2:N:227:ARG:CD	2:N:232:ILE:HD11	2.44	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:B:172:LEU:N	2:B:173:PRO:CD	2.76	0.48
1:M:27:GLU:HA	1:M:60:LYS:CG	2.43	0.48
2:F:166:ARG:O	2:F:167:ASP:HB2	2.14	0.48
2:N:17:SER:HB2	2:P:262:GLN:OE1	2.13	0.48
2:L:38:LEU:C	2:L:40:THR:N	2.67	0.48
2:L:45:HIS:HB3	2:L:100:ASP:HA	1.96	0.48
1:M:37:VAL:HG11	1:M:48:PHE:HB2	1.96	0.48
2:L:227:ARG:HA	2:L:251:GLY:O	2.13	0.48
2:D:173:PRO:O	2:D:256:TYR:HE1	1.97	0.48
1:G:140:LEU:H	1:G:177:LEU:HB2	1.78	0.48
1:E:186:THR:HG21	1:E:199:LYS:HZ1	1.79	0.48
1:E:140:LEU:H	1:E:177:LEU:HB2	1.78	0.48
1:O:79:ARG:HB3	1:O:170:MET:HE3	1.94	0.48
2:D:77:TYR:CE2	2:D:90:THR:HG21	2.49	0.48
2:D:173:PRO:HG3	2:D:179:VAL:CG1	2.40	0.48
1:A:186:THR:CG2	1:A:199:LYS:NZ	2.76	0.48
2:N:218:ALA:HA	2:N:264:THR:HB	1.96	0.48
2:P:164:SER:O	2:P:183:LEU:HD23	2.13	0.48
2:J:267:ASN:HB3	2:J:269:GLN:HE21	1.78	0.48
2:N:96:ASN:N	2:N:96:ASN:HD22	2.12	0.48
1:E:1:GLY:N	1:E:26:ASP:OD1	2.46	0.48
1:K:37:VAL:HG11	1:K:48:PHE:HB2	1.96	0.48
1:I:133:PHE:HD2	1:I:140:LEU:HD21	1.79	0.48
2:L:96:ASN:ND2	2:L:96:ASN:H	2.11	0.48
2:D:227:ARG:HA	2:D:251:GLY:O	2.13	0.48
2:N:45:HIS:HB3	2:N:100:ASP:HA	1.95	0.48
2:L:75:VAL:O	2:L:75:VAL:HG13	2.14	0.48
1:M:41:ASP:HB2	1:M:43:VAL:HG12	1.94	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:173:PRO:O	2:H:256:TYR:HE1	1.97	0.47
1:G:71:THR:HG23	1:G:71:THR:O	2.13	0.47
1:E:156:ASN:C	1:E:158:GLY:H	2.17	0.47
1:E:186:THR:CG2	1:E:199:LYS:NZ	2.76	0.47
1:M:135:ARG:HH22	1:M:181:ALA:CB	2.27	0.47
2:L:164:SER:O	2:L:183:LEU:HD23	2.13	0.47
1:G:1:GLY:N	1:G:26:ASP:CG	2.68	0.47
1:C:134:ARG:NE	1:C:141:THR:HG21	2.28	0.47
2:B:173:PRO:O	2:B:256:TYR:HE1	1.98	0.47
1:K:39:ASN:CG	1:K:43:VAL:HG13	2.33	0.47
1:C:71:THR:O	1:C:71:THR:HG23	2.14	0.47
1:K:135:ARG:HH22	1:K:181:ALA:CB	2.27	0.47
1:I:135:ARG:HH22	1:I:181:ALA:CB	2.27	0.47
2:J:164:SER:O	2:J:183:LEU:HD23	2.14	0.47
2:J:131:LEU:C	2:J:131:LEU:HD23	2.34	0.47
2:D:181:ILE:HB	2:D:252:LEU:HB2	1.96	0.47
1:I:98:LEU:C	1:I:98:LEU:HD13	2.33	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
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:F:163:VAL:HG13	2:F:183:LEU:HD21	1.96	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
1:M:47:ARG:NH2	1:M:74:GLN:NE2	2.59	0.47
1:A:186:THR:HG21	1:A:199:LYS:HZ1	1.79	0.47
2:P:267:ASN:CB	2:P:269:GLN:HE21	2.28	0.47
2:D:184:THR:HG22	2:D:249:SER:CA	2.43	0.47
2:P:227:ARG:CD	2:P:232:ILE:HD11	2.44	0.47
1:I:6:ALA:HB3	1:I:20:LEU:CD1	2.44	0.47
2:N:75:VAL:O	2:N:75:VAL:HG13	2.14	0.47
1:E:71:THR:HG23	1:E:71:THR:O	2.15	0.47
2:P:218:ALA:HA	2:P:264:THR:HB	1.96	0.47
2:N:163:VAL:HA	2:N:185:VAL:CG2	2.36	0.47
2:L:218:ALA:HA	2:L:264:THR:HB	1.96	0.47
1:O:27:GLU:HA	1:O:60:LYS:CG	2.43	0.47
1:O:133:PHE:HD2	1:O:140:LEU:HD21	1.79	0.47
1:E:12:PRO:HB2	1:E:15:GLN:HG2	1.96	0.47
1:O:6:ALA:HB3	1:O:20:LEU:CD1	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:131:LEU:HD23	2:P:131:LEU:C	2.33	0.47
2:F:181:ILE:HB	2:F:252:LEU:HB2	1.97	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:K:178:PRO:O	1:K:179:SER:HB3	2.15	0.47
1:I:185:ILE:O	1:I:202:GLY:N	2.35	0.47
2:B:77:TYR:CE2	2:B:90:THR:HG21	2.50	0.47
1:A:11:TYR:CE2	1:A:69:ASP:HB2	2.50	0.47
2:J:227:ARG:CD	2:J:232:ILE:HD11	2.44	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
2:B:60:ARG:CZ	2:B:60:ARG:HB2	2.45	0.47
1:C:141:THR:HB	1:C:174:THR:CG2	2.41	0.47
2:P:226:THR:CG2	2:P:253:THR:HB	2.43	0.47
2:N:226:THR:CG2	2:N:253:THR:HB	2.42	0.47
1:K:47:ARG:HH22	1:K:74:GLN:NE2	1.92	0.47
1:G:140:LEU:C	1:G:140:LEU:HD23	2.35	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:O:178:PRO:O	1:O:179:SER:HB3	2.15	0.47
1:K:27:GLU:HA	1:K:60:LYS:CG	2.44	0.47
2:F:136:ASN:ND2	2:F:136:ASN:C	2.68	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:J:227:ARG:HA	2:J:251:GLY:O	2.13	0.47
2:P:66:GLY:HA2	2:P:70:ASN:HD22	1.79	0.47
1:C:142:LEU:HD22	1:C:142:LEU:H	1.78	0.47
2:D:240:LEU:HD21	2:D:250:LEU:HD22	1.96	0.47
2:L:179:VAL:O	2:L:179:VAL:HG23	2.15	0.47
1:C:33:ILE:O	1:C:54:LEU:HA	2.15	0.47
1:E:30:THR:HG22	1:E:31:TYR:N	2.30	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:95:LYS:HD3	1:E:95:LYS:N	2.30	0.47
2:D:201:THR:HG23	2:D:203:ASP:H	1.79	0.47
1:M:178:PRO:O	1:M:179:SER:HB3	2.15	0.47
1:K:133:PHE:HD2	1:K:140:LEU:HD21	1.79	0.47
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:I:11:TYR:OH	1:I:69:ASP:HB2	2.14	0.47
2:N:1:PHE:HD1	2:N:144:PHE:CZ	2.33	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1:GLY:N	1:G:26:ASP:OD1	2.48	0.47
1:G:142:LEU:HD22	1:G:142:LEU:H	1.78	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
2:H:41:GLN:NE2	4:H:1627:HOH:O	2.47	0.47
2:N:179:VAL:HG23	2:N:179:VAL:O	2.15	0.47
2:L:13:ILE:HG23	3:L:1504:MAN:C2	2.45	0.47
2:L:224:GLN:HE21	2:L:231:ILE:HD13	1.80	0.47
2:D:211:ASN:C	2:D:211:ASN:ND2	2.67	0.47
1:A:140:LEU:C	1:A:140:LEU:HD23	2.35	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:C:156:ASN:C	1:C:158:GLY:H	2.17	0.47
2:H:201:THR:HG23	2:H:203:ASP:H	1.80	0.47
1:A:140:LEU:H	1:A:177:LEU:HB2	1.79	0.47
2:D:192:ASN:HA	2:D:241:GLY:O	2.15	0.47
2:J:103:TRP:CE2	2:J:105:VAL:HG21	2.50	0.47
2:B:185:VAL:HG11	2:B:276:PHE:CE2	2.50	0.47
1:O:37:VAL:HG11	1:O:48:PHE:HB2	1.96	0.47
2:B:195:TYR:CE1	2:B:238:VAL:HB	2.50	0.47
1:I:37:VAL:HG11	1:I:48:PHE:HB2	1.96	0.47
1:M:61:LYS:O	1:M:62:GLU:HB2	2.15	0.47
2:L:253:THR:HG22	2:L:255:ASN:ND2	2.22	0.46
2:D:201:THR:CG2	2:D:206:ASN:HA	2.29	0.46
1:M:133:PHE:HD2	1:M:140:LEU:HD21	1.79	0.46
2:H:29:ASN:HA	4:H:1629:HOH:O	2.13	0.46
1:G:12:PRO:HD2	1:G:15:GLN:HG3	1.95	0.46
2:L:1:PHE:HD1	2:L:144:PHE:CZ	2.33	0.46
2:J:96:ASN:H	2:J:96:ASN:ND2	2.12	0.46
2:L:250:LEU:HD13	2:L:252:LEU:HD11	1.97	0.46
2:N:96:ASN:ND2	2:N:96:ASN:H	2.13	0.46
2:F:22:VAL:HG23	2:F:22:VAL:O	2.13	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:B:211:ASN:C	2:B:211:ASN:ND2	2.68	0.46
1:I:178:PRO:O	1:I:179:SER:HB3	2.15	0.46
2:H:136:ASN:C	2:H:136:ASN:ND2	2.68	0.46
2:N:38:LEU:C	2:N:40:THR:N	2.67	0.46
1:O:11:TYR:OH	1:O:69:ASP:HB2	2.14	0.46
2:N:66:GLY:HA2	2:N:70:ASN:HD22	1.80	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:H:215:PHE:O	2:H:216:SER:C	2.54	0.46
2:N:53:THR:H	2:N:136:ASN:ND2	2.13	0.46
2:H:60:ARG:CZ	2:H:60:ARG:HB2	2.45	0.46
1:I:95:LYS:N	1:I:95:LYS:HD3	2.30	0.46
2:F:63:ALA:HB1	2:F:67:VAL:HG12	1.96	0.46
1:A:72:ASN:O	1:A:74:GLN:HG3	2.16	0.46
1:O:160:ARG:HG3	1:O:178:PRO:HG3	1.98	0.46
2:J:21:TYR:CB	2:J:151:ASN:HD21	2.24	0.46
1:G:12:PRO:HB2	1:G:15:GLN:HG2	1.96	0.46
1:A:94:ASP:C	1:A:96:SER:H	2.18	0.46
1:I:142:LEU:HB2	1:I:173:SER:O	2.16	0.46
2:B:136:ASN:C	2:B:136:ASN:ND2	2.68	0.46
1:A:12:PRO:CB	1:A:15:GLN:HG3	2.45	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:C:1:GLY:H1	1:C:26:ASP:CG	2.19	0.46
2:H:195:TYR:CE1	2:H:238:VAL:HB	2.49	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:G:33:ILE:O	1:G:54:LEU:HA	2.15	0.46
2:B:113:SER:OG	2:P:81:SER:N	2.47	0.46
2:P:197:LEU:CD1	2:P:225:LEU:HD12	2.42	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
1:C:12:PRO:HB2	1:C:15:GLN:HG2	1.95	0.46
2:P:1:PHE:HD1	2:P:144:PHE:CZ	2.33	0.46
1:E:33:ILE:O	1:E:54:LEU:HA	2.14	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
2:F:88:SER:HA	4:F:1572:HOH:O	2.16	0.46
1:C:30:THR:HG22	1:C:31:TYR:N	2.30	0.46
2:F:60:ARG:CZ	2:F:60:ARG:HB2	2.45	0.46
1:C:140:LEU:C	1:C:140:LEU:HD23	2.35	0.46
2:F:201:THR:HG23	2:F:203:ASP:H	1.80	0.46
2:J:24:LEU:O	2:J:26:PRO:N	2.49	0.46
1:O:177:LEU:HD12	1:O:178:PRO:CD	2.40	0.46
2:N:19:ASN:HD21	2:P:219:GLN:CD	2.19	0.46
1:I:102:THR:H	2:J:269:GLN:HG2	1.80	0.46
1:M:102:THR:H	2:N:269:GLN:HG2	1.80	0.46
2:L:83:PRO:O	2:L:86:THR:HA	2.15	0.46
2:P:250:LEU:HD13	2:P:252:LEU:HD11	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:C:95:LYS:HD3	1:C:95:LYS:N	2.30	0.46
2:P:224:GLN:HE21	2:P:231:ILE:HD13	1.81	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:K:39:ASN:HD21	1:K:43:VAL:CG1	2.18	0.46
1:C:72:ASN:O	1:C:74:GLN:HG3	2.16	0.46
1:A:138:ASN:CA	1:A:177:LEU:HB3	2.46	0.46
1:E:181:ALA:HB1	1:E:182:GLY:H	1.53	0.46
1:K:136:SER:HB2	1:K:139:SER:H	1.81	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:J:208:ILE:HG23	2:J:257:ALA:CB	2.40	0.46
1:I:79:ARG:HB3	1:I:170:MET:HE3	1.96	0.46
2:J:66:GLY:HA2	2:J:70:ASN:HD22	1.80	0.46
2:J:250:LEU:HD13	2:J:252:LEU:HD11	1.96	0.46
2:B:215:PHE:O	2:B:216:SER:C	2.54	0.46
2:B:135:ASN:HD21	2:B:138:ASN:HD21	1.63	0.46
2:J:53:THR:H	2:J:136:ASN:ND2	2.13	0.46
2:J:179:VAL:O	2:J:179:VAL:HG23	2.15	0.46
1:G:95:LYS:HD3	1:G:95:LYS:N	2.31	0.46
1:C:160:ARG:HG2	1:C:178:PRO:HG3	1.98	0.46
1:M:136:SER:HB2	1:M:139:SER:H	1.81	0.46
2:J:203:ASP:OD1	2:J:208:ILE:HD12	2.16	0.46
2:L:184:THR:OG1	2:L:247:ALA:HB1	2.16	0.46
1:K:12:PRO:HB2	1:K:15:GLN:HG3	1.97	0.46
1:G:86:ASN:ND2	1:G:110:ARG:HB2	2.31	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
2:D:131:LEU:HB3	2:D:144:PHE:HB2	1.97	0.46
2:B:13:ILE:HG13	4:B:1545:HOH:O	2.15	0.46
1:K:95:LYS:N	1:K:95:LYS:HD3	2.30	0.46
2:D:67:VAL:CG2	2:D:126:ILE:HG12	2.46	0.46
2:N:24:LEU:O	2:N:26:PRO:N	2.49	0.46
2:P:24:LEU:O	2:P:26:PRO:N	2.49	0.46
1:E:140:LEU:HD23	1:E:140:LEU:C	2.36	0.46
2:L:203:ASP:OD1	2:L:208:ILE:HD12	2.15	0.46
1:M:78:ASP:O	1:M:170:MET:HE1	2.16	0.46
1:O:102:THR:H	2:P:269:GLN:HG2	1.80	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)
2:P:83:PRO:O	2:P:86:THR:HA	2.16	0.46
2:J:175:TYR:N	2:J:176:PRO:CD	2.79	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:N:195:TYR:O	2:N:237:THR:HA	2.16	0.46
2:F:215:PHE:O	2:F:216:SER:C	2.54	0.46
1:G:72:ASN:O	1:G:74:GLN:HG3	2.16	0.46
1:A:160:ARG:HG2	1:A:178:PRO:HG3	1.98	0.46
1:K:142:LEU:HB2	1:K:173:SER:O	2.16	0.46
1:E:94:ASP:C	1:E:96:SER:H	2.19	0.46
2:N:267:ASN:CB	2:N:269:GLN:HE21	2.28	0.46
2:P:103:TRP:CE2	2:P:105:VAL:HG21	2.51	0.46
1:C:1:GLY:N	1:C:26:ASP:CG	2.70	0.46
1:O:57:MET:HA	1:O:61:LYS:CE	2.46	0.46
1:G:129:GLU:HG3	1:G:129:GLU:H	1.52	0.46
1:O:95:LYS:N	1:O:95:LYS:HD3	2.30	0.46
2:P:179:VAL:O	2:P:179:VAL:HG23	2.15	0.46
1:E:72:ASN:O	1:E:74:GLN:HG3	2.16	0.45
1:E:160:ARG:HG2	1:E:178:PRO:HG3	1.98	0.45
2:P:208:ILE:HG23	2:P:257:ALA:CB	2.40	0.45
1:A:86:ASN:ND2	1:A:110:ARG:HB2	2.31	0.45
2:P:184:THR:OG1	2:P:247:ALA:HB1	2.16	0.45
2:L:267:ASN:CB	2:L:269:GLN:HE21	2.28	0.45
1:E:191:ASN:ND2	1:E:195:ALA:HB3	2.31	0.45
2:N:83:PRO:O	2:N:86:THR:HA	2.17	0.45
2:N:250:LEU:HD13	2:N:252:LEU:HD11	1.97	0.45
2:L:250:LEU:CD1	2:L:252:LEU:HD11	2.47	0.45
1:M:57:MET:HA	1:M:61:LYS:CE	2.46	0.45
1:C:28:ASN:O	1:C:29:SER:HB3	2.15	0.45
1:I:57:MET:HA	1:I:61:LYS:CE	2.46	0.45
1:C:94:ASP:C	1:C:96:SER:H	2.19	0.45
2:L:34:LEU:HD12	2:L:35:VAL:N	2.21	0.45
2:J:250:LEU:CD1	2:J:252:LEU:HD11	2.47	0.45
1:E:28:ASN:O	1:E:29:SER:HB3	2.17	0.45
1:K:57:MET:HA	1:K:61:LYS:CE	2.46	0.45
1:C:141:THR:HA	1:C:174:THR:HA	1.98	0.45
2:J:224:GLN:HE21	2:J:231:ILE:HD13	1.80	0.45
1:A:186:THR:HB	1:A:199:LYS:NZ	2.32	0.45
1:I:136:SER:HB2	1:I:139:SER:H	1.81	0.45
2:P:175:TYR:N	2:P:176:PRO:CD	2.80	0.45
2:J:83:PRO:O	2:J:86:THR:HA	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:N:96:ASN:O	2:N:97:SER:HB2	2.17	0.45
1:G:28:ASN:O	1:G:28:ASN:ND2	2.49	0.45
2:D:215:PHE:O	2:D:216:SER:C	2.54	0.45
2:H:240:LEU:HD21	2:H:250:LEU:HD22	1.98	0.45
2:L:53:THR:H	2:L:136:ASN:ND2	2.13	0.45
1:C:162:LEU:HD21	1:C:178:PRO:CD	2.47	0.45
2:F:201:THR:CG2	2:F:206:ASN:HA	2.31	0.45
1:I:177:LEU:HD12	1:I:178:PRO:CD	2.40	0.45
1:M:142:LEU:HB2	1:M:173:SER:O	2.16	0.45
2:F:167:ASP:CG	2:F:168:VAL:HG12	2.37	0.45
1:G:186:THR:HB	1:G:199:LYS:NZ	2.31	0.45
2:P:154:VAL:HG12	2:P:155:VAL:N	2.32	0.45
1:I:12:PRO:HB2	1:I:15:GLN:HG3	1.97	0.45
2:J:155:VAL:HG12	2:J:157:PRO:CD	2.43	0.45
1:C:86:ASN:ND2	1:C:110:ARG:HB2	2.32	0.45
2:F:195:TYR:CE1	2:F:238:VAL:HB	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
1:E:186:THR:CG2	1:E:199:LYS:HZ2	2.30	0.45
1:O:142:LEU:HB2	1:O:173:SER:O	2.16	0.45
2:N:184:THR:OG1	2:N:247:ALA:HB1	2.16	0.45
1:M:12:PRO:HB2	1:M:15:GLN:HG3	1.97	0.45
2:L:103:TRP:CE2	2:L:105:VAL:HG21	2.51	0.45
2:D:5:THR:CG2	2:D:8:GLY:H	2.29	0.45
2:D:158:THR:HG23	4:D:1617:HOH:O	2.15	0.45
2:P:250:LEU:CD1	2:P:252:LEU:HD11	2.47	0.45
2:N:195:TYR:HB2	2:N:275:THR:O	2.17	0.45
1:A:114:TYR:CE2	1:A:149:TYR:HB2	2.51	0.45
1:G:46:GLY:O	1:G:70:ALA:HB3	2.16	0.45
2:D:60:ARG:CZ	2:D:60:ARG:HB2	2.47	0.45
2:J:226:THR:CG2	2:J:253:THR:HB	2.42	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
1:O:61:LYS:O	1:O:62:GLU:HB2	2.15	0.45
1:C:138:ASN:CA	1:C:177:LEU:HB3	2.47	0.45
1:G:94:ASP:C	1:G:96:SER:H	2.18	0.45
1:K:160:ARG:HG3	1:K:178:PRO:HG3	1.98	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:C:167:VAL:HA	1:C:168:PRO:HD2	1.77	0.45
1:G:122:LEU:HD12	1:G:122:LEU:C	2.37	0.45
2:B:184:THR:HB	2:B:247:ALA:HB1	1.98	0.45
1:I:61:LYS:O	1:I:62:GLU:HB2	2.16	0.45
1:O:144:ASN:HB3	1:O:167:VAL:HG12	1.99	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:O:144:ASN:HB3	1:O:167:VAL:CG1	2.47	0.45
1:C:46:GLY:O	1:C:70:ALA:HB3	2.16	0.45
1:I:144:ASN:HB3	1:I:167:VAL:HG12	1.99	0.45
