



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:42 PM UTC

PDB ID : 1RZI / pdb_00001rzi
Title : Crystal structure of human anti-HIV-1 gp120-reactive antibody 47e fab
Authors : Huang, C.C.; Venturi, M.; Majeed, S.; Moore, M.J.; Phogat, S.; Zhang, M.-Y.; Dimitrov, D.S.; Hendrickson, W.A.; Robinson, J.; Sodroski, J.; Wyatt, R.; Choe, H.; Farzan, M.; Kwong, P.D.
Deposited on : 2003-12-24
Resolution : 2.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

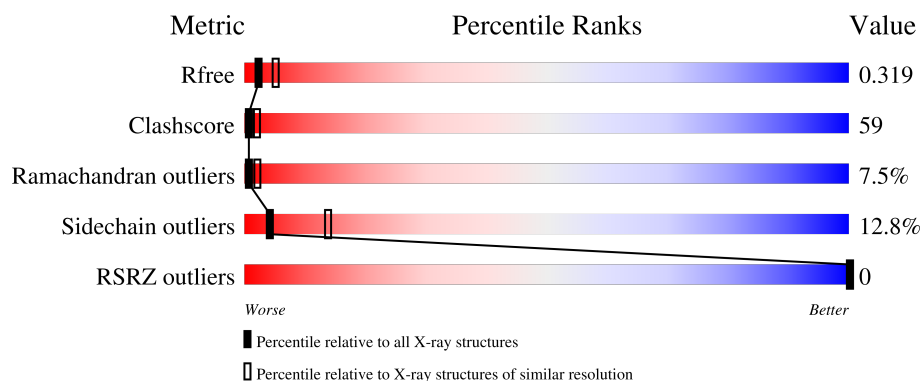
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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.



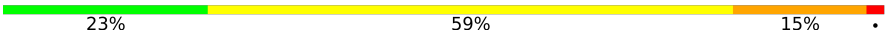
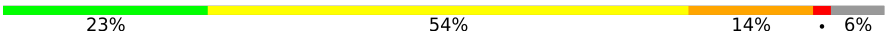
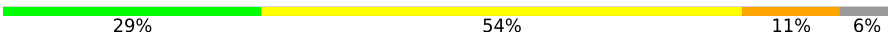
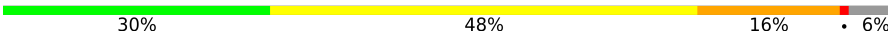
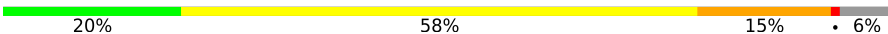
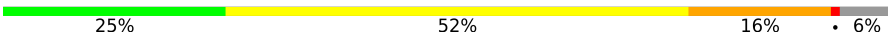
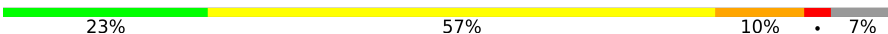
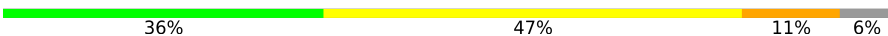
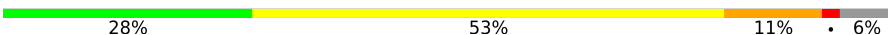
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	212	25% 59% 12% .
1	C	212	26% 51% 22% .
1	E	212	25% 56% 16% .
1	G	212	30% 53% 14% .
1	I	212	29% 56% 15% .

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Mol	Chain	Length	Quality of chain
1	K	212	 26% 57% 13% .
1	M	212	 31% 53% 15% .
1	O	212	 23% 59% 15% .
2	B	230	 23% 54% 14% . 6%
2	D	230	 29% 54% 11% 6%
2	F	230	 30% 48% 16% . 6%
2	H	230	 20% 58% 15% . 6%
2	J	230	 25% 52% 16% . 6%
2	L	230	 23% 57% 10% . 7%
2	N	230	 36% 47% 11% 6%
2	P	230	 28% 53% 11% . 6%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 25973 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 Fab 47e light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	211	Total	C	N	O	S	0	0	0
			1620	1012	272	331	5			
1	C	212	Total	C	N	O	S	0	0	0
			1628	1016	273	334	5			
1	E	211	Total	C	N	O	S	0	0	0
			1620	1012	272	331	5			
1	G	211	Total	C	N	O	S	0	0	0
			1620	1012	272	331	5			
1	I	211	Total	C	N	O	S	0	0	0
			1620	1012	272	331	5			
1	K	211	Total	C	N	O	S	0	0	0
			1620	1012	272	331	5			
1	M	211	Total	C	N	O	S	0	0	0
			1620	1012	272	331	5			
1	O	211	Total	C	N	O	S	0	0	0
			1620	1012	272	331	5			

- Molecule 2 is a protein called Fab 47e heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	216	Total	C	N	O	S	0	0	0
			1576	992	263	314	7			
2	D	216	Total	C	N	O	S	0	0	0
			1576	992	263	314	7			
2	F	217	Total	C	N	O	S	0	0	0
			1586	998	265	316	7			
2	H	216	Total	C	N	O	S	0	0	0
			1576	992	263	314	7			
2	J	216	Total	C	N	O	S	0	0	0
			1576	992	263	314	7			
2	L	215	Total	C	N	O	S	0	0	0
			1572	990	262	313	7			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	N	216	Total	C	N	O	S	0	0	0
			1576	992	263	314	7			
2	P	216	Total	C	N	O	S	0	0	0
			1576	992	263	314	7			

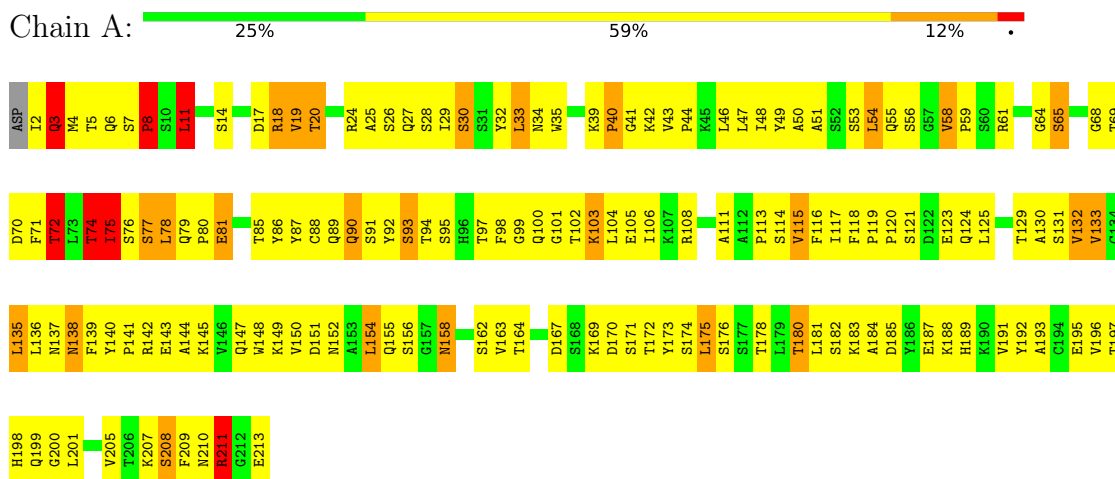
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	34	Total	O	0	0
			34	34		
3	B	29	Total	O	0	0
			29	29		
3	C	25	Total	O	0	0
			25	25		
3	D	27	Total	O	0	0
			27	27		
3	E	26	Total	O	0	0
			26	26		
3	F	18	Total	O	0	0
			18	18		
3	G	23	Total	O	0	0
			23	23		
3	H	31	Total	O	0	0
			31	31		
3	I	21	Total	O	0	0
			21	21		
3	J	17	Total	O	0	0
			17	17		
3	K	21	Total	O	0	0
			21	21		
3	L	20	Total	O	0	0
			20	20		
3	M	23	Total	O	0	0
			23	23		
3	N	31	Total	O	0	0
			31	31		
3	O	22	Total	O	0	0
			22	22		
3	P	23	Total	O	0	0
			23	23		

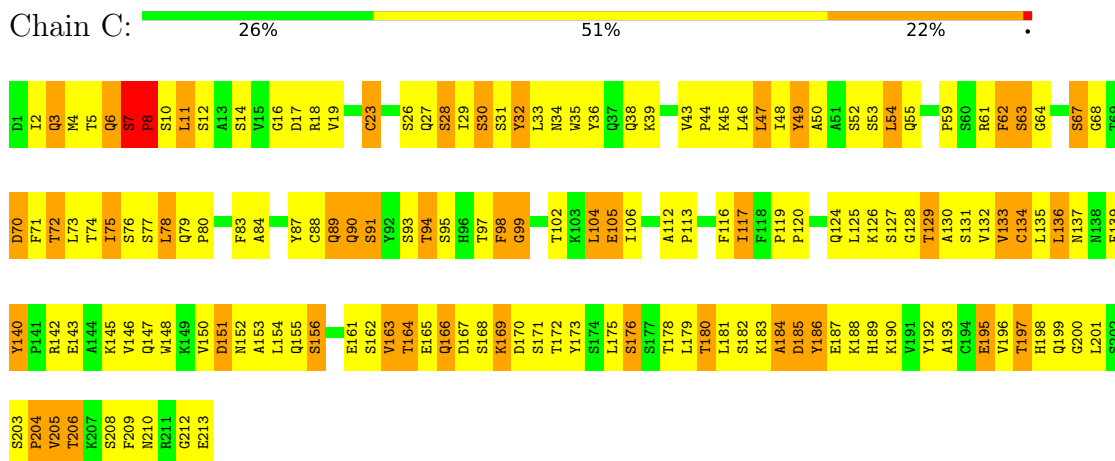
3 Residue-property plots

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

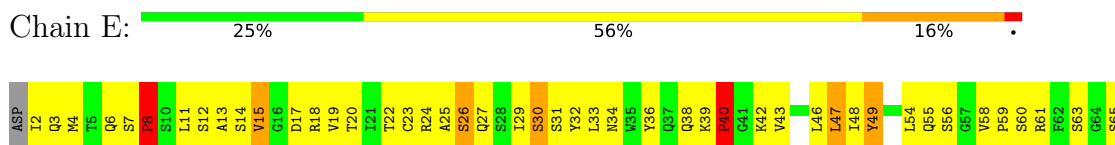
• Molecule 1: Fab 47e light chain

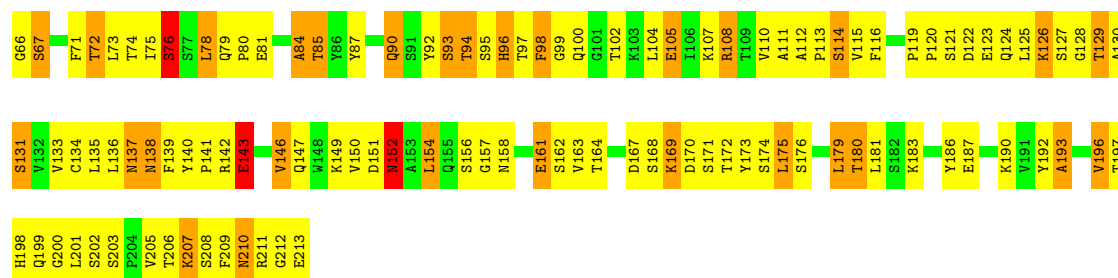


• Molecule 1: Fab 47e light chain

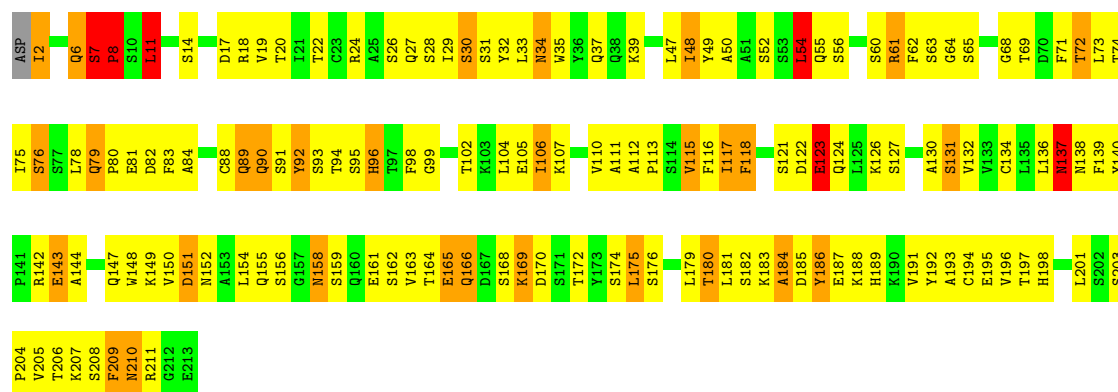


• Molecule 1: Fab 47e light chain

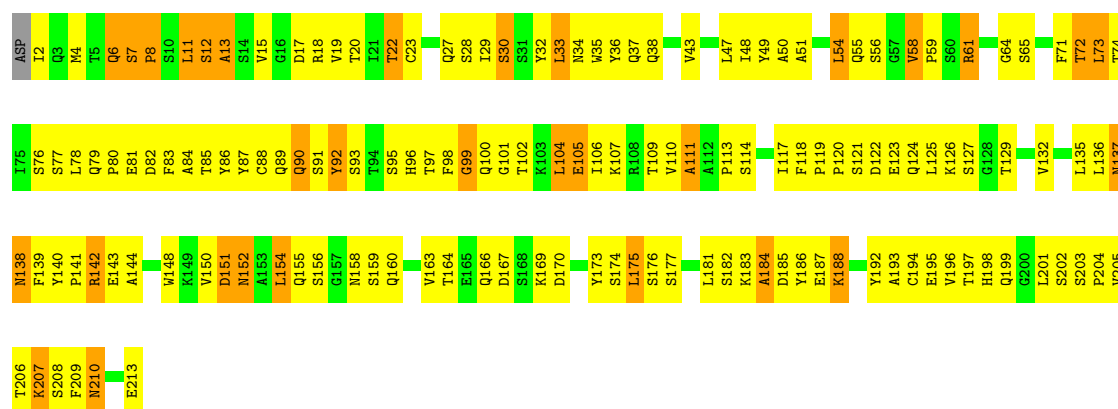




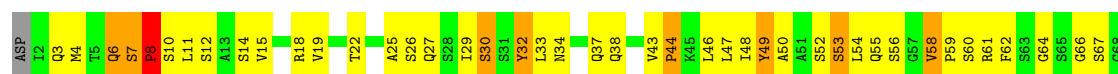
• Molecule 1: Fab 47e light chain

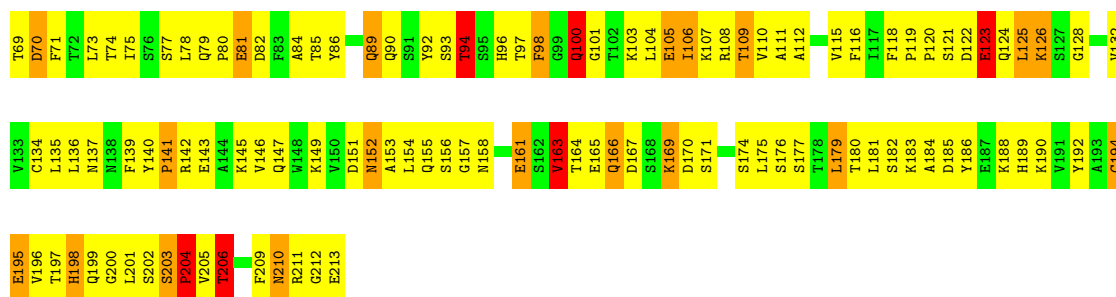


• Molecule 1: Fab 47e light chain



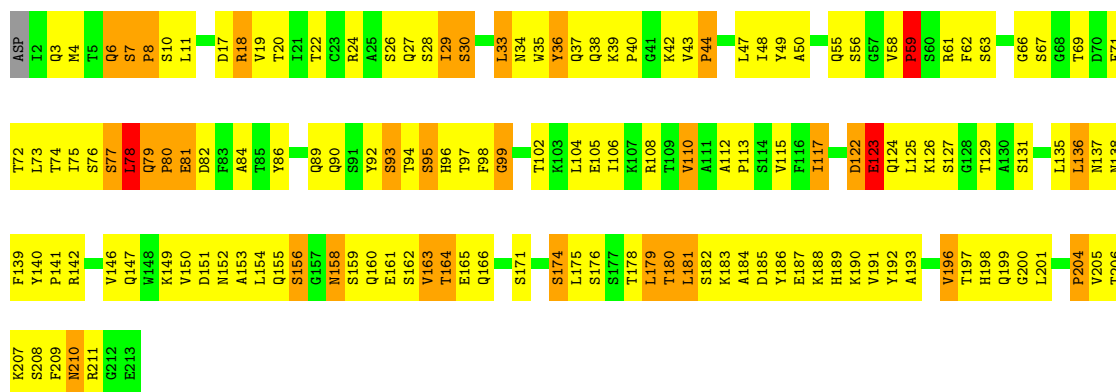
• Molecule 1: Fab 47e light chain





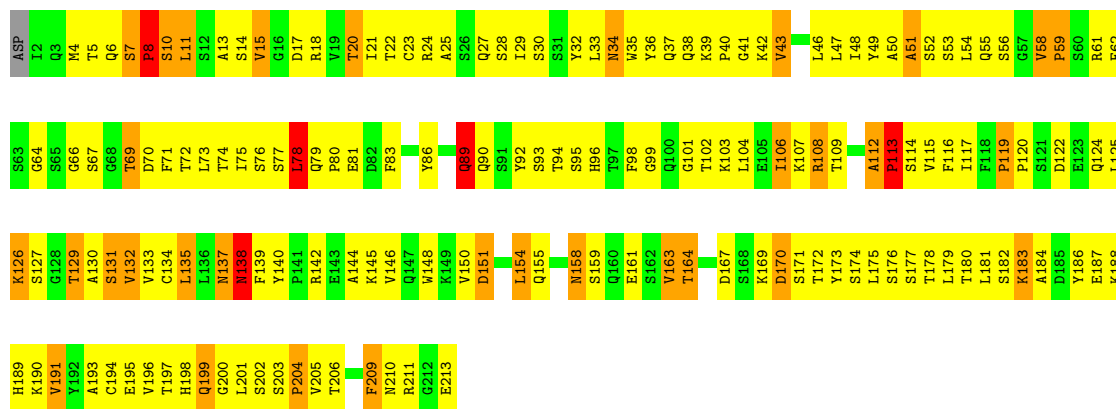
• Molecule 1: Fab 47e light chain

Chain M: 31% 53% 15%



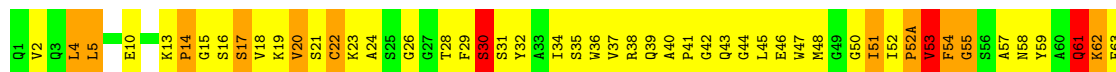
• Molecule 1: Fab 47e light chain

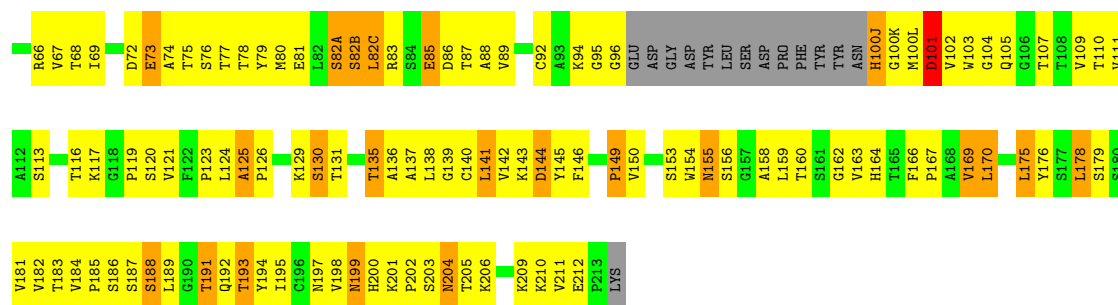
Chain O: 23% 59% 15%



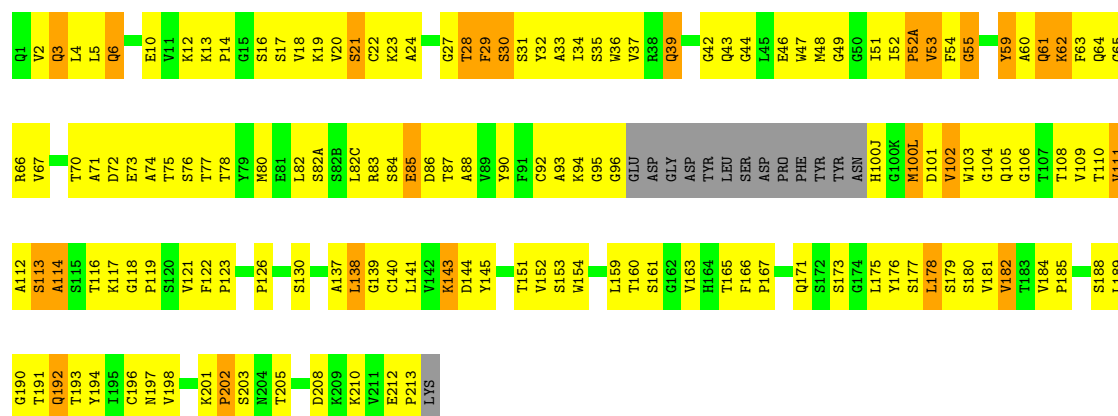
• Molecule 2: Fab 47e heavy chain

Chain B: 23% 54% 14% 6%

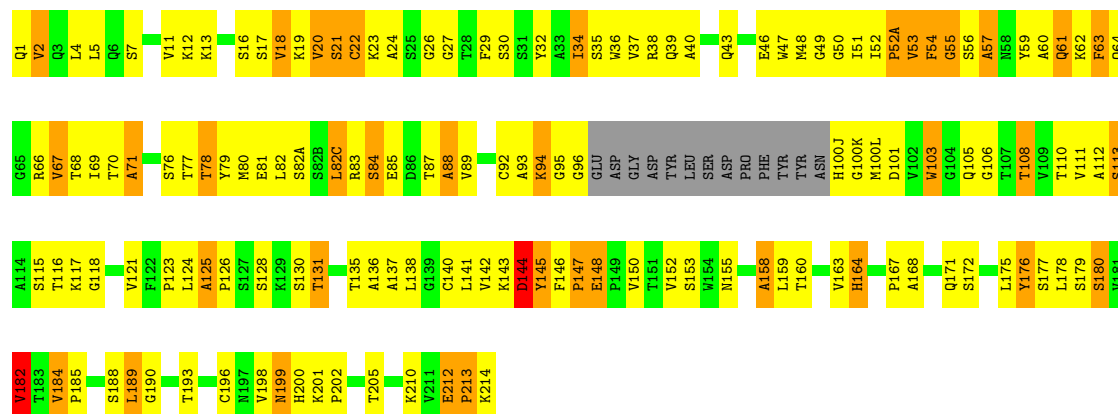




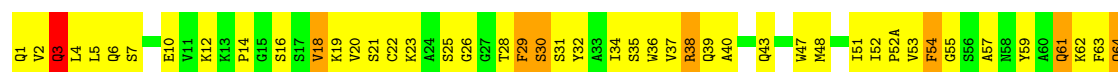
• Molecule 2: Fab 47e heavy chain

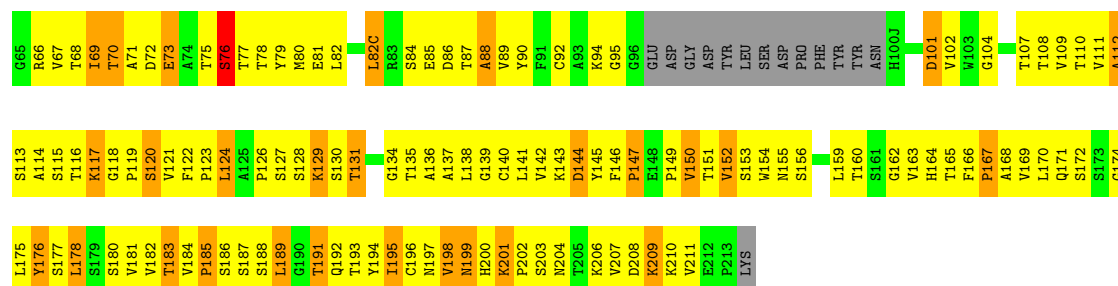


• Molecule 2: Fab 47e heavy chain



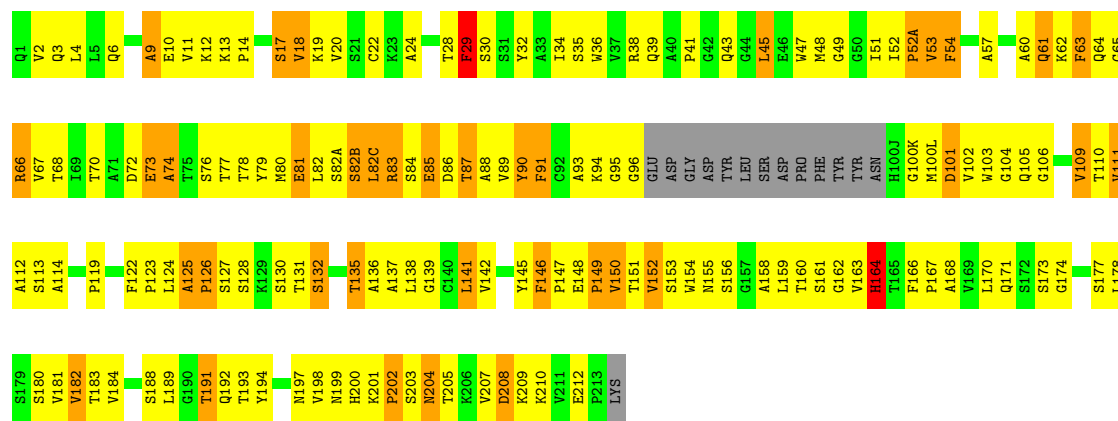
• Molecule 2: Fab 47e heavy chain





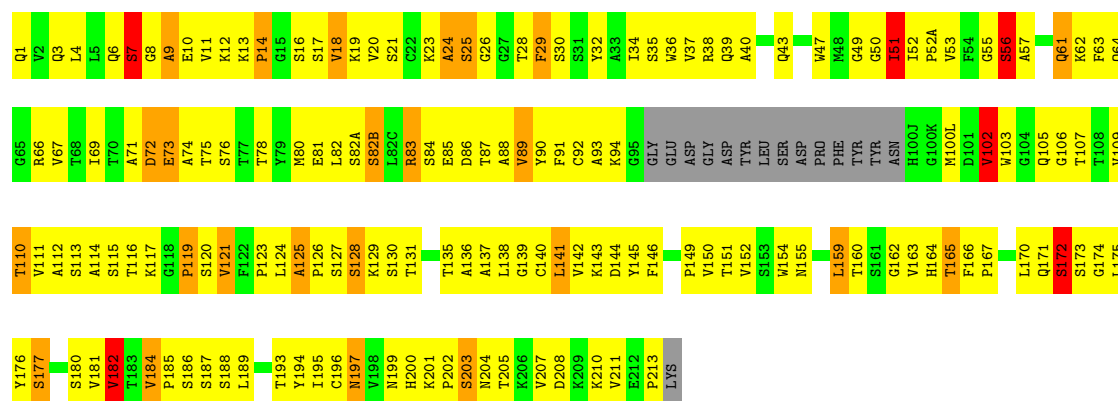
• Molecule 2: Fab 47e heavy chain

Chain J: 25% 52% 16% • 6%



• Molecule 2: Fab 47e heavy chain

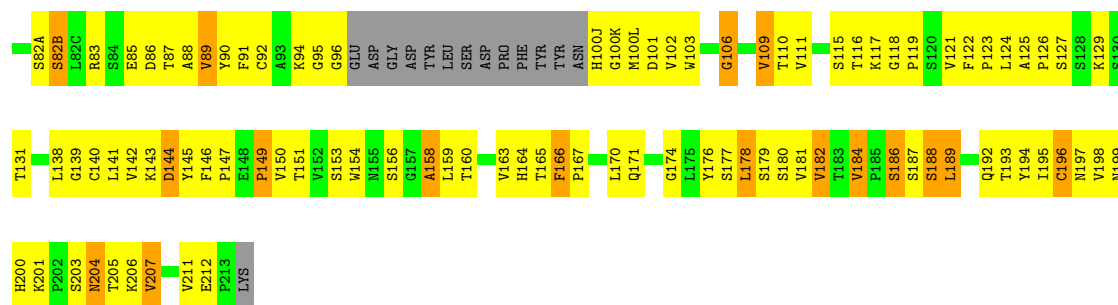
Chain L: 23% 57% 10% • 7%



• Molecule 2: Fab 47e heavy chain

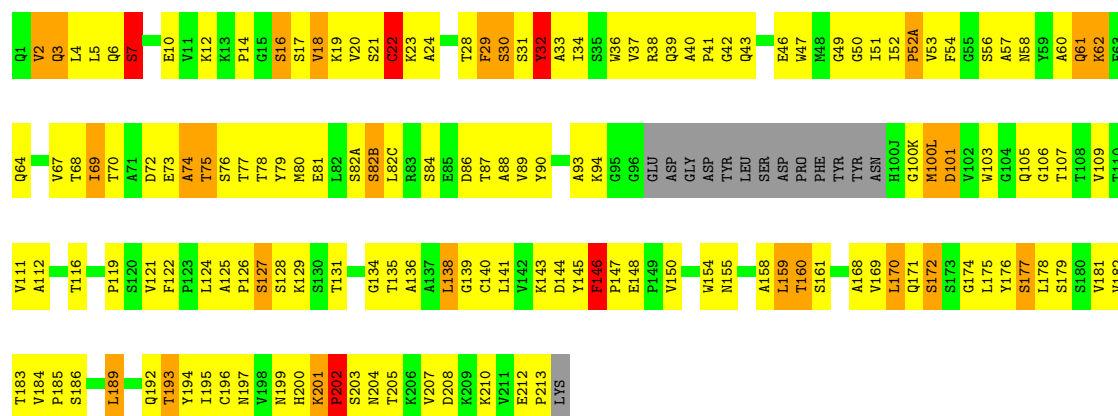
Chain N: 36% 47% 11% 6%





• Molecule 2: Fab 47e heavy chain

Chain P: 28% 53% 11% 6%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	73.43Å 111.64Å 133.31Å 85.48° 90.00° 89.71°	Depositor
Resolution (Å)	20.00 – 2.90 20.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	81.8 (20.00-2.90) 81.2 (20.00-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.97 (at 2.71Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.233 , 0.321 0.232 , 0.319	Depositor DCC