2:J:195:TYR:O	2:J:237:THR:HA	2.16	0.45
2:J:195:TYR:HB2	2:J:275:THR:O	2.16	0.45
2:D:4:LYS:NZ	2:D:4:LYS:HB2	2.31	0.45
2:N:227:ARG:NE	2:N:232:ILE:HD11	2.32	0.45
1:M:47:ARG:HH22	1:M:74:GLN:NE2	1.92	0.45
1:E:186:THR:HB	1:E:199:LYS:NZ	2.32	0.45
2:H:167:ASP:CG	2:H:168:VAL:HG12	2.38	0.45
1:M:149:TYR:CD1	1:M:169:PRO:HD3	2.52	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:C:201:THR:O	1:C:203:VAL:HG23	2.17	0.45
2:B:240:LEU:HD21	2:B:250:LEU:HD22	1.97	0.45
2:F:118:VAL:O	2:F:118:VAL:HG12	2.17	0.45
2:D:38:LEU:C	2:D:40:THR:N	2.69	0.45
2:H:201:THR:CB	2:H:206:ASN:ND2	2.81	0.45
1:O:47:ARG:NH2	1:O:74:GLN:NE2	2.58	0.45
1:G:141:THR:HA	1:G:174:THR:HA	1.99	0.45
2:L:24:LEU:O	2:L:26:PRO:N	2.49	0.45
1:O:136:SER:HB2	1:O:139:SER:H	1.81	0.45
1:C:144:ASN:HB3	1:C:167:VAL:HG12	1.98	0.45
2:L:96:ASN:O	2:L:97:SER:HB2	2.17	0.45
1:A:1:GLY:N	1:A:26:ASP:CG	2.69	0.45
2:N:197:LEU:CD1	2:N:225:LEU:HD12	2.43	0.44
1:A:186:THR:CG2	1:A:199:LYS:HZ2	2.30	0.44
1:E:156:ASN:O	1:E:185:ILE:HA	2.17	0.44
2:N:42:ILE:HG23	2:N:146:TRP:CH2	2.52	0.44
1:C:82:LEU:HD12	1:C:83:PHE:H	1.82	0.44
2:P:227:ARG:NE	2:P:232:ILE:HD11	2.32	0.44
2:P:195:TYR:HB2	2:P:275:THR:O	2.16	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:46:GLY:O	1:E:70:ALA:HB3	2.17	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
2:N:253:THR:HG22	2:N:255:ASN:ND2	2.22	0.44
1:A:102:THR:C	2:B:171:THR:HG22	2.37	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
2:J:184:THR:OG1	2:J:247:ALA:HB1	2.17	0.44
2:J:154:VAL:HG12	2:J:155:VAL:N	2.32	0.44
1:O:82:LEU:HB2	1:O:149:TYR:CE1	2.53	0.44
1:A:144:ASN:HB3	1:A:167:VAL:HG12	1.98	0.44
1:G:144:ASN:HB3	1:G:167:VAL:HG12	1.98	0.44
2:P:96:ASN:O	2:P:97:SER:HB2	2.17	0.44
1:G:28:ASN:O	1:G:29:SER:HB3	2.16	0.44
1:E:201:THR:O	1:E:203:VAL:HG23	2.18	0.44
2:N:224:GLN:HE21	2:N:231:ILE:HD13	1.80	0.44
1:I:39:ASN:OD1	1:I:43:VAL:HG13	2.18	0.44
1:K:177:LEU:HD12	1:K:178:PRO:CD	2.40	0.44
2:J:42:ILE:HG23	2:J:146:TRP:CH2	2.53	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
1:I:57:MET:HA	1:I:61:LYS:HE3	2.00	0.44
1:I:144:ASN:HB3	1:I:167:VAL:CG1	2.48	0.44
1:O:85:MET:O	1:O:110:ARG:HA	2.17	0.44
1:K:85:MET:O	1:K:110:ARG:HA	2.17	0.44
1:K:71:THR:HG23	1:K:71:THR:O	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
2:N:59:GLN:HG3	2:N:132:ARG:HD3	2.00	0.44
2:L:155:VAL:HG12	2:L:157:PRO:CD	2.43	0.44
1:O:186:THR:HB	1:O:199:LYS:NZ	2.32	0.44
2:N:250:LEU:CD1	2:N:252:LEU:HD11	2.47	0.44
1:I:190:ILE:HD12	2:J:279:GLN:HG2	1.99	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:G:201:THR:O	1:G:203:VAL:HG23	2.18	0.44
1:A:47:ARG:NH2	1:A:74:GLN:HB2	2.33	0.44
1:E:141:THR:HA	1:E:174:THR:HA	2.00	0.44
1:O:12:PRO:HD2	1:O:15:GLN:HG3	1.99	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)
2:P:61:GLY:HA3	2:P:86:THR:HG23	2.00	0.44
1:M:190:ILE:HD12	2:N:279:GLN:HG2	2.00	0.44
1:C:28:ASN:O	1:C:28:ASN:ND2	2.51	0.44
1:M:144:ASN:HB3	1:M:167:VAL:CG1	2.47	0.44
1:G:138:ASN:CA	1:G:177:LEU:HB3	2.48	0.44
1:A:177:LEU:HA	1:A:178:PRO:HD2	1.88	0.44
2:P:58:LEU:H	2:P:90:THR:HG21	1.79	0.44
1:G:154:GLU:OE2	1:G:188:ARG:HD3	2.17	0.44
1:M:82:LEU:HB2	1:M:149:TYR:CE1	2.53	0.44
1:E:122:LEU:HD12	1:E:122:LEU:C	2.38	0.44
2:N:168:VAL:O	2:N:168:VAL:HG13	2.18	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:O:71:THR:O	1:O:71:THR:HG23	2.18	0.44
1:M:45:ASP:OD1	1:M:47:ARG:HB2	2.18	0.44
1:K:39:ASN:OD1	1:K:43:VAL:HG13	2.18	0.44
2:P:202:ALA:HB2	2:P:210:THR:CG2	2.34	0.44
1:C:71:THR:O	1:C:73:ASN:N	2.51	0.44
1:E:47:ARG:NH2	1:E:74:GLN:HB2	2.32	0.44
1:K:179:SER:C	1:K:181:ALA:H	2.20	0.44
2:P:42:ILE:HG23	2:P:146:TRP:CH2	2.53	0.44
2:H:192:ASN:HA	2:H:241:GLY:O	2.18	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
1:K:78:ASP:O	1:K:170:MET:HE1	2.18	0.44
2:N:267:ASN:OD1	2:N:269:GLN:NE2	2.51	0.44
2:J:168:VAL:HG13	2:J:168:VAL:O	2.18	0.44
1:E:123:PRO:HA	1:E:124:PRO:HD2	1.84	0.44
2:P:267:ASN:OD1	2:P:269:GLN:NE2	2.50	0.44
2:J:61:GLY:HA3	2:J:86:THR:HG23	1.99	0.44
2:B:184:THR:HA	2:B:248:VAL:O	2.18	0.44
1:M:186:THR:HB	1:M:199:LYS:NZ	2.33	0.44
2:D:5:THR:HG22	2:D:9:THR:N	2.32	0.44
2:J:44:CYS:O	2:J:101:LYS:N	2.50	0.44
2:P:211:ASN:HD22	2:P:212:THR:N	2.16	0.44
2:J:211:ASN:HD22	2:J:212:THR:N	2.16	0.44
1:I:71:THR:HG23	1:I:71:THR:O	2.18	0.44
2:H:4:LYS:HB2	2:H:4:LYS:NZ	2.33	0.44
1:C:186:THR:HB	1:C:199:LYS:NZ	2.32	0.44
1:G:162:LEU:HD21	1:G:178:PRO:CD	2.48	0.44
2:P:59:GLN:HG3	2:P:132:ARG:HD3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:167:ASP:OD1	2:B:168:VAL:HG12	2.18	0.44
2:D:167:ASP:OD1	2:D:168:VAL:HG12	2.18	0.44
1:K:190:ILE:HD12	2:L:279:GLN:HG2	2.00	0.44
2:P:21:TYR:CB	2:P:151:ASN:HD21	2.24	0.44
1:C:12:PRO:CB	1:C:15:GLN:HG3	2.45	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
1:O:190:ILE:HD12	2:P:279:GLN:HG2	2.00	0.44
1:M:144:ASN:HB3	1:M:167:VAL:HG12	1.99	0.44
2:L:211:ASN:HD22	2:L:212:THR:N	2.16	0.44
2:L:227:ARG:NE	2:L:232:ILE:HD11	2.32	0.44
1:K:45:ASP:OD1	1:K:47:ARG:HB2	2.18	0.44
2:L:59:GLN:HG3	2:L:132:ARG:HD3	2.00	0.44
1:A:187:TYR:CD1	1:A:187:TYR:C	2.91	0.44
1:E:154:GLU:OE2	1:E:188:ARG:HD3	2.18	0.44
1:I:160:ARG:HG2	1:I:178:PRO:HG3	2.00	0.44
2:L:42:ILE:HG23	2:L:146:TRP:CH2	2.53	0.44
1:G:156:ASN:O	1:G:185:ILE:HA	2.17	0.44
1:K:149:TYR:CD1	1:K:169:PRO:HD3	2.52	0.44
2:J:95:TYR:HH	2:J:103:TRP:HA	1.83	0.44
2:F:184:THR:HB	2:F:247:ALA:HB1	1.98	0.44
2:H:38:LEU:C	2:H:40:THR:N	2.71	0.44
1:K:144:ASN:HB3	1:K:167:VAL:HG12	1.99	0.44
1:M:71:THR:O	1:M:71:THR:HG23	2.18	0.44
1:C:47:ARG:NH2	1:C:74:GLN:HB2	2.33	0.43
1:A:162:LEU:HD21	1:A:178:PRO:CD	2.47	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
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:N:61:GLY:HA3	2:N:86:THR:HG23	2.00	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:8:GLY:O	2:L:9:THR:C	2.57	0.43
1:E:155:LEU:HD12	1:E:187:TYR:HB3	2.01	0.43
1:O:160:ARG:HG2	1:O:178:PRO:HG3	2.00	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
2:D:184:THR:HA	2:D:248:VAL:O	2.18	0.43
2:H:184:THR:HB	2:H:247:ALA:HB1	1.99	0.43
1:E:31:TYR:O	1:E:56:ALA:HA	2.18	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:H:118:VAL:HG12	2:H:118:VAL:O	2.18	0.43
2:N:211:ASN:HD22	2:N:212:THR:N	2.16	0.43
2:F:201:THR:CB	2:F:206:ASN:ND2	2.81	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:J:267:ASN:OD1	2:J:269:GLN:NE2	2.51	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: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
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:41:GLN:O	2:L:42:ILE:HG13	2.18	0.43
2:D:262:GLN:CA	2:D:262:GLN:HE21	2.25	0.43
1:A:125:ASP:OD1	1:A:126:GLN:N	2.51	0.43
2:L:30:VAL:HG23	2:L:156:VAL:CG1	2.49	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
1:M:50:VAL:HG12	1:M:51:THR:N	2.34	0.43
1:O:39:ASN:OD1	1:O:43:VAL:HG13	2.18	0.43
2:D:167:ASP:CG	2:D:168:VAL:HG12	2.37	0.43
1:K:52:PRO:HG2	1:K:55:PHE:CE2	2.53	0.43
1:O:78:ASP:O	1:O:170:MET:HE1	2.18	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:M:85:MET:O	1:M:110:ARG:HA	2.18	0.43
1:M:39:ASN:OD1	1:M:43:VAL:HG13	2.18	0.43
2:H:5:THR:HG22	2:H:9:THR:N	2.33	0.43
1:G:132:ARG:C	1:G:133:PHE:CD1	2.92	0.43
2:H:167:ASP:OD1	2:H:168:VAL:HG12	2.18	0.43
2:N:41:GLN:O	2:N:42:ILE:HG13	2.19	0.43
1:I:135:ARG:NH2	1:I:181:ALA:CB	2.82	0.43
2:P:41:GLN:O	2:P:42:ILE:HG13	2.18	0.43
2:N:21:TYR:CB	2:N:151:ASN:HD21	2.24	0.43
1:M:182:GLY:O	1:M:183:SER:CB	2.65	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
2:B:221:VAL:HG12	2:B:222:GLY:N	2.33	0.43
1:G:168:PRO:HA	1:G:169:PRO:HD3	1.87	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:227:ARG:NE	2:J:232:ILE:HD11	2.33	0.43
1:A:28:ASN:ND2	1:A:28:ASN:O	2.51	0.43
1:G:155:LEU:HD12	1:G:187:TYR:HB3	2.01	0.43
1:A:201:THR:O	1:A:203:VAL:HG23	2.18	0.43
1:C:186:THR:CG2	1:C:199:LYS:HZ2	2.32	0.43
1:A:141:THR:HA	1:A:174:THR:HA	1.99	0.43
1:O:135:ARG:NH2	1:O:181:ALA:CB	2.81	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:E:125:ASP:OD1	1:E:126:GLN:N	2.51	0.43
2:P:168:VAL:HG13	2:P:168:VAL:O	2.18	0.43
1:O:13:ALA:HB3	1:O:118:ALA:H	1.84	0.43
2:F:184:THR:HA	2:F:248:VAL:O	2.18	0.43
1:O:188:ARG:NH1	1:O:199:LYS:N	2.67	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
2:J:122:ALA:N	2:J:153:ASP:OD1	2.52	0.43
2:B:38:LEU:C	2:B:40:THR:N	2.72	0.43
1:K:41:ASP:C	1:K:43:VAL:H	2.22	0.43
1:G:47:ARG:NH2	1:G:74:GLN:HB2	2.31	0.43
1:A:47:ARG:NH2	1:A:74:GLN:NE2	2.54	0.43
1:A:132:ARG:C	1:A:133:PHE:CD1	2.92	0.43
1:E:187:TYR:C	1:E:187:TYR:CD1	2.92	0.43
2:L:241:GLY:O	2:L:243:VAL:HG23	2.19	0.43
1:I:52:PRO:HG2	1:I:55:PHE:CE2	2.53	0.43
2:N:95:TYR:OH	2:N:103:TRP:CA	2.66	0.43
2:N:241:GLY:O	2:N:243:VAL:HG23	2.19	0.43
1:G:93:MET:HE1	1:G:98:LEU:HD23	2.00	0.43
1:A:31:TYR:O	1:A:56:ALA:HA	2.19	0.43
1:G:31:TYR:O	1:G:56:ALA:HA	2.19	0.43
2:J:197:LEU:CD1	2:J:225:LEU:HD12	2.42	0.43
1:O:45:ASP:OD1	1:O:47:ARG:HB2	2.19	0.43
2:B:167:ASP:CG	2:B:168:VAL:HG12	2.38	0.43
1:M:135:ARG:NH2	1:M:181:ALA:CB	2.81	0.43
1:K:177:LEU:HA	1:K:178:PRO:HD2	1.79	0.43
1:O:52:PRO:HG2	1:O:55:PHE:CE2	2.54	0.43
1:E:122:LEU:HD12	1:E:123:PRO:N	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:5:THR:CG2	2:B:8:GLY:H	2.32	0.43
1:M:57:MET:HA	1:M:61:LYS:HE3	2.00	0.43
1:C:31:TYR:O	1:C:56:ALA:HA	2.18	0.43
1:C:187:TYR:CD1	1:C:187:TYR:C	2.92	0.43
2:B:1:PHE:CG	2:B:133:GLN:HG3	2.54	0.43
2:B:212:THR:O	2:B:269:GLN:HB2	2.19	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
1:K:160:ARG:HG2	1:K:178:PRO:HG3	2.00	0.43
1:C:125:ASP:OD1	1:C:126:GLN:N	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
1:E:28:ASN:ND2	1:E:28:ASN:O	2.52	0.43
2:L:53:THR:H	2:L:136:ASN:HD21	1.67	0.43
2:D:38:LEU:C	2:D:40:THR:H	2.21	0.43
2:J:13:ILE:HG23	3:J:1605:MAN:C2	2.48	0.43
2:B:4:LYS:NZ	2:B:4:LYS:HB2	2.34	0.43
2:P:207:SER:HB3	2:P:233:PRO:HB3	2.01	0.42
2:L:126:ILE:HD11	2:L:150:ALA:HB2	2.01	0.42
2:P:126:ILE:HD11	2:P:150:ALA:HB2	2.01	0.42
1:M:160:ARG:HG2	1:M:178:PRO:HG3	2.01	0.42
1:O:135:ARG:NH2	1:O:181:ALA:HB1	2.34	0.42
1:I:12:PRO:HD2	1:I:15:GLN:HG3	2.00	0.42
1:G:38:GLU:OE1	1:G:110:ARG:NH2	2.46	0.42
2:H:221:VAL:HG12	2:H:222:GLY:N	2.34	0.42
2:B:111:PRO:HB3	2:B:156:VAL:HG21	2.01	0.42
1:M:24:ASN:HB2	1:M:57:MET:HE3	2.00	0.42
1:G:187:TYR:C	1:G:187:TYR:CD1	2.92	0.42
2:J:135:ASN:ND2	3:J:1605:MAN:O4	2.52	0.42
1:G:67:ILE:HD12	1:G:67:ILE:N	2.34	0.42
1:M:77:GLN:NE2	1:M:77:GLN:HA	2.34	0.42
2:H:126:ILE:CD1	2:H:150:ALA:HB2	2.26	0.42
1:M:39:ASN:HD21	1:M:43:VAL:CG1	2.18	0.42
1:O:41:ASP:C	1:O:43:VAL:H	2.22	0.42
2:J:59:GLN:HG3	2:J:132:ARG:HD3	2.00	0.42
1:I:136:SER:C	1:I:177:LEU:HD23	2.39	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
2:L:29:ASN:OD1	2:L:157:PRO:HD2	2.19	0.42
1:K:149:TYR:CG	1:K:169:PRO:HD3	2.54	0.42
2:P:122:ALA:N	2:P:153:ASP:OD1	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:31:TYR:O	1:O:56:ALA:HA	2.19	0.42
2:H:201:THR:HB	2:H:206:ASN:ND2	2.34	0.42
2:D:226:THR:HG22	2:D:255:ASN:HD21	1.84	0.42
1:A:155:LEU:HD12	1:A:187:TYR:HB3	2.01	0.42
1:K:136:SER:C	1:K:177:LEU:HD23	2.39	0.42
2:J:41:GLN:C	2:J:42:ILE:HG13	2.40	0.42
2:L:168:VAL:O	2:L:168:VAL:HG13	2.18	0.42
1:I:13:ALA:HB3	1:I:118:ALA:H	1.84	0.42
1:O:24:ASN:HB2	1:O:57:MET:HE3	2.00	0.42
1:C:117:PRO:O	1:C:120:LEU:HG	2.19	0.42
1:G:117:PRO:O	1:G:120:LEU:HG	2.19	0.42
1:O:50:VAL:HG12	1:O:51:THR:N	2.34	0.42
2:F:4:LYS:NZ	2:F:4:LYS:HB2	2.34	0.42
2:P:223:VAL:CG1	2:P:224:GLN:N	2.82	0.42
2:J:223:VAL:CG1	2:J:224:GLN:N	2.82	0.42
2:D:226:THR:CG2	2:D:255:ASN:HD21	2.32	0.42
1:O:134:ARG:HD2	1:O:141:THR:OG1	2.20	0.42
2:P:41:GLN:C	2:P:42:ILE:HG13	2.40	0.42
2:H:33:ASN:HA	2:H:33:ASN:HD22	1.59	0.42
2:P:29:ASN:OD1	2:P:157:PRO:HD2	2.20	0.42
1:G:10:ILE:O	1:G:12:PRO:HD3	2.19	0.42
2:P:30:VAL:HG23	2:P:156:VAL:CG1	2.49	0.42
1:G:191:ASN:ND2	1:G:195:ALA:HB3	2.32	0.42
2:L:61:GLY:HA3	2:L:86:THR:HG23	2.00	0.42
1:K:13:ALA:HB3	1:K:118:ALA:H	1.84	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:J:8:GLY:O	2:J:9:THR:C	2.57	0.42
1:K:50:VAL:HG12	1:K:51:THR:N	2.34	0.42
2:J:181:ILE:HA	2:J:182:PRO:HD3	1.93	0.42
2:F:240:LEU:HD21	2:F:250:LEU:HD22	2.00	0.42
1:M:41:ASP:C	1:M:43:VAL:H	2.22	0.42
1:I:45:ASP:OD1	1:I:47:ARG:HB2	2.18	0.42
1:O:179:SER:C	1:O:181:ALA:H	2.21	0.42
2:H:136:ASN:N	2:H:136:ASN:HD22	2.18	0.42
2:F:192:ASN:HA	2:F:241:GLY:O	2.19	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: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
2:D:7:ASN:HB2	4:D:1654:HOH:O	2.19	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
2:P:241:GLY:O	2:P:243:VAL:HG23	2.19	0.42
2:N:192:ASN:HA	2:N:241:GLY:O	2.19	0.42
1:E:93:MET:HE1	1:E:98:LEU:HD23	2.01	0.42
1:C:155:LEU:HD12	1:C:187:TYR:HB3	2.01	0.42
2:N:122:ALA:N	2:N:153:ASP:OD1	2.53	0.42
1:A:117:PRO:O	1:A:120:LEU:HG	2.19	0.42
2:H:113:SER:OG	2:L:81:SER:N	2.47	0.42
1:C:132:ARG:C	1:C:133:PHE:CD1	2.93	0.42
2:D:126:ILE:CD1	2:D:150:ALA:HB2	2.24	0.42
1:I:39:ASN:HD21	1:I:43:VAL:CG1	2.18	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:J:20:VAL:CG1	2:J:22:VAL:HG13	2.50	0.42