R_{free} test set	7997 reflections (9.48%)	wwPDB-VP
Wilson B-factor (Å ²)	56.1	Xtriage
Anisotropy	0.401	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 41.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.299 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	25973	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.02% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.81	4/1654 (0.2%)	1.93	30/2244 (1.3%)
1	C	0.70	2/1662 (0.1%)	1.41	25/2255 (1.1%)
1	E	0.68	2/1654 (0.1%)	1.42	29/2244 (1.3%)
1	G	0.63	1/1654 (0.1%)	1.39	20/2244 (0.9%)
1	I	0.76	3/1654 (0.2%)	1.20	16/2244 (0.7%)
1	K	0.70	2/1654 (0.1%)	1.38	23/2244 (1.0%)
1	M	0.73	3/1654 (0.2%)	1.37	19/2244 (0.8%)
1	O	0.75	2/1654 (0.1%)	1.45	29/2244 (1.3%)
2	B	0.57	0/1611	1.06	5/2192 (0.2%)
2	D	0.59	0/1611	1.04	5/2192 (0.2%)
2	F	0.54	0/1621	1.09	13/2203 (0.6%)
2	H	0.52	0/1611	1.05	4/2192 (0.2%)
2	J	0.53	0/1611	1.04	10/2192 (0.5%)
2	L	0.54	0/1607	1.09	13/2187 (0.6%)
2	N	0.58	0/1611	1.09	6/2192 (0.3%)
2	P	0.59	0/1611	1.12	14/2192 (0.6%)
All	All	0.65	19/26134 (0.1%)	1.28	261/35505 (0.7%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
1	K	0	1
All	All	0	2

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	7	SER	CA-C	12.63	1.67	1.52
1	K	10	SER	N-CA	10.46	1.58	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	6	GLN	CA-C	9.62	1.65	1.53
1	C	7	SER	C-O	-8.79	1.12	1.24
1	I	7	SER	C-N	8.01	1.49	1.34
1	E	6	GLN	N-CA	7.97	1.56	1.46
1	C	7	SER	N-CA	7.70	1.56	1.46
1	O	10	SER	CA-C	7.49	1.61	1.52
1	A	3	GLN	CA-C	-7.23	1.43	1.53
1	K	7	SER	C-N	6.78	1.47	1.34
1	E	7	SER	C-O	-6.58	1.17	1.24
1	A	7	SER	CA-C	6.54	1.61	1.53
1	I	6	GLN	CA-C	6.07	1.60	1.52
1	M	10	SER	CA-C	5.99	1.59	1.52
1	O	10	SER	N-CA	5.97	1.53	1.45
1	M	7	SER	CA-C	5.76	1.60	1.52
1	G	7	SER	C-N	5.60	1.44	1.34
1	A	7	SER	C-N	5.50	1.46	1.33
1	A	79	GLN	N-CA	5.08	1.49	1.46

All (261) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	7	SER	CA-C-N	44.53	175.50	119.84
1	A	7	SER	C-N-CA	44.53	175.50	119.84
1	G	7	SER	CA-C-N	21.96	179.71	127.00
1	G	7	SER	C-N-CA	21.96	179.71	127.00
1	M	7	SER	C-N-CD	-21.67	72.93	120.60
1	K	7	SER	CA-C-N	20.88	177.11	127.00
1	K	7	SER	C-N-CA	20.88	177.11	127.00
1	G	7	SER	C-N-CD	-19.01	78.78	120.60
1	O	7	SER	C-N-CD	-18.75	79.34	120.60
1	C	7	SER	CA-C-N	18.66	171.78	127.00
1	C	7	SER	C-N-CA	18.66	171.78	127.00
1	C	7	SER	C-N-CD	-18.65	79.58	120.60
1	K	7	SER	C-N-CD	-18.12	80.74	120.60
1	M	7	SER	CA-C-N	16.70	167.08	127.00
1	M	7	SER	C-N-CA	16.70	167.08	127.00
1	O	7	SER	CA-C-N	14.94	162.87	127.00
1	O	7	SER	C-N-CA	14.94	162.87	127.00
1	E	6	GLN	CA-C-N	-14.88	104.15	123.34
1	E	6	GLN	C-N-CA	-14.88	104.15	123.34
1	I	7	SER	C-N-CD	-14.51	88.68	120.60
1	O	7	SER	N-CA-C	-14.14	90.80	110.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	7	SER	C-N-CD	-13.52	90.85	120.60
1	O	8	PRO	CA-C-N	12.18	143.27	122.81
1	O	8	PRO	C-N-CA	12.18	143.27	122.81
1	I	7	SER	CA-C-N	11.66	155.00	127.00
1	I	7	SER	C-N-CA	11.66	155.00	127.00
1	E	7	SER	N-CA-C	11.63	130.14	108.97
1	I	99	GLY	N-CA-C	-11.49	96.97	112.82
1	E	7	SER	CA-C-N	10.79	152.90	127.00
1	E	7	SER	C-N-CA	10.79	152.90	127.00
1	A	74	THR	CA-C-N	-10.59	110.06	123.19
1	A	74	THR	C-N-CA	-10.59	110.06	123.19
1	K	8	PRO	CA-N-CD	-10.21	97.21	111.50
1	A	7	SER	N-CA-C	-9.81	95.92	110.24
1	K	8	PRO	CA-C-N	9.77	136.78	123.00
1	K	8	PRO	C-N-CA	9.77	136.78	123.00
1	A	8	PRO	CA-N-CD	-9.61	98.55	112.00
1	A	7	SER	C-N-CD	-9.55	85.83	125.00
1	C	7	SER	CA-C-O	-8.97	107.87	120.16
1	E	7	SER	CA-C-O	-8.92	109.03	120.80
2	D	166	PHE	CA-C-N	8.81	129.34	119.83
2	D	166	PHE	C-N-CA	8.81	129.34	119.83
2	F	113	SER	N-CA-C	-8.75	101.43	112.90
1	O	99	GLY	N-CA-C	-8.72	99.15	113.02
1	E	76	SER	N-CA-C	8.65	120.33	111.07
2	L	128	SER	N-CA-C	-8.62	102.47	113.16
1	O	8	PRO	CA-N-CD	-8.60	99.46	111.50
1	G	169	LYS	N-CA-C	8.60	120.34	110.97
2	P	125	ALA	CA-C-N	8.48	128.99	119.92
2	P	125	ALA	C-N-CA	8.48	128.99	119.92
1	C	8	PRO	CA-C-N	8.45	136.42	122.73
1	C	8	PRO	C-N-CA	8.45	136.42	122.73
1	M	137	ASN	N-CA-C	8.33	122.24	110.50
1	I	137	ASN	N-CA-C	8.16	122.04	108.73
1	A	58	VAL	N-CA-C	8.02	115.86	107.76
1	M	8	PRO	CA-N-CD	-7.96	100.36	111.50
2	F	128	SER	N-CA-C	-7.92	103.10	114.12
1	E	137	ASN	N-CA-C	7.91	122.14	109.24
1	C	8	PRO	N-CA-C	7.91	132.67	112.10
1	I	6	GLN	O-C-N	-7.86	114.26	123.22
2	P	144	ASP	N-CA-C	7.83	120.07	110.91
1	E	133	VAL	N-CA-C	7.76	117.47	106.53
1	M	79	GLN	N-CA-C	-7.59	101.40	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	77	SER	N-CA-C	-7.54	97.85	109.24
1	G	8	PRO	CA-N-CD	-7.53	100.96	111.50
1	M	122	ASP	N-CA-C	-7.53	103.07	111.28
1	O	8	PRO	O-C-N	7.51	135.37	121.10
1	M	76	SER	N-CA-C	7.41	121.42	112.38
2	F	212	GLU	CA-C-N	7.39	129.08	119.84
2	F	212	GLU	C-N-CA	7.39	129.08	119.84
1	G	137	ASN	N-CA-C	7.38	121.76	108.48
1	K	100	GLN	N-CA-C	-7.36	103.25	111.28
1	C	206	THR	N-CA-C	7.34	120.39	107.61
1	I	8	PRO	CA-N-CD	-7.31	101.26	111.50
1	G	8	PRO	N-CA-C	7.29	131.06	112.10
2	J	128	SER	N-CA-C	-7.28	103.05	112.23
1	E	6	GLN	CB-CA-C	-7.26	95.98	110.42
1	A	8	PRO	N-CD-CG	7.20	113.99	103.20
2	J	174	GLY	N-CA-C	-7.17	105.89	115.21
1	E	94	THR	N-CA-C	-7.16	104.54	113.28
1	O	191	VAL	N-CA-C	7.16	118.44	107.99
1	C	137	ASN	N-CA-C	7.11	121.27	109.46
2	H	144	ASP	N-CA-C	7.09	119.21	110.91
1	C	169	LYS	N-CA-C	7.09	119.01	111.28
1	A	72	THR	N-CA-C	7.08	120.73	108.76
2	F	84	SER	N-CA-C	-7.03	104.71	113.28
1	G	6	GLN	O-C-N	-7.03	115.02	123.10
1	O	6	GLN	N-CA-C	-7.02	98.87	110.17
2	P	125	ALA	N-CA-C	7.01	118.54	109.64
1	O	7	SER	CA-C-O	-7.00	113.68	120.19
1	K	198	HIS	N-CA-C	6.99	119.96	108.99
1	O	8	PRO	N-CA-CB	6.93	110.23	102.60
1	C	119	PRO	CA-C-N	-6.90	113.20	120.03
1	C	119	PRO	C-N-CA	-6.90	113.20	120.03
1	C	133	VAL	N-CA-C	6.89	117.79	107.80
1	A	115	VAL	N-CA-C	6.84	117.94	110.21
2	P	172	SER	N-CA-C	-6.83	103.06	111.33
1	C	91	SER	N-CA-C	-6.82	102.21	111.55
1	E	171	SER	N-CA-C	6.79	120.54	111.30
2	D	113	SER	N-CA-C	-6.78	105.01	113.55
1	M	106	ILE	N-CA-C	6.77	117.82	108.89
1	E	193	ALA	N-CA-C	6.76	119.60	108.99
2	H	120	SER	N-CA-C	-6.75	100.80	110.59
1	G	61	ARG	N-CA-C	-6.73	105.18	113.19
1	O	132	VAL	N-CA-C	-6.71	102.63	110.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	125	ALA	CA-C-N	6.70	128.22	119.84
2	J	125	ALA	C-N-CA	6.70	128.22	119.84
1	K	163	VAL	N-CA-C	6.70	117.45	108.27
1	E	30	SER	CB-CA-C	-6.70	108.86	116.63
2	B	144	ASP	N-CA-C	6.68	118.73	110.91
2	J	82(C)	LEU	N-CA-C	6.67	120.38	109.24
2	J	54	PHE	N-CA-C	6.63	117.23	107.88
2	L	18	VAL	N-CA-C	6.62	119.88	108.90
2	N	207	VAL	N-CA-C	6.60	116.51	108.06
1	A	99	GLY	N-CA-C	-6.55	102.54	112.89
1	K	134	CYS	N-CA-C	-6.55	100.83	110.52
1	C	99	GLY	N-CA-C	-6.53	101.13	111.18
2	N	166	PHE	CA-C-N	6.50	126.89	119.93
2	N	166	PHE	C-N-CA	6.50	126.89	119.93
1	C	19	VAL	N-CA-C	6.49	117.46	108.12
1	M	6	GLN	N-CA-C	6.48	119.47	107.60
1	M	8	PRO	CA-C-N	6.42	133.22	121.85
1	M	8	PRO	C-N-CA	6.42	133.22	121.85
1	E	8	PRO	CA-N-CD	-6.41	102.53	111.50
2	L	172	SER	N-CA-C	-6.39	105.12	113.17
2	D	143	LYS	N-CA-C	6.39	120.11	109.95
1	E	7	SER	CB-CA-C	-6.37	100.81	110.87
1	K	123	GLU	N-CA-C	-6.36	104.07	112.34
1	G	151	ASP	N-CA-C	-6.35	105.11	112.86
2	F	125	ALA	CA-C-N	6.34	126.25	119.85
2	F	125	ALA	C-N-CA	6.34	126.25	119.85
1	A	75	ILE	CA-C-N	6.33	133.63	121.54
1	A	75	ILE	C-N-CA	6.33	133.63	121.54
1	K	206	THR	N-CA-C	6.28	120.38	107.37
1	I	7	SER	N-CA-C	6.28	128.62	107.32
2	H	167	PRO	N-CA-C	-6.26	102.01	111.41
1	C	7	SER	O-C-N	-6.24	114.14	121.32
1	O	170	ASP	N-CA-C	6.24	117.92	110.44
1	K	98	PHE	CB-CA-C	-6.23	107.45	116.54
1	C	203	SER	CA-C-N	6.15	127.53	119.84
1	C	203	SER	C-N-CA	6.15	127.53	119.84
1	E	169	LYS	N-CA-C	6.15	120.40	113.02
1	E	29	ILE	N-CA-C	-6.15	107.00	112.90
1	I	151	ASP	N-CA-C	-6.15	103.33	111.02
1	O	109	THR	N-CA-C	6.14	118.23	110.24
1	C	134	CYS	N-CA-C	-6.14	100.91	110.42
1	A	7	SER	CA-C-O	-6.13	114.33	120.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	121	VAL	N-CA-C	6.12	116.69	107.75
1	C	106	ILE	N-CA-C	6.07	116.43	107.15
2	B	143	LYS	N-CA-C	6.06	118.51	108.99
1	M	196	VAL	N-CA-C	6.05	116.64	108.17
1	G	72	THR	N-CA-C	6.04	118.96	108.76
1	O	58	VAL	CA-C-N	6.03	127.37	119.84
1	O	58	VAL	C-N-CA	6.03	127.37	119.84
2	P	174	GLY	N-CA-C	-6.00	106.74	114.85
1	I	7	SER	CA-C-O	-5.98	113.12	119.22
2	L	184	VAL	CA-C-N	5.97	127.31	119.84
2	L	184	VAL	C-N-CA	5.97	127.31	119.84
2	N	188	SER	N-CA-C	5.96	117.45	111.07
1	M	206	THR	N-CA-C	5.96	118.94	107.44
1	M	115	VAL	N-CA-C	5.90	117.70	109.55
1	E	196	VAL	N-CA-C	5.82	114.99	106.55
1	A	163	VAL	N-CA-C	5.82	116.66	108.17
1	E	96	HIS	N-CA-C	-5.82	101.44	110.10
1	E	146	VAL	N-CA-C	5.80	116.15	107.51
1	G	99	GLY	N-CA-C	-5.78	103.74	112.41
1	A	53	SER	N-CA-C	5.77	118.99	107.62
1	A	133	VAL	N-CA-C	5.77	117.06	108.23
2	P	124	LEU	N-CA-C	-5.75	101.60	109.71
2	P	128	SER	N-CA-C	-5.73	106.42	113.41
1	C	182	SER	N-CA-C	-5.72	102.83	110.55
1	E	78	LEU	N-CA-C	5.71	118.30	110.24
1	A	78	LEU	N-CA-C	5.69	118.75	109.59
1	O	8	PRO	CB-CA-C	-5.68	97.79	112.00
1	M	29	ILE	N-CA-C	-5.63	105.94	112.98
1	K	6	GLN	CB-CA-C	-5.63	101.68	112.43
2	N	92	CYS	N-CA-C	-5.62	99.50	109.06
1	K	58	VAL	N-CA-C	5.62	114.14	107.73
1	A	208	SER	N-CA-C	5.61	115.96	108.38
2	D	92	CYS	N-CA-C	-5.60	98.87	110.80
1	K	194	CYS	N-CA-C	-5.60	100.27	109.40
2	L	73	GLU	N-CA-C	5.59	117.45	111.36
1	K	94	THR	N-CA-C	-5.58	106.82	113.97
1	K	8	PRO	N-CA-CB	5.58	108.74	102.60
1	O	10	SER	N-CA-C	5.55	118.63	109.85
2	P	75	THR	N-CA-C	-5.55	104.93	112.26
1	G	123	GLU	N-CA-C	-5.54	105.33	111.71
1	E	99	GLY	N-CA-C	-5.54	103.01	112.64
1	A	58	VAL	CA-C-N	5.52	125.52	119.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	58	VAL	C-N-CA	5.52	125.52	119.89
1	O	30	SER	CB-CA-C	-5.52	110.23	116.63
1	I	58	VAL	CA-C-N	5.50	126.72	119.84
1	I	58	VAL	C-N-CA	5.50	126.72	119.84
2	J	122	PHE	CA-C-N	5.49	125.76	119.83
2	J	122	PHE	C-N-CA	5.49	125.76	119.83
2	P	101	ASP	N-CA-C	5.47	117.67	111.11
2	P	139	GLY	N-CA-C	5.46	118.22	110.74
1	K	115	VAL	N-CA-C	5.46	116.09	108.89
1	O	137	ASN	N-CA-C	5.46	118.13	109.24
2	J	132	SER	N-CA-C	-5.44	107.29	114.31
1	O	163	VAL	N-CA-C	5.43	116.80	108.71
1	M	95	SER	N-CA-C	-5.42	99.25	110.80
2	L	102	VAL	N-CA-C	5.41	115.78	107.77
1	G	203	SER	CA-C-N	5.38	126.57	119.84
1	G	203	SER	C-N-CA	5.38	126.57	119.84
2	B	82(C)	LEU	N-CA-C	5.38	118.08	110.50
1	K	81	GLU	N-CA-C	-5.37	105.95	112.88
1	M	174	SER	N-CA-C	-5.37	101.59	109.81
1	I	61	ARG	N-CA-C	-5.36	106.90	113.50
2	F	69	ILE	N-CA-C	5.35	115.57	107.75
1	A	137	ASN	N-CA-C	5.35	117.96	109.24
1	E	134	CYS	N-CA-C	-5.34	103.48	110.53
2	P	122	PHE	CA-C-N	5.31	126.47	119.84
2	P	122	PHE	C-N-CA	5.31	126.47	119.84
1	K	169	LYS	N-CA-C	5.30	117.49	111.02
1	O	89	GLN	N-CA-C	5.29	117.05	108.26
1	G	165	GLU	N-CA-C	-5.29	102.69	110.52
2	F	176	TYR	N-CA-C	5.28	117.53	110.35
2	B	4	LEU	CA-C-N	-5.28	115.37	123.07
2	B	4	LEU	C-N-CA	-5.28	115.37	123.07
1	M	99	GLY	N-CA-C	-5.27	104.99	112.37
1	C	126	LYS	N-CA-C	-5.26	105.66	111.71
1	G	156	SER	N-CA-C	5.26	118.77	107.67
2	L	120	SER	N-CA-C	-5.26	101.59	109.95
2	H	108	THR	N-CA-C	5.25	117.03	108.63
1	G	131	SER	N-CA-C	5.24	117.20	108.02
2	F	144	ASP	N-CA-C	5.24	121.96	110.80
2	N	26	GLY	N-CA-C	5.22	125.56	113.18
1	A	54	LEU	N-CA-C	5.22	118.13	110.30
2	L	125	ALA	CA-C-N	5.20	125.18	120.03
2	L	125	ALA	C-N-CA	5.20	125.18	120.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	98	PHE	CB-CA-C	-5.19	105.01	113.37
2	L	83	ARG	N-CA-C	-5.19	101.40	109.24
1	O	119	PRO	CA-C-N	-5.18	114.64	120.14
1	O	119	PRO	C-N-CA	-5.18	114.64	120.14
1	G	195	GLU	N-CA-C	5.18	116.70	108.67
1	A	5	THR	N-CA-C	5.16	116.94	108.52
1	A	78	LEU	CA-C-N	-5.16	116.53	123.96
1	A	78	LEU	C-N-CA	-5.16	116.53	123.96
1	I	105	GLU	N-CA-C	-5.15	101.36	109.50
1	O	96	HIS	N-CA-C	5.15	117.56	108.24
1	K	106	ILE	N-CA-C	5.14	115.63	108.84
1	O	78	LEU	N-CA-C	5.14	121.74	110.80
1	G	115	VAL	N-CA-C	5.13	117.23	109.12
2	J	101	ASP	N-CA-C	5.13	119.43	112.04
1	K	137	ASN	N-CA-C	5.13	117.76	108.69
1	C	151	ASP	N-CA-C	-5.12	105.68	112.24
1	I	104	LEU	N-CA-C	-5.11	102.20	110.32
1	A	80	PRO	CA-C-N	5.09	130.88	121.52
1	A	80	PRO	C-N-CA	5.09	130.88	121.52
2	P	121	VAL	N-CA-C	5.09	115.64	108.36
1	I	12	SER	N-CA-C	-5.07	103.23	110.59
1	E	207	LYS	N-CA-C	-5.07	102.29	110.14
1	E	8	PRO	CA-C-N	5.06	132.74	121.81
1	E	8	PRO	C-N-CA	5.06	132.74	121.81
2	F	18	VAL	N-CA-C	5.05	113.86	107.70
1	O	126	LYS	N-CA-C	-5.05	105.91	111.71
2	F	148	GLU	N-CA-C	-5.04	102.70	110.01
2	L	56	SER	N-CA-C	-5.03	100.10	110.80
2	F	131	THR	N-CA-C	5.02	115.61	107.23
1	E	114	SER	N-CA-C	-5.01	101.08	109.24