1:M:134:ARG:HD2	1:M:141:THR:OG1	2.20	0.42
2:J:184:THR:HA	2:J:248:VAL:O	2.19	0.42
1:M:149:TYR:CG	1:M:169:PRO:HD3	2.54	0.42
2:B:116:GLY:HA2	2:B:189:LYS:CE	2.47	0.42
2:P:169:THR:OG1	2:P:181:ILE:HG23	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:I:28:ASN:O	1:I:29:SER:CB	2.68	0.42
1:M:31:TYR:O	1:M:56:ALA:HA	2.20	0.42
2:D:118:VAL:HG12	2:D:118:VAL:O	2.19	0.42
2:D:212:THR:O	2:D:269:GLN:HB2	2.20	0.42
1:M:177:LEU:HD12	1:M:178:PRO:CD	2.40	0.42
1:I:135:ARG:CZ	1:I:177:LEU:HD21	2.50	0.42
1:A:122:LEU:HD12	1:A:123:PRO:N	2.35	0.42
2:L:95:TYR:OH	2:L:103:TRP:CA	2.66	0.42
1:K:156:ASN:C	1:K:158:GLY:N	2.73	0.42
1:E:142:LEU:HD22	1:E:142:LEU:N	2.34	0.42
1:A:142:LEU:N	1:A:142:LEU:HD22	2.35	0.42
2:D:135:ASN:HD21	2:D:138:ASN:HD21	1.66	0.42
2:N:8:GLY:O	2:N:9:THR:C	2.57	0.42
1:A:67:ILE:N	1:A:67:ILE:HD12	2.34	0.42
1:I:50:VAL:HG12	1:I:51:THR:N	2.34	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:212:THR:O	2:F:269:GLN:HB2	2.20	0.42
1:M:135:ARG:CZ	1:M:177:LEU:HD21	2.50	0.42
1:I:135:ARG:NH2	1:I:181:ALA:HB1	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:58:LEU:H	2:J:90:THR:HG21	1.79	0.42
2:F:136:ASN:H	2:F:136:ASN:ND2	2.17	0.42
2:P:222:GLY:C	2:P:257:ALA:HB3	2.40	0.42
2:P:184:THR:HA	2:P:248:VAL:O	2.19	0.42
2:L:48:TYR:HB2	2:L:52:ILE:CD1	2.48	0.42
1:C:122:LEU:C	1:C:122:LEU:HD12	2.38	0.42
1:I:122:LEU:CD1	1:I:126:GLN:HB3	2.50	0.42
2:L:30:VAL:HG12	2:L:31:GLY:N	2.34	0.42
1:O:117:PRO:O	1:O:119:LYS:N	2.53	0.42
1:I:117:PRO:O	1:I:119:LYS:N	2.53	0.42
1:I:188:ARG:NH1	1:I:199:LYS:H	2.18	0.42
1:K:57:MET:HA	1:K:61:LYS:HE3	2.00	0.42
2:J:13:ILE:HG23	3:J:1605:MAN:O2	2.20	0.42
1:A:107:ILE:HG12	4:A:213:HOH:O	2.19	0.42
1:I:41:ASP:C	1:I:43:VAL:H	2.22	0.42
2:N:41:GLN:C	2:N:42:ILE:HG13	2.40	0.42
2:L:58:LEU:H	2:L:90:THR:HG21	1.78	0.42
2:D:221:VAL:HG12	2:D:222:GLY:N	2.35	0.42
2:P:95:TYR:OH	2:P:103:TRP:CA	2.66	0.42
2:P:14:GLY:HA2	2:P:142:PHE:CZ	2.55	0.42
1:I:188:ARG:NH1	1:I:199:LYS:N	2.67	0.42
2:L:96:ASN:HD22	2:L:96:ASN:N	2.10	0.42
1:M:108:ILE:HB	2:N:275:THR:HG23	2.02	0.42
2:D:215:PHE:HD1	2:D:267:ASN:OD1	2.03	0.42
2:N:169:THR:OG1	2:N:181:ILE:HG23	2.20	0.42
1:O:77:GLN:HA	1:O:77:GLN:NE2	2.35	0.42
1:I:31:TYR:O	1:I:56:ALA:HA	2.20	0.42
2:J:207:SER:HB3	2:J:233:PRO:HB3	2.01	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:A:94:ASP:OD1	2:B:168:VAL:HG11	2.20	0.42
1:O:136:SER:C	1:O:177:LEU:HD23	2.39	0.42
1:K:134:ARG:HD2	1:K:141:THR:OG1	2.20	0.42
1:C:94:ASP:OD1	2:D:168:VAL:HG11	2.20	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:C:122:LEU:HD12	1:C:123:PRO:N	2.35	0.42
2:F:221:VAL:HG12	2:F:222:GLY:N	2.35	0.42
1:O:13:ALA:CB	1:O:117:PRO:HA	2.50	0.42
1:O:156:ASN:C	1:O:158:GLY:N	2.73	0.42
2:F:111:PRO:HB3	2:F:156:VAL:HG21	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:226:THR:HG22	2:B:255:ASN:HD21	1.84	0.41
1:A:71:THR:O	1:A:73:ASN:N	2.51	0.41
2:J:163:VAL:HA	2:J:185:VAL:CG2	2.36	0.41
1:E:132:ARG:C	1:E:133:PHE:CD1	2.93	0.41
2:N:184:THR:HA	2:N:248:VAL:O	2.20	0.41
2:D:90:THR:HG23	2:D:91:PRO:N	2.34	0.41
2:L:14:GLY:HA2	2:L:142:PHE:CZ	2.54	0.41
1:M:156:ASN:C	1:M:158:GLY:N	2.73	0.41
1:K:28:ASN:O	1:K:29:SER:CB	2.68	0.41
1:C:142:LEU:N	1:C:142:LEU:HD22	2.34	0.41
2:J:136:ASN:HD22	2:J:136:ASN:N	2.18	0.41
2:F:38:LEU:C	2:F:40:THR:H	2.22	0.41
2:P:8:GLY:O	2:P:9:THR:C	2.57	0.41
2:L:122:ALA:N	2:L:153:ASP:OD1	2.53	0.41
2:L:64:TYR:CE1	2:L:128:VAL:HG23	2.55	0.41
1:C:67:ILE:HD12	1:C:67:ILE:N	2.34	0.41
1:I:77:GLN:HA	1:I:77:GLN:NE2	2.35	0.41
1:E:67:ILE:HD12	1:E:67:ILE:N	2.34	0.41
2:B:201:THR:CB	2:B:206:ASN:ND2	2.83	0.41
2:F:170:VAL:C	2:F:172:LEU:N	2.73	0.41
2:J:126:ILE:HD11	2:J:150:ALA:HB2	2.02	0.41
1:M:136:SER:C	1:M:177:LEU:HD23	2.40	0.41
1:I:134:ARG:HD2	1:I:141:THR:OG1	2.20	0.41
2:D:136:ASN:HD22	2:D:136:ASN:N	2.16	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:K:122:LEU:CD1	1:K:126:GLN:HB3	2.50	0.41
2:P:116:GLY:O	2:P:156:VAL:O	2.38	0.41
2:P:30:VAL:HG12	2:P:31:GLY:N	2.34	0.41
2:J:116:GLY:O	2:J:156:VAL:O	2.38	0.41
2:N:14:GLY:HA2	2:N:142:PHE:CZ	2.55	0.41
2:J:53:THR:H	2:J:136:ASN:HD21	1.68	0.41
2:J:140:ASP:OD1	3:J:1605:MAN:O3	2.31	0.41
1:E:117:PRO:O	1:E:120:LEU:HG	2.20	0.41
2:P:19:ASN:OD1	2:P:147:ASN:HB2	2.20	0.41
2:J:165:ALA:O	2:J:166:ARG:C	2.59	0.41
1:C:181:ALA:HB1	1:C:182:GLY:H	1.53	0.41
2:N:207:SER:HB3	2:N:233:PRO:HB3	2.01	0.41
2:D:201:THR:HB	2:D:206:ASN:ND2	2.36	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:185:ILE:O	1:M:202:GLY:N	2.35	0.41
2:B:192:ASN:HA	2:B:241:GLY:O	2.20	0.41
1:E:12:PRO:CB	1:E:15:GLN:HG3	2.48	0.41
1:O:122:LEU:CD1	1:O:126:GLN:HB3	2.50	0.41
2:L:116:GLY:O	2:L:156:VAL:O	2.38	0.41
1:M:188:ARG:NH1	1:M:199:LYS:H	2.17	0.41
1:I:156:ASN:C	1:I:158:GLY:N	2.73	0.41
2:N:1:PHE:CD1	2:N:133:GLN:HG3	2.54	0.41
2:J:227:ARG:HG2	2:J:232:ILE:HD11	2.02	0.41
1:O:28:ASN:O	1:O:29:SER:CB	2.68	0.41
1:G:142:LEU:HD22	1:G:142:LEU:N	2.34	0.41
2:L:44:CYS:O	2:L:101:LYS:N	2.50	0.41
2:N:165:ALA:O	2:N:166:ARG:C	2.59	0.41
1:K:77:GLN:HA	1:K:77:GLN:NE2	2.35	0.41
2:F:126:ILE:CD1	2:F:150:ALA:HB2	2.25	0.41
2:B:170:VAL:C	2:B:172:LEU:N	2.74	0.41
1:O:135:ARG:CZ	1:O:177:LEU:HD21	2.50	0.41
1:K:135:ARG:CZ	1:K:177:LEU:HD21	2.50	0.41
2:D:136:ASN:H	2:D:136:ASN:ND2	2.17	0.41
1:G:186:THR:CG2	1:G:199:LYS:HZ2	2.33	0.41
2:J:19:ASN:OD1	2:J:147:ASN:HB2	2.20	0.41
1:C:38:GLU:OE1	1:C:110:ARG:NH2	2.46	0.41
1:I:13:ALA:CB	1:I:117:PRO:HA	2.50	0.41
2:P:227:ARG:HG2	2:P:232:ILE:HD11	2.03	0.41
2:J:250:LEU:CB	2:J:252:LEU:HG	2.50	0.41
2:P:53:THR:H	2:P:136:ASN:HD21	1.66	0.41
2:F:162:ASP:HB3	2:F:186:TYR:CZ	2.55	0.41
1:K:31:TYR:O	1:K:56:ALA:HA	2.19	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
2:F:201:THR:HB	2:F:206:ASN:ND2	2.35	0.41
1:O:39:ASN:HD21	1:O:43:VAL:CG1	2.18	0.41
1:I:140:LEU:C	1:I:140:LEU:HD23	2.41	0.41
2:L:184:THR:HA	2:L:248:VAL:O	2.20	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
1:O:108:ILE:HB	2:P:275:THR:HG23	2.03	0.41
2:L:169:THR:OG1	2:L:181:ILE:HG23	2.20	0.41
2:F:138:ASN:HD22	2:F:138:ASN:C	2.23	0.41
1:C:178:PRO:O	1:C:179:SER:HB3	2.20	0.41
1:K:140:LEU:C	1:K:140:LEU:HD23	2.41	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:L:222:GLY:C	2:L:257:ALA:HB3	2.41	0.41
2:J:29:ASN:OD1	2:J:157:PRO:HD2	2.20	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:B:5:THR:HG22	2:B:9:THR:N	2.35	0.41
2:J:169:THR:OG1	2:J:181:ILE:HG23	2.20	0.41
2:P:44:CYS:O	2:P:101:LYS:N	2.51	0.41
1:K:99:THR:C	1:K:100:GLU:HG3	2.41	0.41
1:A:178:PRO:O	1:A:179:SER:HB3	2.21	0.41
1:M:135:ARG:HH12	1:M:177:LEU:HD11	1.82	0.41
2:N:22:VAL:HG12	2:N:41:GLN:HG3	2.02	0.41
2:N:20:VAL:CG1	2:N:22:VAL:HG13	2.50	0.41
1:O:140:LEU:HD23	1:O:140:LEU:C	2.41	0.41
2:L:20:VAL:CG1	2:L:22:VAL:HG13	2.50	0.41
2:N:90:THR:HG23	2:N:91:PRO:O	2.21	0.41
2:N:19:ASN:OD1	2:N:147:ASN:HB2	2.21	0.41
1:C:183:SER:C	1:C:185:ILE:N	2.74	0.41
2:N:227:ARG:HG2	2:N:232:ILE:HD11	2.03	0.41
2:P:67:VAL:CG2	2:P:126:ILE:HG23	2.36	0.41
1:I:133:PHE:HB3	1:I:134:ARG:H	1.70	0.41
1:E:94:ASP:OD1	2:F:168:VAL:HG11	2.20	0.41
1:G:183:SER:C	1:G:185:ILE:N	2.74	0.41
1:A:51:THR:HA	1:A:52:PRO:C	2.41	0.41
1:M:13:ALA:CB	1:M:117:PRO:HA	2.50	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
2:B:207:SER:HB3	2:B:233:PRO:HB3	2.02	0.41
2:H:215:PHE:HD1	2:H:267:ASN:OD1	2.03	0.41
2:N:53:THR:H	2:N:136:ASN:HD21	1.67	0.41
2:B:215:PHE:HD1	2:B:267:ASN:OD1	2.04	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
2:D:1:PHE:CG	2:D:133:GLN:HG3	2.56	0.41
1:G:107:ILE:HG12	4:G:216:HOH:O	2.21	0.41
2:P:165:ALA:O	2:P:166:ARG:C	2.59	0.41
2:H:201:THR:CB	2:H:206:ASN:HD22	2.34	0.41
2:B:226:THR:CG2	2:B:255:ASN:HD21	2.33	0.41
1:G:140:LEU:CD2	1:G:140:LEU:C	2.89	0.41
1:G:71:THR:O	1:G:73:ASN:N	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:THR:O	1:A:174:THR:CG2	2.68	0.41
1:A:181:ALA:HB1	1:A:182:GLY:H	1.53	0.41
2:H:212:THR:O	2:H:269:GLN:HB2	2.20	0.41
2:N:67:VAL:HG21	2:N:126:ILE:CG2	2.36	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:J:20:VAL:CG2	2:J:42:ILE:HD11	2.50	0.41
1:M:133:PHE:HB3	1:M:134:ARG:H	1.71	0.41
2:F:168:VAL:HG22	2:F:168:VAL:O	2.21	0.41
2:F:92:ARG:NH1	2:F:92:ARG:CG	2.83	0.41
2:N:222:GLY:C	2:N:257:ALA:HB3	2.41	0.41
2:J:222:GLY:C	2:J:257:ALA:HB3	2.41	0.41
2:P:262:GLN:HE21	2:P:262:GLN:HA	1.86	0.41
2:L:262:GLN:HA	2:L:262:GLN:HE21	1.85	0.41
2:B:33:ASN:HA	2:B:33:ASN:HD22	1.60	0.41
2:N:262:GLN:HA	2:N:262:GLN:HE21	1.85	0.41
2:D:116:GLY:HA2	2:D:189:LYS:CE	2.47	0.41
1:K:126:GLN:O	1:K:126:GLN:HG2	2.21	0.41
1:M:13:ALA:HB3	1:M:118:ALA:H	1.84	0.41
1:M:117:PRO:O	1:M:119:LYS:N	2.53	0.41
1:E:198:PRO:O	1:E:200:MET:HG2	2.21	0.41
1:A:198:PRO:O	1:A:200:MET:HG2	2.21	0.41
2:N:136:ASN:HD22	2:N:136:ASN:N	2.18	0.41
2:N:64:TYR:CE1	2:N:128:VAL:HG23	2.56	0.41
1:A:129:GLU:H	1:A:129:GLU:HG3	1.51	0.41
1:M:140:LEU:HD23	1:M:140:LEU:C	2.41	0.41
1:M:142:LEU:HD22	1:M:142:LEU:N	2.35	0.41
1:K:80:GLU:HG3	1:K:148:TYR:HA	2.03	0.41
1:A:27:GLU:CG	1:A:60:LYS:HD2	2.49	0.41
1:E:167:VAL:HA	1:E:168:PRO:HD2	1.75	0.41
2:P:175:TYR:CZ	2:P:263:VAL:HB	2.56	0.41
2:D:5:THR:N	2:D:9:THR:O	2.51	0.41
1:C:198:PRO:O	1:C:200:MET:HG2	2.21	0.41
2:P:120:ILE:O	2:P:153:ASP:HA	2.21	0.41
2:F:135:ASN:HD21	2:F:138:ASN:HD21	1.67	0.41
2:L:165:ALA:O	2:L:166:ARG:C	2.59	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
2:N:202:ALA:HB2	2:N:210:THR:CG2	2.34	0.40
1:I:142:LEU:HD22	1:I:142:LEU:N	2.36	0.40
1:O:185:ILE:O	1:O:202:GLY: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:P:52:ILE:HD12	3:P:1607:MAN:H61	2.04	0.40
2:F:90:THR:HG23	2:F:91:PRO:N	2.35	0.40
1:O:182:GLY:O	1:O:183:SER:CB	2.65	0.40
1:M:126:GLN:O	1:M:126:GLN:HG2	2.21	0.40
1:C:168:PRO:HA	1:C:169:PRO:HD3	1.87	0.40
2:L:175:TYR:CZ	2:L:263:VAL:HB	2.57	0.40
2:N:46:ASN:HD22	2:N:96:ASN:HA	1.86	0.40
2:D:138:ASN:C	2:D:138:ASN:HD22	2.24	0.40
2:N:128:VAL:HG12	2:N:128:VAL:O	2.21	0.40
2:L:19:ASN:OD1	2:L:147:ASN:HB2	2.21	0.40
2:H:162:ASP:HB3	2:H:186:TYR:CZ	2.56	0.40
2:H:170:VAL:C	2:H:172:LEU:N	2.74	0.40
2:H:168:VAL:HG22	2:H:168:VAL:O	2.22	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
2:L:41:GLN:C	2:L:42:ILE:HG13	2.40	0.40
1:G:51:THR:HA	1:G:52:PRO:C	2.41	0.40
1:M:101:ASN:ND2	2:N:268:VAL:N	2.69	0.40
1:I:80:GLU:HG3	1:I:148:TYR:HA	2.03	0.40
2:B:90:THR:HG23	2:B:91:PRO:N	2.36	0.40
2:N:175:TYR:CZ	2:N:263:VAL:HB	2.56	0.40
1:C:191:ASN:ND2	1:C:195:ALA:HB3	2.34	0.40
1:G:198:PRO:O	1:G:200:MET:HG2	2.21	0.40
2:D:111:PRO:HB3	2:D:156:VAL:HG21	2.02	0.40
2:B:138:ASN:HD22	2:B:138:ASN:C	2.24	0.40
1:I:108:ILE:HB	2:J:275:THR:HG23	2.02	0.40
1:O:99:THR:C	1:O:100:GLU:HG3	2.42	0.40
2:H:228:ASN:HD22	2:H:228:ASN:N	2.19	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:O:193:TYR:HB3	2:P:157:PRO:HG3	2.03	0.40
1:A:167:VAL:HA	1:A:168:PRO:HD2	1.76	0.40
1:G:167:VAL:HA	1:G:168:PRO:HD2	1.76	0.40
1:A:82:LEU:HD12	1:A:83:PHE:H	1.84	0.40
2:P:128:VAL:HG12	2:P:128:VAL:O	2.21	0.40
2:N:223:VAL:CG1	2:N:224:GLN:N	2.83	0.40
1:G:178:PRO:O	1:G:179:SER:HB3	2.21	0.40
1:A:155:LEU:HA	1:A:186:THR:O	2.22	0.40
2:N:24:LEU:O	2:N:152:ASN:ND2	2.51	0.40
1:E:155:LEU:HA	1:E:186:THR:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:142:LEU:N	1:K:142:LEU:HD22	2.36	0.40
2:P:11:ILE:HA	2:P:12:PRO:HD2	1.89	0.40
2:J:22:VAL:HG12	2:J:41:GLN:HG3	2.03	0.40
2:B:136:ASN:HD22	2:B:136:ASN:N	2.18	0.40
1:K:8:ARG:NH1	1:K:190:ILE:CG2	2.85	0.40
1:O:103:LEU:HD23	2:P:181:ILE:HD11	2.03	0.40
1:G:191:ASN:O	1:G:194:GLY:N	2.46	0.40
2:J:46:ASN:HD22	2:J:96:ASN:HA	1.86	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:P:106:ALA:CB	2:P:108:TYR:HE1	2.35	0.40
2:H:1:PHE:CG	2:H:133:GLN:HG3	2.57	0.40
1:E:129:GLU:HG3	1:E:129:GLU:H	1.52	0.40
2:N:231:ILE:CG2	2:N:232:ILE:N	2.85	0.40
2:L:231:ILE:CG2	2:L:232:ILE:N	2.84	0.40
2:N:209:PHE:CE2	2:N:272:ILE:HG23	2.57	0.40
1:E:47:ARG:NH2	1:E:74:GLN:NE2	2.55	0.40
1:A:140:LEU:C	1:A:140:LEU:CD2	2.90	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
2:L:22:VAL:HG12	2:L:41:GLN:HG3	2.02	0.40
2:L:90:THR:HG23	2:L:91:PRO:O	2.22	0.40
1:O:101:ASN:ND2	2:P:268:VAL:N	2.69	0.40
1:M:193:TYR:HB3	2:N:157:PRO:HG3	2.04	0.40
2:B:262:GLN:CA	2:B:262:GLN:HE21	2.25	0.40
1:I:78:ASP:O	1:I:170:MET:HE1	2.20	0.40
2:F:116:GLY:HA2	2:F:189:LYS:CE	2.47	0.40
1:O:126:GLN:O	1:O:126:GLN:HG2	2.21	0.40
2:J:120:ILE:O	2:J:153:ASP:HA	2.21	0.40
2:B:118:VAL:HG12	2:B:118:VAL:O	2.20	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	7
1	C	203/205 (99%)	164 (81%)	28 (14%)	11 (5%)	2	7
1	E	203/205 (99%)	163 (80%)	29 (14%)	11 (5%)	2	7
1	G	203/205 (99%)	164 (81%)	28 (14%)	11 (5%)	2	7
1	I	203/205 (99%)	162 (80%)	29 (14%)	12 (6%)	2	5
1	K	203/205 (99%)	162 (80%)	29 (14%)	12 (6%)	2	5
1	M	203/205 (99%)	162 (80%)	29 (14%)	12 (6%)	2	5
1	O	203/205 (99%)	163 (80%)	28 (14%)	12 (6%)	2	5
2	B	277/279 (99%)	244 (88%)	24 (9%)	9 (3%)	5	17
2	D	277/279 (99%)	243 (88%)	24 (9%)	10 (4%)	4	14
2	F	277/279 (99%)	244 (88%)	23 (8%)	10 (4%)	4	14
2	H	277/279 (99%)	243 (88%)	24 (9%)	10 (4%)	4	14
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%)	2	6

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%)	12	33
1	C	176/176 (100%)	159 (90%)	17 (10%)	10	29
1	E	176/176 (100%)	160 (91%)	16 (9%)	12	33
1	G	176/176 (100%)	160 (91%)	16 (9%)	12	33
1	I	176/176 (100%)	165 (94%)	11 (6%)	22	53
1	K	176/176 (100%)	164 (93%)	12 (7%)	20	49
1	M	176/176 (100%)	165 (94%)	11 (6%)	22	53
1	O	176/176 (100%)	165 (94%)	11 (6%)	22	53
2	B	226/226 (100%)	208 (92%)	18 (8%)	15	40
2	D	226/226 (100%)	208 (92%)	18 (8%)	15	40
2	F	226/226 (100%)	207 (92%)	19 (8%)	14	37
2	H	226/226 (100%)	207 (92%)	19 (8%)	14	37
2	J	226/226 (100%)	214 (95%)	12 (5%)	28	61
2	L	226/226 (100%)	214 (95%)	12 (5%)	28	61
2	N	226/226 (100%)	214 (95%)	12 (5%)	28	61
2	P	226/226 (100%)	213 (94%)	13 (6%)	25	57
All	All	3216/3216 (100%)	2983 (93%)	233 (7%)	18	45

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 carbohydrates in this entry.