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	140	TYR	Sidechain
1	K	49	TYR	Sidechain

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	1620	0	1575	202	0
1	C	1628	0	1582	179	0
1	E	1620	0	1575	173	0
1	G	1620	0	1575	211	0
1	I	1620	0	1575	191	0
1	K	1620	0	1575	215	0
1	M	1620	0	1575	173	0
1	O	1620	0	1575	175	0
2	B	1576	0	1554	213	0
2	D	1576	0	1554	178	0
2	F	1586	0	1567	219	0
2	H	1576	0	1554	259	0
2	J	1576	0	1554	215	0
2	L	1572	0	1551	216	0
2	N	1576	0	1554	145	0
2	P	1576	0	1554	176	0
3	A	34	0	0	4	0
3	B	29	0	0	3	0
3	C	25	0	0	6	0
3	D	27	0	0	0	0
3	E	26	0	0	2	0
3	F	18	0	0	2	0
3	G	23	0	0	3	0
3	H	31	0	0	2	0
3	I	21	0	0	2	0
3	J	17	0	0	2	0
3	K	21	0	0	3	0
3	L	20	0	0	3	0
3	M	23	0	0	4	0
3	N	31	0	0	2	0
3	O	22	0	0	1	0
3	P	23	0	0	0	0
All	All	25973	0	25049	2996	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 59.