5.6 Ligand geometry

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	MAN	B	1500	-	12,12,12	0.40	0	17,17,17	0.39	0
3	MAN	D	1601	-	12,12,12	0.35	0	17,17,17	0.53	0
3	MAN	F	1502	-	12,12,12	0.43	0	17,17,17	0.61	0
3	MAN	H	1603	-	12,12,12	0.43	0	17,17,17	0.52	0
3	MAN	J	1605	-	12,12,12	0.27	0	17,17,17	0.35	0
3	MAN	L	1504	-	12,12,12	0.28	0	17,17,17	0.44	0
3	MAN	N	1506	-	12,12,12	0.23	0	17,17,17	0.43	0
3	MAN	P	1607	-	12,12,12	0.27	0	17,17,17	0.39	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	B	1500	-	-	0/2/22/22	0/1/1/1
3	MAN	D	1601	-	-	0/2/22/22	0/1/1/1
3	MAN	F	1502	-	-	0/2/22/22	0/1/1/1
3	MAN	H	1603	-	-	0/2/22/22	0/1/1/1
3	MAN	J	1605	-	-	0/2/22/22	0/1/1/1
3	MAN	L	1504	-	-	0/2/22/22	0/1/1/1
3	MAN	N	1506	-	-	0/2/22/22	0/1/1/1
3	MAN	P	1607	-	-	0/2/22/22	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	J	1605	MAN	4	0
3	L	1504	MAN	2	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(Å²)	Q<0.9
1	A	205/205 (100%)	0.55	11 (5%)	29	19	20, 55, 108, 132	0
1	C	205/205 (100%)	0.52	13 (6%)	23	14	20, 57, 108, 130	0
1	E	205/205 (100%)	0.45	5 (2%)	62	50	20, 59, 108, 129	0
1	G	205/205 (100%)	0.50	18 (8%)	12	6	19, 58, 110, 132	0
1	I	205/205 (100%)	4.00	147 (71%)	0	0	20, 168, 190, 196	0
1	K	205/205 (100%)	4.85	175 (85%)	0	0	20, 171, 195, 198	0
1	M	205/205 (100%)	4.62	167 (81%)	0	0	20, 170, 193, 198	0
1	O	205/205 (100%)	4.05	150 (73%)	0	0	20, 168, 193, 198	0
2	B	279/279 (100%)	0.34	6 (2%)	65	54	17, 40, 79, 114	0
2	D	279/279 (100%)	0.34	7 (2%)	61	48	18, 41, 80, 116	0
2	F	279/279 (100%)	0.26	4 (1%)	78	69	18, 41, 83, 112	0
2	H	279/279 (100%)	0.32	6 (2%)	65	54	17, 42, 83, 114	0
2	J	279/279 (100%)	2.09	107 (38%)	0	0	51, 112, 192, 200	0
2	L	279/279 (100%)	2.42	124 (44%)	0	0	56, 113, 190, 200	0
2	N	279/279 (100%)	2.65	144 (51%)	0	0	53, 115, 193, 200	0
2	P	279/279 (100%)	2.19	111 (39%)	0	0	50, 112, 191, 200	0
All	All	3872/3872 (100%)	1.80	1195 (30%)	1	0	17, 85, 186, 200	0

All (1195) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	48	PHE	17.9
1	I	102	THR	16.8
1	M	102	THR	15.7
2	L	270	SER	15.5
1	K	95	LYS	15.3

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Mol	Chain	Res	Type	RSRZ
1	M	150	LEU	14.5
1	K	102	THR	14.3
1	K	205	GLU	13.9
1	M	183	SER	13.9
1	K	65	LEU	13.9
1	M	95	LYS	13.4
1	O	103	LEU	13.2
1	K	69	ASP	12.8
1	M	133	PHE	12.7
1	M	71	THR	12.7
1	K	127	ALA	12.7
1	O	48	PHE	12.6
1	O	71	THR	12.6
1	K	101	ASN	12.5
1	O	162	LEU	12.5
1	M	179	SER	12.2
2	L	202	ALA	12.2
2	J	256	TYR	12.1
1	I	127	ALA	12.1
2	N	179	VAL	12.1
1	I	95	LYS	12.1
1	I	205	GLU	11.9
2	P	256	TYR	11.9
1	K	174	THR	11.8
1	O	67	ILE	11.8
1	K	104	GLN	11.7
1	O	105	LEU	11.7
1	K	98	LEU	11.7
1	M	93	MET	11.6
1	K	170	MET	11.6
2	L	271	ILE	11.6
1	M	18	VAL	11.5
1	O	95	LYS	11.5
1	K	184	ASN	11.5
1	K	48	PHE	11.3
1	I	174	THR	11.2
1	O	184	ASN	11.0
2	P	215	PHE	11.0
2	P	218	ALA	10.9
1	M	105	LEU	10.9
2	N	168	VAL	10.8
1	K	150	LEU	10.8

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Mol	Chain	Res	Type	RSRZ
1	M	184	ASN	10.7
1	M	162	LEU	10.6
1	K	183	SER	10.6
1	K	18	VAL	10.5
1	K	135	ARG	10.4
1	M	55	PHE	10.4
1	M	201	THR	10.2
2	N	218	ALA	10.2
1	M	65	LEU	10.1
2	P	214	SER	10.0
2	J	268	VAL	9.9
1	M	104	GLN	9.9
1	O	201	THR	9.9
1	O	104	GLN	9.9
2	J	215	PHE	9.9
1	K	93	MET	9.9
1	O	96	SER	9.8
2	P	263	VAL	9.8
1	M	205	GLU	9.7
2	L	256	TYR	9.7
1	K	71	THR	9.7
1	M	135	ARG	9.5
2	L	168	VAL	9.5
1	M	174	THR	9.5
2	J	217	PRO	9.5
1	I	67	ILE	9.5
2	N	271	ILE	9.5
1	I	135	ARG	9.5
2	P	272	ILE	9.5
2	N	181	ILE	9.4
1	K	133	PHE	9.3
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	137	ALA	9.1
1	I	69	ASP	9.1
1	K	94	ASP	9.1
1	O	94	ASP	9.1
1	K	67	ILE	9.0
1	I	184	ASN	9.0
2	N	267	ASN	9.0

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Mol	Chain	Res	Type	RSRZ
1	I	150	LEU	9.0
1	M	101	ASN	9.0
2	J	179	VAL	9.0
2	J	213	ALA	9.0
1	K	103	LEU	8.9
2	N	175	TYR	8.9
1	M	47	ARG	8.8
1	K	185	ILE	8.8
1	K	201	THR	8.7
1	K	55	PHE	8.7
2	P	217	PRO	8.7
2	P	202	ALA	8.7
2	N	207	SER	8.7
2	P	179	VAL	8.7
2	L	268	VAL	8.7
1	I	101	ASN	8.7
1	K	20	LEU	8.6
1	K	106	ALA	8.6
2	N	268	VAL	8.6
2	L	223	VAL	8.6
1	I	131	LEU	8.5
1	K	128	ALA	8.5
1	I	94	ASP	8.5
1	O	102	THR	8.5
1	M	116	ARG	8.4
1	I	170	MET	8.4
2	L	116	GLY	8.4
1	M	148	TYR	8.4
1	O	20	LEU	8.4
1	K	34	GLN	8.4
1	O	174	THR	8.2
1	M	185	ILE	8.2
1	I	128	ALA	8.1
2	P	211	ASN	8.1
2	J	212	THR	8.1
1	O	177	LEU	8.1
2	N	174	ASP	8.1
1	M	137	ALA	8.1
1	O	127	ALA	8.1
2	J	204	ALA	8.1
1	I	162	LEU	8.1
1	I	48	PHE	8.0

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Mol	Chain	Res	Type	RSRZ
1	K	157	ALA	8.0
1	K	162	LEU	8.0
2	N	211	ASN	8.0
1	M	151	THR	8.0
1	O	183	SER	7.9
1	M	98	LEU	7.9
2	N	272	ILE	7.9
1	M	128	ALA	7.9
1	O	18	VAL	7.9
2	N	219	GLN	7.9
2	N	172	LEU	7.9
1	M	70	ALA	7.9
1	I	186	THR	7.8
1	I	20	LEU	7.8
1	I	183	SER	7.8
1	K	173	SER	7.8
1	K	138	ASN	7.8
2	N	270	SER	7.8
1	I	93	MET	7.7
1	K	37	VAL	7.7
2	N	260	GLY	7.7
2	N	256	TYR	7.7
2	N	214	SER	7.7
1	K	19	GLN	7.7
2	P	271	ILE	7.6
1	O	55	PHE	7.6
2	P	213	ALA	7.6
1	O	69	ASP	7.6
1	M	67	ILE	7.6
1	K	200	MET	7.6
1	M	87	VAL	7.6
1	I	201	THR	7.6
1	O	205	GLU	7.6
1	M	155	LEU	7.5
1	M	94	ASP	7.5
1	M	127	ALA	7.5
2	N	202	ALA	7.5
1	K	68	LEU	7.5
1	M	178	PRO	7.5
1	O	135	ARG	7.5
1	O	136	SER	7.5
1	M	152	VAL	7.5

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Mol	Chain	Res	Type	RSRZ
1	I	35	SER	7.4
1	K	105	LEU	7.4
2	N	261	GLY	7.4
2	P	212	THR	7.3
1	M	100	GLU	7.3
2	P	261	GLY	7.3
1	O	87	VAL	7.3
2	J	175	TYR	7.3
1	I	98	LEU	7.3
1	O	133	PHE	7.3
1	I	117	PRO	7.2
2	P	270	SER	7.2
1	I	33	ILE	7.2
1	K	92	SER	7.2
1	I	4	LEU	7.2
2	L	222	GLY	7.2
1	I	151	THR	7.1
1	K	36	TRP	7.1
1	M	52	PRO	7.1
1	I	157	ALA	7.1
1	O	35	SER	7.1
2	J	225	LEU	7.0
1	K	35	SER	7.0
1	M	11	TYR	7.0
1	M	91	PRO	7.0
1	K	74	GLN	7.0
2	L	182	PRO	7.0
1	M	51	THR	6.9
2	P	268	VAL	6.9
1	M	203	VAL	6.9
1	O	21	ALA	6.9
1	O	98	LEU	6.9
2	J	257	ALA	6.9
1	I	142	LEU	6.8
1	I	55	PHE	6.8
2	J	271	ILE	6.8
2	L	181	ILE	6.8
2	L	272	ILE	6.8
2	N	20	VAL	6.8
1	K	96	SER	6.8
1	M	69	ASP	6.7
2	P	216	SER	6.7

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Mol	Chain	Res	Type	RSRZ
1	O	91	PRO	6.7
1	K	9	VAL	6.7
1	O	50	VAL	6.7
1	I	148	TYR	6.7
2	P	219	GLN	6.7
1	O	7	THR	6.7
1	O	93	MET	6.7
1	I	18	VAL	6.7
1	I	21	ALA	6.7
2	N	222	GLY	6.7
1	K	4	LEU	6.7
1	K	181	ALA	6.6
1	O	47	ARG	6.6
2	L	219	GLN	6.6
1	O	84	TRP	6.6
1	M	177	LEU	6.6
1	I	104	GLN	6.6
1	I	83	PHE	6.5
1	O	128	ALA	6.5
2	N	266	GLY	6.5
2	J	218	ALA	6.5
2	N	215	PHE	6.5
2	P	225	LEU	6.5
2	J	223	VAL	6.5
2	L	232	ILE	6.5
2	P	222	GLY	6.5
2	P	221	VAL	6.5
2	J	202	ALA	6.5
1	O	185	ILE	6.4
1	O	179	SER	6.4
2	N	170	VAL	6.4
2	L	213	ALA	6.4
2	J	22	VAL	6.4
1	I	85	MET	6.4
1	M	85	MET	6.4
1	I	68	LEU	6.4
2	N	178	SER	6.4
1	K	172	GLU	6.4
1	I	7	THR	6.4
1	K	87	VAL	6.4
2	N	248	VAL	6.4
1	O	52	PRO	6.4

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Mol	Chain	Res	Type	RSRZ
1	I	158	GLY	6.3
1	I	136	SER	6.3
1	K	83	PHE	6.3
1	O	158	GLY	6.3
2	P	207	SER	6.3
1	I	103	LEU	6.3
2	N	264	THR	6.2
1	M	12	PRO	6.2
1	M	167	VAL	6.2
1	O	11	TYR	6.2
1	O	33	ILE	6.2
2	P	181	ILE	6.2
1	I	56	ALA	6.2
1	I	172	GLU	6.2
1	M	106	ALA	6.2
1	K	179	SER	6.2
2	L	267	ASN	6.2
1	K	152	VAL	6.2
1	M	33	ILE	6.1
2	N	169	THR	6.1
1	O	198	PRO	6.1
1	K	38	GLU	6.1
2	N	166	ARG	6.1
1	C	178	PRO	6.1
2	J	181	ILE	6.1
1	I	71	THR	6.1
1	I	96	SER	6.1
2	L	266	GLY	6.1
2	N	263	VAL	6.1
1	K	10	ILE	6.1
2	L	119	ALA	6.1
1	I	70	ALA	6.1
1	O	85	MET	6.0
2	L	207	SER	6.0
2	L	230	THR	6.0
1	O	70	ALA	6.0
1	O	106	ALA	6.0
2	N	22	VAL	6.0
2	L	225	LEU	6.0
2	J	20	VAL	5.9
1	K	33	ILE	5.9
2	P	20	VAL	5.9

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Mol	Chain	Res	Type	RSRZ
1	M	140	LEU	5.9
2	L	215	PHE	5.9
2	N	182	PRO	5.9
2	N	223	VAL	5.9
2	L	269	GLN	5.9
1	M	165	ALA	5.9
2	L	166	ARG	5.9
1	K	54	LEU	5.9
1	O	4	LEU	5.9
1	K	11	TYR	5.9
1	K	194	GLY	5.9
1	O	137	ALA	5.9
1	M	34	GLN	5.9
1	O	143	ILE	5.8
1	I	87	VAL	5.8
1	K	85	MET	5.8
1	I	19	GLN	5.8
2	L	67	VAL	5.8
1	M	143	ILE	5.8
1	O	140	LEU	5.8
1	M	66	ARG	5.8
1	K	136	SER	5.8
1	M	90	ILE	5.8
2	J	261	GLY	5.8
1	K	177	LEU	5.8
2	L	120	ILE	5.7
1	I	84	TRP	5.7
1	I	181	ALA	5.7
2	J	214	SER	5.7
2	L	126	ILE	5.7
1	K	70	ALA	5.7
1	M	160	ARG	5.7
1	I	11	TYR	5.7
2	N	213	ALA	5.7
1	K	142	LEU	5.7
1	O	142	LEU	5.7
1	K	114	TYR	5.6
1	M	29	SER	5.6
1	M	136	SER	5.6
2	P	223	VAL	5.6
2	P	262	GLN	5.6
2	J	222	GLY	5.6

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Mol	Chain	Res	Type	RSRZ
1	O	178	PRO	5.6
1	M	103	LEU	5.6
2	L	229	GLY	5.6
2	L	211	ASN	5.6
1	K	90	ILE	5.6
2	N	116	GLY	5.6
1	K	176	LYS	5.6
1	M	7	THR	5.6
2	N	212	THR	5.6
1	O	83	PHE	5.5
1	I	167	VAL	5.5
2	J	273	GLY	5.5
2	N	188	ALA	5.5
1	K	7	THR	5.5
2	L	210	THR	5.5
2	P	210	THR	5.5
2	P	166	ARG	5.5
1	M	180	ASP	5.5
1	M	170	MET	5.5
2	L	214	SER	5.5
1	K	21	ALA	5.5
1	K	155	LEU	5.5
1	O	176	LYS	5.5
1	O	203	VAL	5.5
1	K	53	PRO	5.4
2	L	170	VAL	5.4
1	M	200	MET	5.4
2	L	53	THR	5.4
1	O	34	GLN	5.4
2	L	260	GLY	5.4
1	K	167	VAL	5.4
1	K	203	VAL	5.4
1	K	166	LEU	5.4
1	I	179	SER	5.4
1	I	200	MET	5.4
2	L	273	GLY	5.4
2	P	170	VAL	5.4
1	I	177	LEU	5.3
2	P	53	THR	5.3
1	K	16	LYS	5.3
2	N	225	LEU	5.3
2	J	210	THR	5.3