All (2996) 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:A:11:LEU:CD2	1:A:104:LEU:HD22	1.56	1.32
1:A:11:LEU:CD2	1:A:104:LEU:CD2	2.20	1.18
1:E:199:GLN:HA	1:I:199:GLN:HE22	1.12	1.15
2:H:150:VAL:HG22	2:H:151:THR:H	1.11	1.14
1:O:113:PRO:HB3	1:O:139:PHE:HB3	1.29	1.13
1:I:32:TYR:HB3	1:I:91:SER:HB2	1.29	1.12
2:H:68:THR:HB	2:H:81:GLU:HB3	1.30	1.11
1:G:7:SER:HB3	1:G:8:PRO:HD2	1.26	1.11
2:L:119:PRO:HB3	2:L:145:TYR:HB3	1.25	1.11
2:D:17:SER:HB3	2:D:82(A):SER:HA	1.34	1.10
2:P:126:PRO:HG3	2:P:138:LEU:HB3	1.34	1.09
2:B:159:LEU:HD21	2:B:182:VAL:HG21	1.33	1.08
2:J:2:VAL:HG21	2:J:94:LYS:HZ3	1.15	1.07
2:F:64:GLN:HG3	2:L:116:THR:HB	1.37	1.05
1:G:90:GLN:HE22	1:G:93:SER:HB3	1.17	1.05
1:K:190:LYS:HG2	1:K:210:ASN:HB2	1.38	1.05
2:N:126:PRO:HG3	2:N:138:LEU:HB3	1.39	1.05
2:H:199:ASN:HD22	2:H:200:HIS:N	1.56	1.04
1:E:199:GLN:HA	1:I:199:GLN:NE2	1.72	1.04
2:F:87:THR:HG23	2:F:110:THR:HA	1.37	1.04
2:H:124:LEU:HD21	2:H:141:LEU:HB2	1.35	1.04
2:L:38:ARG:NH2	2:L:86:ASP:HA	1.73	1.03
1:K:123:GLU:H	1:K:123:GLU:CD	1.66	1.02
2:H:153:SER:HB2	2:H:197:ASN:HB2	1.42	1.02
2:F:145:TYR:HE1	2:F:150:VAL:HB	1.25	1.01
1:E:151:ASP:O	1:E:152:ASN:HB2	1.59	1.01
1:K:142:ARG:HH12	1:K:163:VAL:HG11	1.22	1.01
1:A:211:ARG:HB2	1:A:211:ARG:HH11	1.26	1.00
2:H:124:LEU:HB2	2:H:139:GLY:HA3	1.40	1.00
2:J:83:ARG:HB3	2:J:85:GLU:HG3	1.41	1.00
1:A:46:LEU:HD23	1:A:55:GLN:HE21	1.26	1.00
2:J:61:GLN:H	2:J:61:GLN:NE2	1.59	0.98
1:O:89:GLN:HE22	2:P:100(L):MET:HE1	1.28	0.98
2:L:163:VAL:HG22	2:L:182:VAL:HB	1.44	0.98
1:C:34:ASN:HD22	1:C:89:GLN:HE21	1.07	0.98
2:F:2:VAL:HG21	2:F:32:TYR:HE1	1.24	0.98
2:D:17:SER:CB	2:D:82(A):SER:HA	1.94	0.97
2:D:94:LYS:HD3	2:D:102:VAL:HG11	1.46	0.97
1:A:11:LEU:HD22	1:A:104:LEU:CD2	1.92	0.97
1:M:113:PRO:HD3	1:M:198:HIS:HD1	1.30	0.97
2:H:124:LEU:HD21	2:H:141:LEU:CB	1.94	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:61:GLN:HE21	2:J:61:GLN:N	1.60	0.96
1:A:11:LEU:HD23	1:A:104:LEU:HD22	1.43	0.96
2:L:3:GLN:H	2:L:25:SER:HB3	1.30	0.96
2:D:12:LYS:HG3	2:D:18:VAL:HB	1.45	0.96
2:P:51:ILE:HB	2:P:57:ALA:HB2	1.45	0.96
2:D:163:VAL:HG22	2:D:182:VAL:HB	1.45	0.96
2:J:4:LEU:HB3	2:J:24:ALA:HB2	1.48	0.96
1:O:37:GLN:HB2	1:O:47:LEU:HD11	1.47	0.96
2:F:199:ASN:C	2:F:199:ASN:HD22	1.74	0.95
2:B:192:GLN:NE2	2:B:193:THR:H	1.65	0.95
2:B:199:ASN:HD22	2:B:200:HIS:N	1.64	0.95
1:K:179:LEU:HD12	1:K:180:THR:N	1.82	0.94
1:A:11:LEU:HD23	1:A:104:LEU:CD2	1.94	0.94
2:N:1:GLN:HG3	2:N:2:VAL:H	1.30	0.94
2:B:123:PRO:HD3	2:B:209:LYS:HE2	1.49	0.93
1:G:123:GLU:H	1:G:123:GLU:CD	1.76	0.93
2:H:73:GLU:H	2:H:73:GLU:CD	1.77	0.93
2:L:152:VAL:HG11	2:L:180:SER:CB	1.98	0.93
1:I:185:ASP:HA	1:I:188:LYS:HD2	1.50	0.93
2:J:17:SER:HB3	2:J:82(A):SER:HA	1.51	0.93
2:F:24:ALA:HB3	2:F:76:SER:HB2	1.51	0.93
1:G:113:PRO:HB3	1:G:139:PHE:CD1	2.03	0.93
1:E:116:PHE:HB2	1:E:135:LEU:HB3	1.50	0.92
2:B:138:LEU:HD23	2:B:138:LEU:H	1.34	0.92
2:J:131:THR:HG22	2:J:136:ALA:HA	1.48	0.92
2:L:126:PRO:HG3	2:L:138:LEU:HB3	1.52	0.92
2:J:2:VAL:HG21	2:J:94:LYS:NZ	1.83	0.92
2:D:165:THR:HG23	2:D:180:SER:HB2	1.50	0.92
2:F:29:PHE:HZ	2:F:71:ALA:HB1	1.31	0.92
1:I:38:GLN:O	1:I:84:ALA:HB1	1.69	0.92
2:P:201:LYS:HB3	2:P:202:PRO:HD3	1.52	0.91
1:I:2:ILE:CD1	1:I:93:SER:HB2	2.00	0.91
1:A:158:ASN:H	1:A:158:ASN:HD22	1.13	0.91
2:B:2:VAL:HA	2:B:26:GLY:HA3	1.52	0.91
1:K:210:ASN:HD22	1:K:210:ASN:N	1.66	0.91
2:F:32:TYR:HB3	2:F:94:LYS:HG3	1.53	0.91
2:L:94:LYS:HB3	2:L:102:VAL:HG13	1.51	0.90
1:E:11:LEU:HD12	1:E:104:LEU:HD22	1.52	0.90
1:O:167:ASP:OD1	1:O:169:LYS:HG2	1.71	0.90
2:D:18:VAL:HG12	2:D:82(C):LEU:HD11	1.51	0.90
1:G:116:PHE:CD2	2:H:130:SER:HA	2.05	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:150:VAL:HG22	2:H:151:THR:N	1.87	0.90
1:A:158:ASN:H	1:A:158:ASN:ND2	1.67	0.90
1:E:199:GLN:CA	1:I:199:GLN:HE22	1.83	0.89
1:G:136:LEU:HD11	1:G:196:VAL:HG21	1.54	0.89
1:E:147:GLN:HE22	1:I:11:LEU:CD2	1.84	0.89
2:F:24:ALA:CB	2:F:29:PHE:HB2	2.03	0.89
1:G:107:LYS:HA	1:G:140:TYR:OH	1.72	0.89
2:H:68:THR:CB	2:H:81:GLU:HB3	2.03	0.89
1:I:142:ARG:HG2	1:I:142:ARG:HH11	1.36	0.89
1:O:124:GLN:NE2	1:O:131:SER:OG	2.05	0.89
1:G:47:LEU:HD23	1:G:48:ILE:HG13	1.55	0.88
1:G:90:GLN:NE2	1:G:93:SER:HB3	1.86	0.88
1:O:66:GLY:HA3	1:O:71:PHE:HA	1.54	0.88
1:C:11:LEU:HD21	1:O:154:LEU:HD12	1.54	0.88
1:G:7:SER:CB	1:G:8:PRO:HD2	1.95	0.88
1:I:2:ILE:HD11	1:I:93:SER:HB2	1.54	0.88
2:L:138:LEU:C	2:L:138:LEU:HD12	1.99	0.88
2:J:11:VAL:HG21	2:J:147:PRO:HG3	1.56	0.88
2:B:192:GLN:HE21	2:B:193:THR:H	0.90	0.87
2:P:192:GLN:HE21	2:P:193:THR:H	1.21	0.87
1:A:20:THR:HG23	1:A:74:THR:HG23	1.56	0.87
2:D:171:GLN:HE21	2:D:177:SER:HB2	1.38	0.87
1:C:183:LYS:O	1:C:187:GLU:HG3	1.74	0.87
2:B:192:GLN:HE21	2:B:193:THR:N	1.73	0.87
1:I:61:ARG:CZ	1:I:79:GLN:HG3	2.05	0.86
2:J:126:PRO:HG3	2:J:138:LEU:HB3	1.57	0.86
2:N:52(A):PRO:O	2:N:53:VAL:HB	1.75	0.86
1:K:190:LYS:O	1:K:210:ASN:HA	1.76	0.86
1:M:175:LEU:HD23	1:M:176:SER:N	1.89	0.86
1:A:11:LEU:HD21	1:A:104:LEU:HD22	1.55	0.86
2:J:47:TRP:HE1	2:J:100(L):MET:HE1	1.38	0.86
2:H:119:PRO:HB3	2:H:145:TYR:HB3	1.58	0.86
1:I:210:ASN:HD22	1:I:210:ASN:N	1.72	0.86
2:L:119:PRO:CB	2:L:145:TYR:HB3	2.04	0.86
1:M:4:MET:CB	1:M:99:GLY:HA2	2.06	0.86
2:P:34:ILE:HG21	2:P:78:THR:HG21	1.55	0.85
2:P:29:PHE:HB3	2:P:76:SER:HB2	1.58	0.85
2:B:87:THR:HG23	2:B:110:THR:HA	1.56	0.85
1:M:4:MET:HB2	1:M:99:GLY:HA2	1.58	0.85
1:E:61:ARG:CZ	1:E:79:GLN:HG3	2.07	0.85
2:H:186:SER:O	2:H:189:LEU:HG	1.75	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:13:LYS:HD3	2:F:113:SER:HA	1.56	0.85
2:F:126:PRO:HD2	2:F:213:PRO:HA	1.57	0.85
1:C:29:ILE:HD11	1:C:33:LEU:HB2	1.58	0.85
2:H:19:LYS:HA	2:H:80:MET:O	1.77	0.85
2:P:197:ASN:HA	2:P:208:ASP:OD2	1.76	0.85
2:B:40:ALA:HB3	2:B:43:GLN:HE21	1.41	0.84
2:J:123:PRO:HD3	2:J:209:LYS:HG2	1.58	0.84
2:N:200:HIS:HB3	2:N:205:THR:OG1	1.77	0.84
2:H:200:HIS:CE1	2:H:202:PRO:HD2	2.12	0.84
2:B:62:LYS:HA	2:N:83:ARG:HH22	1.41	0.84
2:B:199:ASN:HD22	2:B:199:ASN:C	1.85	0.84
1:C:212:GLY:O	1:C:213:GLU:HG3	1.76	0.84
2:N:154:TRP:CZ3	2:N:196:CYS:HB3	2.11	0.84
1:K:19:VAL:HG23	1:K:78:LEU:HD21	1.58	0.84
1:A:201:LEU:HD13	1:A:205:VAL:HG23	1.58	0.84
2:P:100(L):MET:H	2:P:100(L):MET:HE3	1.42	0.84
1:C:4:MET:HB2	1:C:98:PHE:O	1.77	0.84
2:H:124:LEU:HB2	2:H:139:GLY:CA	2.07	0.84
2:F:121:VAL:HG11	2:F:198:VAL:HG21	1.58	0.84
2:F:64:GLN:CG	2:L:116:THR:HB	2.07	0.84
1:E:48:ILE:HD12	1:E:73:LEU:HD13	1.58	0.83
2:D:126:PRO:HG3	2:D:138:LEU:HB3	1.60	0.83
1:K:11:LEU:HD12	1:K:104:LEU:HD22	1.60	0.83
2:P:2:VAL:HG22	2:P:3:GLN:H	1.41	0.83
2:F:2:VAL:HG21	2:F:32:TYR:CE1	2.13	0.83
1:M:33:LEU:HD11	1:M:35:TRP:NE1	1.94	0.83
1:M:18:ARG:HB2	1:M:18:ARG:HH11	1.41	0.83
2:D:6:GLN:HA	2:D:21:SER:O	1.79	0.83
2:F:61:GLN:HG3	2:F:62:LYS:H	1.42	0.83
1:E:110:VAL:HG22	1:E:141:PRO:HD3	1.61	0.83
1:I:54:LEU:HD12	1:I:55:GLN:N	1.93	0.83