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Mol	Chain	Res	Type	RSRZ
2	J	260	GLY	5.3
1	O	92	SER	5.3
1	K	148	TYR	5.3
2	L	124	SER	5.3
1	M	5	GLY	5.2
2	J	272	ILE	5.2
2	P	260	GLY	5.2
1	K	6	ALA	5.2
1	M	74	GLN	5.2
1	K	116	ARG	5.2
2	N	230	THR	5.2
1	O	9	VAL	5.2
2	J	211	ASN	5.2
1	I	198	PRO	5.2
2	P	267	ASN	5.2
1	K	132	ARG	5.1
2	N	242	ALA	5.1
2	L	20	VAL	5.1
1	K	29	SER	5.1
1	K	186	THR	5.1
2	J	207	SER	5.1
1	M	138	ASN	5.1
1	O	167	VAL	5.1
1	I	106	ALA	5.1
1	I	165	ALA	5.1
1	M	68	LEU	5.1
1	O	74	GLN	5.1
1	K	47	ARG	5.1
2	J	115	ALA	5.0
2	L	257	ALA	5.0
1	I	116	ARG	5.0
2	P	174	ASP	5.0
1	M	4	LEU	5.0
2	L	175	TYR	5.0
2	N	199	GLY	5.0
1	I	47	ARG	5.0
1	M	53	PRO	5.0
1	K	64	THR	5.0
1	O	148	TYR	5.0
1	M	171	GLY	5.0
2	P	266	GLY	5.0
1	O	101	ASN	5.0

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Mol	Chain	Res	Type	RSRZ
1	O	131	LEU	4.9
1	K	31	TYR	4.9
1	K	151	THR	4.9
1	K	196	LEU	4.9
1	O	152	VAL	4.9
2	J	15	GLY	4.9
1	I	105	LEU	4.9
2	N	18	ALA	4.9
2	J	148	ILE	4.9
2	N	269	GLN	4.9
1	O	53	PRO	4.9
1	I	176	LYS	4.9
1	I	54	LEU	4.8
1	I	137	ALA	4.8
1	M	96	SER	4.8
2	L	252	LEU	4.8
2	P	104	PRO	4.8
1	K	160	ARG	4.8
1	M	172	GLU	4.8
2	P	22	VAL	4.8
1	M	35	SER	4.8
2	P	28	VAL	4.8
1	M	129	GLU	4.7
2	N	233	PRO	4.7
1	K	117	PRO	4.7
1	K	120	LEU	4.7
1	K	100	GLU	4.7
2	N	177	GLY	4.7
1	O	19	GLN	4.7
1	I	10	ILE	4.7
2	L	148	ILE	4.7
2	N	24	LEU	4.6
1	O	116	ARG	4.6
2	P	273	GLY	4.6
1	M	92	SER	4.6
2	P	169	THR	4.6
2	N	209	PHE	4.6
1	K	99	THR	4.6
1	M	117	PRO	4.6
2	N	148	ILE	4.6
1	O	97	LYS	4.6
2	N	257	ALA	4.6

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Mol	Chain	Res	Type	RSRZ
1	I	203	VAL	4.6
1	K	126	GLN	4.6
2	P	264	THR	4.6
1	I	6	ALA	4.5
1	K	91	PRO	4.5
1	K	158	GLY	4.5
1	O	180	ASP	4.5
2	J	124	SER	4.5
1	K	57	MET	4.5
1	I	50	VAL	4.5
2	N	221	VAL	4.5
2	L	218	ALA	4.5
1	I	36	TRP	4.5
1	M	173	SER	4.5
1	I	9	VAL	4.5
1	I	99	THR	4.5
2	L	191	GLN	4.5
1	M	84	TRP	4.5
2	J	267	ASN	4.5
1	M	54	LEU	4.5
1	O	99	THR	4.5
2	J	219	GLN	4.5
1	O	187	TYR	4.5
2	P	115	ALA	4.5
1	I	160	ARG	4.5
1	O	200	MET	4.4
1	K	109	SER	4.4
1	O	170	MET	4.4
1	M	9	VAL	4.4
1	K	66	ARG	4.4
2	N	259	THR	4.4
1	K	178	PRO	4.4
1	M	83	PHE	4.4
2	N	53	THR	4.4
1	M	17	GLN	4.4
1	M	157	ALA	4.4
2	L	18	ALA	4.4
2	N	258	ARG	4.4
1	M	45	ASP	4.4
1	M	145	PRO	4.4
2	P	168	VAL	4.4
1	K	140	LEU	4.4

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Mol	Chain	Res	Type	RSRZ
1	I	185	ILE	4.4
1	O	49	ILE	4.4
1	K	119	LYS	4.4
1	I	34	GLN	4.4
1	M	99	THR	4.4
2	L	185	VAL	4.4
2	N	201	THR	4.4
2	J	216	SER	4.4
2	J	166	ARG	4.4
1	K	58	LYS	4.4
1	M	79	ARG	4.4
2	L	150	ALA	4.4
1	O	114	TYR	4.4
1	G	178	PRO	4.3
1	O	151	THR	4.3
2	N	228	ASN	4.3
1	I	132	ARG	4.3
1	K	159	THR	4.3
2	N	197	LEU	4.3
1	K	171	GLY	4.3
1	G	177	LEU	4.3
1	K	121	ALA	4.3
2	L	115	ALA	4.3
2	L	250	LEU	4.3
2	P	148	ILE	4.3
1	O	172	GLU	4.2
1	I	122	LEU	4.2
1	M	36	TRP	4.2
2	L	33	ASN	4.2
1	M	121	ALA	4.2
2	P	191	GLN	4.2
1	O	122	LEU	4.2
2	L	217	PRO	4.2
2	L	212	THR	4.2
1	I	143	ILE	4.2
2	L	104	PRO	4.2
2	N	217	PRO	4.2
2	N	234	ALA	4.2
2	L	278	TYR	4.2
1	K	122	LEU	4.2
2	J	30	VAL	4.2
2	N	195	TYR	4.2

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Mol	Chain	Res	Type	RSRZ
1	K	202	GLY	4.1
1	M	186	THR	4.1
1	K	56	ALA	4.1
1	I	31	TYR	4.1
2	J	150	ALA	4.1
2	N	229	GLY	4.1
1	M	6	ALA	4.1
1	K	180	ASP	4.1
1	I	120	LEU	4.1
2	N	176	PRO	4.1
1	I	152	VAL	4.1
1	M	31	TYR	4.1
1	O	165	ALA	4.1
2	L	129	LEU	4.1
2	J	279	GLN	4.1
1	M	158	GLY	4.1
2	L	221	VAL	4.1
1	M	120	LEU	4.1
2	P	230	THR	4.1
2	L	28	VAL	4.0
1	I	121	ALA	4.0
1	I	114	TYR	4.0
2	N	42	ILE	4.0
2	L	15	GLY	4.0
1	K	198	PRO	4.0
2	P	177	GLY	4.0
2	N	124	SER	4.0
1	K	189	THR	4.0
2	P	172	LEU	4.0
1	I	187	TYR	4.0
2	J	232	ILE	4.0
2	L	174	ASP	4.0
2	N	262	GLN	4.0
1	I	8	ARG	4.0
2	L	245	THR	4.0
1	I	166	LEU	4.0
1	O	186	THR	4.0
1	K	22	VAL	4.0
2	B	172	LEU	4.0
1	K	84	TRP	4.0
1	I	173	SER	4.0
1	K	143	ILE	4.0

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Mol	Chain	Res	Type	RSRZ
1	M	109	SER	4.0
2	N	278	TYR	4.0
1	K	79	ARG	3.9
2	H	215	PHE	3.9
1	K	192	ASP	3.9
1	O	90	ILE	3.9
1	K	82	LEU	3.9
1	I	37	VAL	3.9
2	P	257	ALA	3.9
1	K	187	TYR	3.9
2	N	210	THR	3.9
1	O	72	ASN	3.9
1	O	57	MET	3.9
1	I	22	VAL	3.9
1	K	199	LYS	3.9
1	M	199	LYS	3.9
2	J	258	ARG	3.9
2	F	172	LEU	3.9
2	P	36	VAL	3.9
2	N	191	GLN	3.9
2	J	240	LEU	3.9
2	P	175	TYR	3.9
1	I	161	VAL	3.9
2	N	243	VAL	3.9
2	N	254	ALA	3.9
1	M	166	LEU	3.8
1	M	37	VAL	3.8
1	O	121	ALA	3.8
1	K	49	ILE	3.8
1	M	189	THR	3.8
2	J	270	SER	3.8
1	M	176	LYS	3.8
1	K	123	PRO	3.8
2	L	93	VAL	3.8
2	J	169	THR	3.8
2	J	137	TYR	3.8
2	J	263	VAL	3.8
2	N	36	VAL	3.8
2	L	24	LEU	3.8
2	L	42	ILE	3.8
1	M	168	PRO	3.8
2	J	255	ASN	3.8

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Mol	Chain	Res	Type	RSRZ
2	N	239	SER	3.8
2	N	112	VAL	3.8
1	I	100	GLU	3.8
2	N	232	ILE	3.8
2	N	249	SER	3.8
2	J	53	THR	3.8
1	O	22	VAL	3.8
1	M	187	TYR	3.8
2	N	137	TYR	3.8
1	O	58	LYS	3.7
1	K	24	ASN	3.7
1	O	8	ARG	3.7
2	L	224	GLN	3.7
1	K	129	GLU	3.7
2	N	216	SER	3.7
2	N	255	ASN	3.7
2	N	115	ALA	3.7
1	I	74	GLN	3.7
1	M	132	ARG	3.7
2	N	200	THR	3.7
2	J	254	ALA	3.7
1	A	161	VAL	3.7
1	I	138	ASN	3.7
1	A	93	MET	3.7
1	M	27	GLU	3.7
1	M	10	ILE	3.7
1	M	21	ALA	3.7
2	N	250	LEU	3.7
2	L	146	TRP	3.7
1	O	51	THR	3.7
1	M	131	LEU	3.7
1	I	115	TYR	3.7
2	J	67	VAL	3.6
2	P	255	ASN	3.6
2	P	196	TYR	3.6
2	J	174	ASP	3.6
1	O	109	SER	3.6
1	M	16	LYS	3.6
1	O	27	GLU	3.6
1	O	100	GLU	3.6
2	P	204	ALA	3.6
2	J	118	VAL	3.6

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Mol	Chain	Res	Type	RSRZ
1	I	16	LYS	3.6
2	P	193	LEU	3.6
2	N	203	ASP	3.6
1	K	190	ILE	3.6
2	L	244	GLY	3.6
1	O	64	THR	3.6
1	M	122	LEU	3.6
2	J	252	LEU	3.6
2	N	33	ASN	3.6
2	F	215	PHE	3.6
2	P	242	ALA	3.6
1	K	17	GLN	3.6
1	M	2	VAL	3.6
2	P	33	ASN	3.6
1	M	49	ILE	3.6
1	O	23	THR	3.6
2	L	106	ALA	3.6
1	M	20	LEU	3.6
2	P	120	ILE	3.5
1	K	88	LYS	3.5
2	N	189	LYS	3.5
2	N	16	GLY	3.5
1	M	130	LYS	3.5
2	J	278	TYR	3.5
2	D	165	ALA	3.5
1	O	66	ARG	3.5
1	I	129	GLU	3.5
1	I	159	THR	3.5
1	K	73	ASN	3.5
1	M	64	THR	3.5
2	P	232	ILE	3.5
1	O	38	GLU	3.5
2	L	255	ASN	3.5
2	D	172	LEU	3.5
1	I	38	GLU	3.5
1	I	64	THR	3.5
1	I	125	ASP	3.5
1	O	155	LEU	3.5
1	K	112	LYS	3.5
1	M	164	ASN	3.5
1	M	190	ILE	3.5
1	M	192	ASP	3.5

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Mol	Chain	Res	Type	RSRZ
2	L	54	ASP	3.5
1	O	6	ALA	3.5
2	J	191	GLN	3.5
1	O	199	LYS	3.5
1	O	89	ALA	3.4
2	P	186	TYR	3.4
2	J	168	VAL	3.4
2	N	244	GLY	3.4
1	I	180	ASP	3.4
2	L	167	ASP	3.4
1	O	189	THR	3.4
2	P	250	LEU	3.4
2	J	157	PRO	3.4
1	M	196	LEU	3.4
2	N	245	THR	3.4
2	H	172	LEU	3.4
1	M	163	GLU	3.4
1	I	32	LEU	3.4
1	K	161	VAL	3.4
2	P	195	TYR	3.4
1	O	160	ARG	3.4
1	O	166	LEU	3.4
1	O	157	ALA	3.4
2	N	231	ILE	3.4
2	N	15	GLY	3.4
1	O	68	LEU	3.4
2	L	248	VAL	3.4
1	A	178	PRO	3.3
1	I	23	THR	3.3
2	J	120	ILE	3.3
1	K	78	ASP	3.3
2	J	178	SER	3.3
2	L	80	SER	3.3
1	O	32	LEU	3.3
2	N	123	GLY	3.3
2	L	179	VAL	3.3
1	A	177	LEU	3.3
2	N	237	THR	3.3
2	P	258	ARG	3.3
1	I	109	SER	3.3
2	L	22	VAL	3.3
1	O	138	ASN	3.3

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Mol	Chain	Res	Type	RSRZ
1	K	169	PRO	3.3
2	L	264	THR	3.3
2	J	104	PRO	3.3
1	I	199	LYS	3.3
1	M	119	LYS	3.3
1	M	125	ASP	3.3
1	M	198	PRO	3.3
2	L	204	ALA	3.3
1	M	50	VAL	3.2
2	J	28	VAL	3.2
1	O	119	LYS	3.2
1	O	17	GLN	3.2
1	I	30	THR	3.2
1	I	79	ARG	3.2
1	I	2	VAL	3.2
1	I	196	LEU	3.2
1	K	139	SER	3.2
2	P	137	TYR	3.2
2	J	116	GLY	3.2
2	N	167	ASP	3.2
2	L	187	CYS	3.2
1	I	189	THR	3.2
1	M	112	LYS	3.2
1	O	107	ILE	3.2
1	M	38	GLU	3.2
1	I	92	SER	3.2
1	O	194	GLY	3.2
2	J	186	TYR	3.2
1	K	8	ARG	3.2
1	O	54	LEU	3.2
2	J	170	VAL	3.2
2	N	180	PRO	3.2
2	L	183	LEU	3.1
2	N	187	CYS	3.1
2	N	205	GLY	3.1
1	K	134	ARG	3.1
2	H	165	ALA	3.1
2	N	265	ALA	3.1
2	L	137	TYR	3.1
1	M	15	GLN	3.1
2	N	277	VAL	3.1
2	P	116	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
2	P	54	ASP	3.1
2	J	236	ASN	3.1
1	K	2	VAL	3.1
1	C	72	ASN	3.1
1	I	156	ASN	3.1
2	N	279	GLN	3.1
1	K	168	PRO	3.1
2	L	263	VAL	3.1
2	J	230	THR	3.1
2	J	24	LEU	3.1
2	N	183	LEU	3.1
2	P	109	LEU	3.1
2	P	234	ALA	3.1
1	I	66	ARG	3.1
1	M	202	GLY	3.1
2	N	104	PRO	3.1
2	N	108	TYR	3.1
2	N	146	TRP	3.1
1	K	113	LEU	3.1
1	M	175	VAL	3.1
1	M	8	ARG	3.0
2	J	126	ILE	3.0
1	C	160	ARG	3.0
1	M	30	THR	3.0
1	E	178	PRO	3.0
1	I	178	PRO	3.0
2	L	144	PHE	3.0
2	N	120	ILE	3.0
1	M	114	TYR	3.0
2	N	163	VAL	3.0
2	P	178	SER	3.0
2	L	279	GLN	3.0
1	O	78	ASP	3.0
2	P	30	VAL	3.0
1	O	196	LEU	3.0
2	N	52	ILE	3.0
1	C	132	ARG	3.0
1	I	53	PRO	3.0
2	D	215	PHE	3.0
2	L	276	PHE	3.0
1	G	176	LYS	3.0
2	L	163	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
2	P	199	GLY	3.0
1	M	19	GLN	3.0
2	J	250	LEU	3.0
2	N	193	LEU	3.0
1	I	81	SER	3.0
2	L	216	SER	3.0
1	K	5	GLY	3.0
1	M	161	VAL	3.0
2	P	265	ALA	3.0
1	I	58	LYS	3.0
2	J	47	ASP	3.0
2	N	173	PRO	3.0
2	P	182	PRO	3.0
1	K	111	ILE	3.0
2	P	67	VAL	3.0
2	J	33	ASN	3.0
1	I	119	LYS	2.9
1	K	51	THR	2.9
2	L	169	THR	2.9
2	H	261	GLY	2.9
2	N	14	GLY	2.9
1	M	22	VAL	2.9
2	J	146	TRP	2.9
2	P	236	ASN	2.9
1	K	141	THR	2.9
2	N	276	PHE	2.9
1	M	111	ILE	2.9
1	I	140	LEU	2.9
2	J	119	ALA	2.9
2	L	102	PRO	2.9
1	O	173	SER	2.9
1	M	126	GLN	2.9
1	M	149	TYR	2.9
2	D	171	THR	2.9
2	D	175	TYR	2.9
2	L	123	GLY	2.9
1	A	176	LYS	2.9
1	O	197	THR	2.9
2	L	68	LEU	2.9
2	L	262	GLN	2.9
2	L	277	VAL	2.9
2	P	163	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	M	62	GLU	2.9
1	O	79	ARG	2.9
2	P	259	THR	2.9
2	L	186	TYR	2.9
1	A	140	LEU	2.8
2	J	80	SER	2.8
1	I	82	LEU	2.8
1	K	30	THR	2.8
2	N	157	PRO	2.8
2	J	195	TYR	2.8
2	L	258	ARG	2.8
1	M	73	ASN	2.8
1	O	63	ASN	2.8
2	B	215	PHE	2.8
2	H	175	TYR	2.8
1	M	97	LYS	2.8
1	O	26	ASP	2.8
2	L	61	GLY	2.8
2	P	126	ILE	2.8
1	G	135	ARG	2.8
1	G	158	GLY	2.8
1	M	32	LEU	2.8
2	J	93	VAL	2.8
1	O	60	LYS	2.8
2	L	47	ASP	2.8
1	O	202	GLY	2.8
1	K	145	PRO	2.8
1	O	175	VAL	2.8
2	N	206	ASN	2.8
2	P	18	ALA	2.8
2	N	1	PHE	2.8
2	N	171	THR	2.8
1	K	14	GLY	2.8
1	O	31	TYR	2.7
1	I	72	ASN	2.7
2	N	251	GLY	2.7
2	L	208	ILE	2.7
1	I	27	GLU	2.7
2	J	220	GLY	2.7
2	P	24	LEU	2.7
2	F	175	TYR	2.7
1	E	176	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
2	J	221	VAL	2.7
2	L	36	VAL	2.7
2	N	54	ASP	2.7
1	I	113	LEU	2.7
2	J	183	LEU	2.7
1	O	112	LYS	2.7
1	K	175	VAL	2.7
1	I	171	GLY	2.7
2	N	252	LEU	2.7
2	N	126	ILE	2.7
1	K	204	MET	2.7
1	M	159	THR	2.7
2	L	172	LEU	2.7
1	O	73	ASN	2.7
2	L	195	TYR	2.7
2	N	238	VAL	2.7
1	K	12	PRO	2.7
1	O	29	SER	2.7
2	N	185	VAL	2.7
2	P	93	VAL	2.7
1	K	15	GLN	2.6
1	M	58	LYS	2.6
1	C	1	GLY	2.6
2	J	266	GLY	2.6
1	O	10	ILE	2.6
2	J	163	VAL	2.6
2	L	209	PHE	2.6
2	N	21	TYR	2.6
2	P	269	GLN	2.6
1	I	107	ILE	2.6
2	J	248	VAL	2.6
2	N	204	ALA	2.6
2	L	261	GLY	2.6
2	P	176	PRO	2.6
1	I	134	ARG	2.6
2	N	149	TYR	2.6
1	I	155	LEU	2.6
1	K	63	ASN	2.6
2	L	228	ASN	2.6
2	L	52	ILE	2.6
1	M	142	LEU	2.6
1	I	46	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	132	ARG	2.6
1	I	90	ILE	2.6
2	J	182	PRO	2.6
1	K	61	LYS	2.6
1	M	56	ALA	2.6
1	O	56	ALA	2.6
2	N	150	ALA	2.6
1	M	23	THR	2.6
2	P	240	LEU	2.6
1	O	161	VAL	2.6
2	P	185	VAL	2.6
1	I	89	ALA	2.5
1	K	149	TYR	2.5
1	M	134	ARG	2.5
1	I	97	LYS	2.5
2	P	249	SER	2.5
2	L	157	PRO	2.5
2	P	1	PHE	2.5
1	I	194	GLY	2.5
1	O	132	ARG	2.5
2	P	47	ASP	2.5
1	M	57	MET	2.5
2	L	95	TYR	2.5
1	K	60	LYS	2.5
1	G	140	LEU	2.5
1	M	72	ASN	2.5
1	K	23	THR	2.5
2	N	50	GLU	2.5
1	M	193	TYR	2.5
2	P	108	TYR	2.5
1	C	182	GLY	2.5
2	F	165	ALA	2.5
2	J	42	ILE	2.5
2	J	264	THR	2.5
1	I	1	GLY	2.5
1	I	49	ILE	2.5
2	L	125	LEU	2.5
1	M	86	ASN	2.5
1	O	117	PRO	2.5
2	N	7	ASN	2.5
1	G	155	LEU	2.5
1	I	3	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
2	P	171	THR	2.5
1	K	1	GLY	2.5
2	P	278	TYR	2.5
2	J	269	GLN	2.5
1	M	26	ASP	2.5
2	J	125	LEU	2.5
1	K	118	ALA	2.5
1	M	60	LYS	2.5
1	O	159	THR	2.5
1	O	62	GLU	2.5
1	M	78	ASP	2.5
1	K	52	PRO	2.5
2	J	7	ASN	2.5
2	L	49	PRO	2.5
1	K	131	LEU	2.4
2	J	193	LEU	2.4
2	N	274	VAL	2.4
1	C	135	ARG	2.4
1	K	27	GLU	2.4
2	L	16	GLY	2.4
1	O	36	TRP	2.4
2	J	18	ALA	2.4
2	N	10	ALA	2.4
2	P	248	VAL	2.4
1	O	204	MET	2.4
2	J	167	ASP	2.4
1	G	72	ASN	2.4
1	M	24	ASN	2.4
2	J	102	PRO	2.4
1	M	107	ILE	2.4
1	M	44	LYS	2.4
1	O	61	LYS	2.4
2	P	164	SER	2.4
1	I	91	PRO	2.4
1	M	3	ALA	2.4
2	J	11	ILE	2.4
2	N	28	VAL	2.4
2	L	109	LEU	2.4
1	G	1	GLY	2.4
2	J	229	GLY	2.4
2	D	166	ARG	2.4
1	G	162	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
2	J	1	PHE	2.4
2	J	176	PRO	2.4
2	P	173	PRO	2.4
1	K	163	GLU	2.4
2	L	231	ILE	2.4
1	I	175	VAL	2.3
1	K	50	VAL	2.3
1	K	97	LYS	2.3
2	L	127	ALA	2.3
2	P	119	ALA	2.3
1	K	25	ASN	2.3
1	M	82	LEU	2.3
2	N	240	LEU	2.3
1	K	62	GLU	2.3
1	K	130	LYS	2.3
1	O	126	GLN	2.3
2	L	162	ASP	2.3
2	L	118	VAL	2.3
2	N	190	SER	2.3
1	K	3	ALA	2.3
1	G	167	VAL	2.3
2	J	16	GLY	2.3
2	N	117	GLY	2.3
2	J	54	ASP	2.3
2	N	47	ASP	2.3
2	N	48	TYR	2.3
1	O	123	PRO	2.3
1	O	3	ALA	2.3
1	O	113	LEU	2.3
1	K	124	PRO	2.3
2	J	203	ASP	2.3
1	K	89	ALA	2.3
2	N	119	ALA	2.3
1	I	51	THR	2.3
2	P	220	GLY	2.3
2	L	240	LEU	2.2
2	P	183	LEU	2.2
2	L	176	PRO	2.2
1	G	183	SER	2.2
1	M	14	GLY	2.2
2	P	245	THR	2.2
1	O	75	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
2	L	76	LYS	2.2
1	C	93	MET	2.2
1	G	205	GLU	2.2
2	L	103	TRP	2.2
2	N	27	VAL	2.2
1	I	108	ILE	2.2
2	P	252	LEU	2.2
2	P	209	PHE	2.2
1	M	118	ALA	2.2
2	B	165	ALA	2.2
2	L	254	ALA	2.2
1	I	190	ILE	2.2
1	K	153	THR	2.2
1	K	32	LEU	2.2
1	I	17	GLN	2.2
2	P	206	ASN	2.2
1	C	176	LYS	2.2
2	P	103	TRP	2.2
2	D	167	ASP	2.2
2	L	37	ASP	2.2
2	N	37	ASP	2.2
1	A	179	SER	2.2
2	B	164	SER	2.2
2	N	164	SER	2.2
2	N	246	SER	2.2
1	I	202	GLY	2.2
2	J	185	VAL	2.2
2	N	30	VAL	2.2
2	J	172	LEU	2.2
2	B	175	TYR	2.2
2	P	279	GLN	2.2
1	M	204	MET	2.2
2	J	171	THR	2.2
1	G	98	LEU	2.1
2	P	52	ILE	2.1
2	P	131	LEU	2.1
2	P	253	THR	2.2
2	J	208	ILE	2.1
1	O	182	GLY	2.1
2	L	173	PRO	2.1
2	L	48	TYR	2.1
1	C	129	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
2	P	254	ALA	2.1
1	C	177	LEU	2.1
2	N	67	VAL	2.1
1	K	108	ILE	2.1
2	P	14	GLY	2.1
1	O	25	ASN	2.1
1	A	157	ALA	2.1
2	J	127	ALA	2.1
2	P	165	ALA	2.1
1	C	179	SER	2.1
1	E	140	LEU	2.1
1	O	153	THR	2.1
1	A	135	ARG	2.1
1	I	73	ASN	2.1
1	M	123	PRO	2.1
2	P	48	TYR	2.1
2	J	162	ASP	2.1
2	L	203	ASP	2.1
1	G	132	ARG	2.1
1	G	159	THR	2.1
2	L	56	VAL	2.1
1	O	12	PRO	2.1
2	N	247	ALA	2.1
1	K	110	ARG	2.1
1	M	139	SER	2.1
1	O	134	ARG	2.1
2	N	125	LEU	2.1
1	K	72	ASN	2.1
1	O	139	SER	2.1
2	L	117	GLY	2.1
1	G	93	MET	2.1
1	K	125	ASP	2.1
2	L	60	ARG	2.1
1	A	205	GLU	2.1
1	O	171	GLY	2.1
2	N	129	LEU	2.1
2	J	187	CYS	2.1
2	N	273	GLY	2.1
1	K	165	ALA	2.1
2	J	234	ALA	2.1
1	K	28	ASN	2.0
2	P	201	THR	2.0

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Mol	Chain	Res	Type	RSRZ
1	E	160	ARG	2.0
1	E	135	ARG	2.0
1	O	108	ILE	2.0
2	B	167	ASP	2.0
1	C	142	LEU	2.0
1	I	118	ALA	2.0
1	I	112	LYS	2.0
1	K	115	TYR	2.0
2	P	200	THR	2.0
1	M	28	ASN	2.0
1	M	89	ALA	2.0
1	G	160	ARG	2.0
2	H	163	VAL	2.0
2	J	277	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(\AA^2)	Q<0.9
3	MAN	D	1601	12/12	0.98	0.19	0.07	28,36,41,41	0
3	MAN	P	1607	12/12	0.90	0.26	0.02	110,112,116,117	0
3	MAN	F	1502	12/12	0.95	0.19	-0.04	29,35,41,41	0
3	MAN	H	1603	12/12	0.96	0.16	-0.05	28,34,39,39	0
3	MAN	J	1605	12/12	0.88	0.25	-0.28	96,100,105,106	0
3	MAN	L	1504	12/12	0.81	0.23	-0.79	96,99,103,106	0
3	MAN	B	1500	12/12	0.97	0.15	-0.80	30,35,39,39	0
3	MAN	N	1506	12/12	0.91	0.18	-1.22	90,94,100,101	0

6.5 Other polymers [i](#)

There are no such residues in this entry.