1:A:198:HIS:ND1	1:A:200:GLY:N	2.27	0.82
2:F:29:PHE:CZ	2:F:71:ALA:HB1	2.13	0.82
2:H:150:VAL:CG2	2:H:151:THR:H	1.90	0.82
1:M:33:LEU:HD11	1:M:35:TRP:HE1	1.44	0.82
1:A:89:GLN:HB2	1:A:98:PHE:CE2	2.15	0.82
2:H:52(A):PRO:HG3	2:H:71:ALA:CB	2.10	0.82
1:M:67:SER:HA	1:M:71:PHE:CE2	2.14	0.82
1:C:12:SER:HA	1:C:105:GLU:HG3	1.61	0.82
1:M:209:PHE:C	1:M:210:ASN:HD22	1.86	0.82
1:C:50:ALA:HB3	1:C:53:SER:HB3	1.61	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:165:THR:HG23	2:H:180:SER:HB2	1.62	0.82
1:A:158:ASN:HD22	1:A:158:ASN:N	1.76	0.82
1:E:11:LEU:HD23	1:I:156:SER:HB2	1.61	0.82
1:C:38:GLN:O	1:C:84:ALA:HB1	1.80	0.82
1:E:39:LYS:HG2	1:E:84:ALA:HB2	1.61	0.81
2:L:87:THR:HA	2:L:109:VAL:O	1.80	0.81
1:K:186:TYR:CE2	1:K:211:ARG:HD3	2.14	0.81
1:O:39:LYS:HB3	1:O:40:PRO:CD	2.09	0.81
1:G:11:LEU:HD12	1:G:104:LEU:CD2	2.09	0.81
2:J:64:GLN:HB3	2:L:204:ASN:OD1	1.79	0.81
2:J:4:LEU:HA	2:J:24:ALA:HA	1.63	0.81
2:P:5:LEU:O	2:P:22:CYS:HA	1.80	0.81
1:A:33:LEU:HD11	1:A:35:TRP:NE1	1.96	0.81
1:M:123:GLU:N	1:M:123:GLU:OE2	2.12	0.81
2:B:30:SER:O	2:B:53:VAL:HG22	1.81	0.81
1:O:135:LEU:CD1	2:P:181:VAL:HG21	2.11	0.81
2:H:19:LYS:HE3	2:H:79:TYR:HB3	1.63	0.80
2:P:50:GLY:O	2:P:57:ALA:HB1	1.79	0.80
1:G:175:LEU:C	1:G:175:LEU:HD23	2.05	0.80
1:I:73:LEU:HD12	1:I:74:THR:H	1.47	0.80
2:N:153:SER:OG	2:N:197:ASN:HB2	1.80	0.80
1:A:189:HIS:O	1:A:211:ARG:HD3	1.81	0.80
2:H:36:TRP:CE3	2:H:80:MET:HG3	2.16	0.80
2:D:163:VAL:CG2	2:D:182:VAL:HB	2.11	0.80
1:I:73:LEU:HD12	1:I:74:THR:N	1.96	0.80
1:O:124:GLN:O	1:O:127:SER:HB2	1.82	0.80
1:I:48:ILE:HD13	1:I:64:GLY:N	1.96	0.80
2:N:118:GLY:HA3	2:N:205:THR:HG21	1.62	0.80
1:E:209:PHE:C	1:E:210:ASN:HD22	1.90	0.80
2:B:200:HIS:CE1	2:B:202:PRO:HB2	2.17	0.79
2:F:89:VAL:HG22	2:F:108:THR:HG23	1.64	0.79
2:H:130:SER:HB2	2:H:137:ALA:HB3	1.63	0.79
2:P:100(L):MET:HE3	2:P:100(L):MET:N	1.97	0.79
1:K:4:MET:HB2	1:K:98:PHE:O	1.81	0.79
2:H:200:HIS:ND1	2:H:202:PRO:HD2	1.97	0.79
2:P:126:PRO:CG	2:P:138:LEU:HB3	2.10	0.79
2:H:36:TRP:HB2	2:H:69:ILE:HD11	1.63	0.79
2:P:131:THR:HG22	2:P:136:ALA:HB2	1.63	0.79
1:K:163:VAL:O	2:L:167:PRO:HG2	1.82	0.79
1:M:179:LEU:HD12	1:M:180:THR:N	1.97	0.79
2:J:6:GLN:HB2	2:J:105:GLN:HG2	1.65	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:60:ALA:O	2:P:64:GLN:HG3	1.81	0.79
2:F:141:LEU:HD12	2:F:178:LEU:O	1.83	0.79
1:I:29:ILE:HA	1:I:92:TYR:CD2	2.17	0.79
2:L:119:PRO:HD2	2:L:205:THR:HG21	1.63	0.78
2:N:119:PRO:HB2	2:N:142:VAL:HG13	1.62	0.78
1:K:152:ASN:HD22	1:K:152:ASN:N	1.79	0.78
2:N:3:GLN:C	2:N:4:LEU:HD23	2.08	0.78
1:A:135:LEU:HG	1:A:136:LEU:N	1.98	0.78
2:B:69:ILE:HG12	2:B:80:MET:HG2	1.63	0.78
1:C:116:PHE:HD2	2:D:130:SER:HB2	1.48	0.78
1:G:113:PRO:HB3	1:G:139:PHE:HD1	1.47	0.78
1:K:29:ILE:HB	1:K:92:TYR:HB2	1.65	0.78
1:A:193:ALA:HB2	1:A:208:SER:HB3	1.65	0.78
1:K:164:THR:CG2	1:K:174:SER:H	1.96	0.78
2:H:7:SER:HB3	2:H:21:SER:H	1.49	0.78
1:I:142:ARG:HG3	1:I:163:VAL:HG11	1.66	0.78
1:I:126:LYS:N	1:I:126:LYS:HD2	1.99	0.78
2:D:138:LEU:HD11	2:D:182:VAL:HG13	1.67	0.77
2:F:145:TYR:CE1	2:F:150:VAL:HB	2.16	0.77
1:M:142:ARG:HH12	1:M:163:VAL:HG21	1.48	0.77
1:O:7:SER:CB	1:O:8:PRO:HD3	2.15	0.77
1:O:11:LEU:HB3	1:O:104:LEU:HD22	1.64	0.77
1:A:124:GLN:HE22	1:A:131:SER:H	1.32	0.77
1:E:20:THR:HG23	1:E:74:THR:OG1	1.84	0.77
1:K:156:SER:O	1:K:158:ASN:N	2.18	0.77
1:K:98:PHE:HE1	2:L:47:TRP:HB2	1.49	0.77
2:H:51:ILE:HB	2:H:57:ALA:HB2	1.66	0.77
2:F:17:SER:CB	2:F:82(A):SER:HA	2.15	0.77
2:B:188:SER:HA	2:B:191:THR:HG23	1.67	0.77
2:L:87:THR:HG23	2:L:110:THR:HA	1.66	0.77
1:C:185:ASP:O	1:C:188:LYS:HB2	1.84	0.76
1:A:90:GLN:HG3	1:A:97:THR:H	1.50	0.76
2:F:111:VAL:O	2:F:111:VAL:HG12	1.85	0.76
2:P:29:PHE:CB	2:P:76:SER:HB2	2.15	0.76
2:F:37:VAL:HG22	2:F:47:TRP:HA	1.65	0.76
1:I:209:PHE:C	1:I:210:ASN:HD22	1.93	0.76
2:L:182:VAL:HG22	2:L:184:VAL:HG13	1.66	0.76
2:B:170:LEU:HD13	2:B:176:TYR:CE1	2.21	0.76
2:D:51:ILE:HG12	2:D:52:ILE:H	1.49	0.76
2:H:53:VAL:HB	2:H:54:PHE:CE1	2.20	0.76
1:I:54:LEU:HD11	1:I:58:VAL:HB	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:193:ALA:CB	1:M:208:SER:HB3	2.16	0.76
1:A:19:VAL:HG13	1:M:154:LEU:HB2	1.66	0.76
2:P:192:GLN:HE21	2:P:193:THR:N	1.83	0.76
2:P:200:HIS:HD2	2:P:202:PRO:HD2	1.51	0.76
1:A:46:LEU:CD2	1:A:55:GLN:HE21	1.99	0.76
1:E:154:LEU:HD22	1:E:154:LEU:H	1.48	0.76
1:G:73:LEU:HD23	1:G:73:LEU:C	2.11	0.76
2:J:63:PHE:O	2:J:67:VAL:HG12	1.86	0.76
2:P:70:THR:OG1	2:P:79:TYR:HB2	1.85	0.76
2:D:51:ILE:HG12	2:D:52:ILE:N	2.01	0.76
2:H:94:LYS:HE2	2:H:95:GLY:C	2.12	0.75
2:H:141:LEU:HD12	2:H:142:VAL:N	2.02	0.75
1:C:124:GLN:HG2	1:C:129:THR:O	1.87	0.75
1:I:184:ALA:O	1:I:188:LYS:HG3	1.86	0.75
2:J:47:TRP:NE1	2:J:100(L):MET:HE1	2.01	0.75
2:J:2:VAL:CG2	2:J:94:LYS:HZ3	1.98	0.75
2:L:151:THR:OG1	2:L:199:ASN:HB3	1.87	0.75
2:N:94:LYS:HB3	2:N:102:VAL:HG13	1.68	0.75
1:A:117:ILE:HG23	1:A:117:ILE:O	1.87	0.75
1:E:198:HIS:CE1	1:E:200:GLY:H	2.05	0.75
1:O:89:GLN:NE2	2:P:100(L):MET:HE1	2.02	0.75
1:A:183:LYS:O	1:A:187:GLU:HG3	1.87	0.75
2:H:117:LYS:HD3	2:H:118:GLY:O	1.87	0.75
1:M:198:HIS:HD2	1:M:199:GLN:H	1.32	0.75
2:D:71:ALA:HB2	2:D:78:THR:HG22	1.69	0.75
2:F:200:HIS:CD2	2:F:202:PRO:HD2	2.22	0.75
2:J:80:MET:HE1	2:J:82:LEU:HB2	1.68	0.75
1:K:210:ASN:N	1:K:210:ASN:ND2	2.33	0.75
2:L:123:PRO:CB	2:L:211:VAL:HG22	2.17	0.74
1:C:29:ILE:HG13	1:C:29:ILE:O	1.85	0.74
1:G:122:ASP:O	1:G:126:LYS:HD3	1.86	0.74
2:B:23:LYS:HD3	2:B:24:ALA:N	2.02	0.74
2:F:94:LYS:HE2	2:F:95:GLY:C	2.10	0.74
1:G:163:VAL:HG22	1:G:175:LEU:HB2	1.68	0.74
2:H:154:TRP:O	2:H:155:ASN:HB2	1.85	0.74
2:B:126:PRO:HG3	2:B:138:LEU:HB3	1.66	0.74
1:C:62:PHE:O	1:C:63:SER:HB3	1.87	0.74
1:E:61:ARG:NE	1:E:79:GLN:HG3	2.01	0.74
1:I:139:PHE:HD2	1:I:198:HIS:NE2	1.85	0.74
2:N:126:PRO:HG3	2:N:138:LEU:CB	2.14	0.74
2:N:178:LEU:C	2:N:178:LEU:HD12	2.12	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:2:VAL:HG23	2:F:27:GLY:H	1.52	0.74
1:K:29:ILE:HG21	1:K:90:GLN:HG3	1.66	0.74
2:P:189:LEU:HD13	2:P:213:PRO:HG3	1.69	0.74
2:L:6:GLN:HA	2:L:21:SER:O	1.87	0.74
2:N:154:TRP:CH2	2:N:196:CYS:HB3	2.22	0.74
1:C:46:LEU:HD22	2:D:100(L):MET:H	1.51	0.74
2:D:64:GLN:HG3	2:N:116:THR:HB	1.70	0.74
1:E:147:GLN:HE22	1:I:11:LEU:HD21	1.53	0.74
2:D:36:TRP:CE2	2:D:80:MET:HB2	2.23	0.74
2:L:50:GLY:O	2:L:57:ALA:HB1	1.87	0.74
1:M:149:LYS:HG3	1:M:154:LEU:HD13	1.68	0.74
2:H:153:SER:HB2	2:H:197:ASN:CB	2.17	0.74
1:M:39:LYS:HG2	1:M:84:ALA:HB2	1.68	0.74
1:O:39:LYS:HB3	1:O:40:PRO:HD2	1.68	0.74
1:A:117:ILE:HD13	1:A:208:SER:HA	1.70	0.73
1:K:195:GLU:HB2	1:K:206:THR:HG23	1.68	0.73
2:B:131:THR:HG22	2:B:136:ALA:CB	2.18	0.73
1:C:116:PHE:HB3	2:D:130:SER:HB2	1.70	0.73
2:N:61:GLN:O	2:N:64:GLN:HB2	1.88	0.73
1:A:29:ILE:O	1:A:30:SER:HB3	1.88	0.73
1:A:124:GLN:NE2	1:A:131:SER:H	1.84	0.73
1:A:162:SER:OG	2:B:167:PRO:HD2	1.87	0.73
2:D:85:GLU:CD	2:D:85:GLU:H	1.97	0.73
2:J:30:SER:HA	2:J:52(A):PRO:HB2	1.70	0.73
1:K:52:SER:O	1:K:53:SER:C	2.30	0.73
1:K:26:SER:OG	1:K:27:GLN:OE1	2.05	0.73
2:L:13:LYS:HD3	2:L:113:SER:HA	1.69	0.73
2:J:12:LYS:HD2	2:J:18:VAL:HB	1.71	0.73
1:A:11:LEU:CD2	1:A:104:LEU:HD23	2.18	0.73
1:I:2:ILE:HB	1:I:90:GLN:HE21	1.54	0.73
2:H:146:PHE:HB2	2:H:175:LEU:HD22	1.69	0.72
1:O:54:LEU:HD12	1:O:55:GLN:H	1.52	0.72
1:A:33:LEU:HD13	1:A:33:LEU:C	2.13	0.72
2:H:150:VAL:HG23	2:H:199:ASN:O	1.89	0.72
1:A:54:LEU:H	1:A:54:LEU:HD12	1.54	0.72
1:C:112:ALA:HB1	1:C:201:LEU:HG	1.71	0.72
2:F:94:LYS:C	2:F:94:LYS:HD3	2.14	0.72
1:G:7:SER:CB	1:G:8:PRO:CD	2.60	0.72
1:G:33:LEU:HD21	1:G:88:CYS:HB2	1.72	0.72
2:L:127:SER:O	2:L:131:THR:HG23	1.89	0.72
2:P:61:GLN:HA	2:P:64:GLN:OE1	1.90	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:170:LEU:HD12	2:L:171:GLN:H	1.53	0.72
2:D:210:LYS:HE2	2:D:212:GLU:HG3	1.69	0.72
1:I:138:ASN:HA	1:I:173:TYR:O	1.89	0.72
1:M:33:LEU:HD22	1:M:34:ASN:N	2.04	0.72
2:H:136:ALA:O	2:H:183:THR:HA	1.88	0.72
2:J:94:LYS:HG2	2:J:95:GLY:N	2.04	0.72
1:I:167:ASP:OD1	1:I:169:LYS:HD3	1.89	0.72
1:K:111:ALA:O	1:K:139:PHE:HA	1.89	0.72
2:L:30:SER:O	2:L:53:VAL:HG23	1.90	0.72
1:A:133:VAL:HG22	1:A:178:THR:HG23	1.72	0.72
2:D:117:LYS:HG3	2:D:118:GLY:O	1.90	0.72
2:F:57:ALA:HB1	2:F:59:TYR:HE2	1.54	0.72
1:I:65:SER:HB2	1:I:72:THR:HG22	1.72	0.72
1:G:116:PHE:HD2	2:H:130:SER:HA	1.52	0.71
1:G:121:SER:HB2	1:G:123:GLU:OE1	1.90	0.71
2:H:134:GLY:O	2:H:186:SER:N	2.23	0.71
2:L:3:GLN:N	2:L:25:SER:HB3	2.04	0.71
2:N:156:SER:HA	2:N:197:ASN:HD21	1.54	0.71
2:P:200:HIS:CD2	2:P:202:PRO:HD2	2.24	0.71
1:A:136:LEU:HD21	1:A:196:VAL:HG11	1.72	0.71
2:D:197:ASN:HD22	2:D:208:ASP:CG	1.98	0.71
1:I:117:ILE:HD12	1:I:207:LYS:O	1.89	0.71
2:N:159:LEU:HD21	2:N:182:VAL:HG21	1.72	0.71
2:P:4:LEU:HD11	2:P:94:LYS:HB2	1.71	0.71
2:B:40:ALA:CB	2:B:43:GLN:HE21	2.02	0.71
2:F:2:VAL:CG2	2:F:27:GLY:H	2.03	0.71
2:H:48:MET:HE3	2:H:63:PHE:CE2	2.25	0.71
2:B:94:LYS:HD2	2:B:102:VAL:CG1	2.20	0.71
1:E:114:SER:HB2	1:E:137:ASN:HB3	1.72	0.71
2:F:83:ARG:HH12	2:J:62:LYS:HB3	1.56	0.71
1:O:182:SER:O	1:O:184:ALA:N	2.23	0.71
2:B:92:CYS:O	2:B:92:CYS:SG	2.49	0.71
1:K:167:ASP:OD1	1:K:169:LYS:HG2	1.90	0.71
1:O:200:GLY:O	1:O:201:LEU:HD23	1.91	0.71
2:L:38:ARG:HH22	2:L:86:ASP:HA	1.56	0.71
1:M:190:LYS:O	1:M:210:ASN:HA	1.90	0.71
1:A:28:SER:HA	1:A:69:THR:HG22	1.72	0.71
1:E:162:SER:OG	2:F:167:PRO:HD2	1.90	0.71
1:G:184:ALA:O	1:G:188:LYS:HG3	1.90	0.71
1:I:113:PRO:HB3	1:I:139:PHE:HB3	1.72	0.71
1:M:191:VAL:HG22	1:M:210:ASN:ND2	2.06	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:123:GLU:CD	1:G:123:GLU:N	2.46	0.70
1:I:54:LEU:HD12	1:I:55:GLN:H	1.54	0.70
1:M:19:VAL:HG12	1:M:20:THR:N	2.04	0.70
1:E:201:LEU:HD13	1:E:205:VAL:HG23	1.72	0.70
2:F:171:GLN:NE2	2:F:177:SER:HB2	2.05	0.70
2:L:152:VAL:HG11	2:L:180:SER:HB2	1.72	0.70
2:N:178:LEU:HD12	2:N:179:SER:N	2.05	0.70
2:D:72:ASP:OD1	2:D:74:ALA:HB3	1.91	0.70
1:E:32:TYR:HD1	1:E:92:TYR:CD1	2.10	0.70
2:L:159:LEU:HD12	2:L:160:THR:N	2.05	0.70
1:M:176:SER:HB3	2:N:166:PHE:CE1	2.27	0.70
1:G:106:ILE:HD12	1:G:106:ILE:H	1.57	0.70
2:H:124:LEU:HG	2:H:141:LEU:H	1.56	0.70
1:E:120:PRO:HB3	1:E:131:SER:H	1.56	0.70
1:G:201:LEU:HD13	1:G:205:VAL:HG23	1.73	0.70
1:M:210:ASN:HD22	1:M:210:ASN:N	1.85	0.70
1:O:94:THR:HG23	1:O:95:SER:N	2.07	0.70
1:C:34:ASN:HD22	1:C:89:GLN:NE2	1.86	0.70
2:H:29:PHE:CG	2:H:76:SER:HB2	2.27	0.70
2:N:63:PHE:HB3	2:N:67:VAL:HG11	1.71	0.70
2:D:65:GLY:HA3	2:N:203:SER:HB2	1.74	0.70
2:J:151:THR:O	2:J:152:VAL:HG23	1.91	0.70
1:K:123:GLU:CD	1:K:123:GLU:N	2.46	0.70
2:L:202:PRO:O	2:L:203:SER:HB3	1.92	0.70
1:M:113:PRO:HB3	1:M:139:PHE:HB3	1.73	0.70
1:O:135:LEU:HD11	2:P:181:VAL:HG21	1.72	0.70
2:F:71:ALA:HA	2:F:77:THR:O	1.91	0.70
1:K:29:ILE:O	1:K:30:SER:HB3	1.90	0.70
1:M:19:VAL:HG12	1:M:20:THR:H	1.57	0.70
1:A:89:GLN:HB2	1:A:98:PHE:CD2	2.27	0.70
1:C:142:ARG:HH22	1:C:163:VAL:HG21	1.55	0.70
1:E:210:ASN:N	1:E:210:ASN:ND2	2.38	0.70
2:F:24:ALA:HB1	3:F:222:HOH:O	1.90	0.70
1:G:79:GLN:HE21	1:G:79:GLN:HA	1.56	0.70
2:H:193:THR:HG23	2:H:210:LYS:HE3	1.74	0.70
2:J:67:VAL:HG22	2:J:68:THR:N	2.07	0.70
1:K:38:GLN:O	1:K:84:ALA:HB1	1.92	0.70
2:L:63:PHE:HB3	2:L:67:VAL:HG11	1.74	0.70
1:M:140:TYR:HA	1:M:141:PRO:O	1.92	0.70
2:J:51:ILE:CD1	2:J:57:ALA:HB2	2.22	0.70
1:M:198:HIS:CD2	1:M:199:GLN:H	2.09	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:121:VAL:HG21	2:N:198:VAL:HG21	1.72	0.70
1:C:34:ASN:ND2	1:C:89:GLN:HE21	1.86	0.69
1:G:138:ASN:HA	1:G:172:THR:HB	1.74	0.69
2:H:19:LYS:HE2	2:H:79:TYR:CD2	2.27	0.69
1:A:14:SER:HB2	1:A:17:ASP:OD1	1.91	0.69
2:B:209:LYS:HG3	2:B:210:LYS:H	1.58	0.69
2:F:105:GLN:HG2	2:F:106:GLY:N	2.07	0.69
2:F:199:ASN:C	2:F:199:ASN:ND2	2.48	0.69
2:H:138:LEU:HD12	2:H:139:GLY:N	2.06	0.69
1:I:143:GLU:O	1:I:198:HIS:HD2	1.74	0.69
2:H:29:PHE:O	2:H:31:SER:N	2.25	0.69
2:H:94:LYS:HE2	2:H:95:GLY:O	1.91	0.69
1:I:6:GLN:HE22	1:I:87:TYR:HA	1.56	0.69
1:I:30:SER:HA	3:I:226:HOH:O	1.91	0.69
2:N:63:PHE:HB3	2:N:67:VAL:CG1	2.22	0.69
2:H:199:ASN:HD22	2:H:199:ASN:C	1.98	0.69
2:L:6:GLN:OE1	2:L:91:PHE:HA	1.91	0.69
1:O:170:ASP:O	1:O:172:THR:HG23	1.91	0.69
1:C:184:ALA:O	1:C:185:ASP:C	2.35	0.69
2:F:47:TRP:CH2	2:F:49:GLY:HA2	2.27	0.69
1:I:142:ARG:HG2	1:I:142:ARG:NH1	2.05	0.69
1:K:121:SER:O	1:K:124:GLN:HB3	1.92	0.69
1:M:193:ALA:HB2	1:M:208:SER:HB3	1.75	0.69
2:J:4:LEU:HD12	2:J:4:LEU:O	1.93	0.69
1:K:140:TYR:HA	1:K:141:PRO:O	1.93	0.69
2:L:116:THR:CG2	2:L:203:SER:HB3	2.23	0.69
2:B:51:ILE:HG12	2:B:52:ILE:N	2.08	0.69
1:C:14:SER:HB2	1:C:17:ASP:OD1	1.91	0.69
1:C:116:PHE:CD2	2:D:130:SER:HB2	2.26	0.69
2:P:143:LYS:HA	2:P:177:SER:OG	1.92	0.69
2:D:18:VAL:HG22	2:D:19:LYS:N	2.07	0.69
1:G:179:LEU:HG	1:G:181:LEU:HD11	1.74	0.69
2:H:38:ARG:HB3	2:H:90:TYR:CD2	2.27	0.69
2:J:17:SER:HB3	2:J:82(A):SER:CA	2.23	0.69
1:K:179:LEU:HD12	1:K:179:LEU:C	2.16	0.69
2:P:51:ILE:HB	2:P:57:ALA:CB	2.20	0.69
2:B:119:PRO:HB3	2:B:145:TYR:CD2	2.28	0.69
1:G:39:LYS:HD3	1:G:84:ALA:HB2	1.73	0.69
2:L:200:HIS:HB3	2:L:205:THR:HB	1.75	0.69
2:B:124:LEU:HD12	2:B:139:GLY:C	2.18	0.69
2:L:116:THR:HG22	2:L:203:SER:HB3	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:132:VAL:HB	1:G:179:LEU:HB3	1.75	0.68
1:K:175:LEU:HD23	1:K:176:SER:N	2.09	0.68
1:A:116:PHE:CD1	1:A:135:LEU:HD23	2.27	0.68
1:C:6:GLN:O	1:C:7:SER:O	2.11	0.68
1:M:151:ASP:O	1:M:153:ALA:N	2.26	0.68
1:E:119:PRO:HB3	1:E:209:PHE:CZ	2.28	0.68
2:J:67:VAL:HG22	2:J:68:THR:H	1.57	0.68
1:M:29:ILE:HD11	1:M:33:LEU:HB2	1.75	0.68
2:H:51:ILE:HD11	2:H:55:GLY:HA2	1.74	0.68
2:H:197:ASN:O	2:H:198:VAL:C	2.37	0.68
1:C:7:SER:HB2	1:C:102:THR:OG1	1.94	0.68
2:F:24:ALA:HB1	2:F:29:PHE:HB2	1.73	0.68
1:A:18:ARG:HH11	1:A:18:ARG:HB2	1.58	0.68
2:F:68:THR:HB	2:F:81:GLU:HB3	1.74	0.68
2:F:63:PHE:HB3	2:F:67:VAL:HG12	1.75	0.68
1:I:193:ALA:HB2	1:I:208:SER:HB3	1.74	0.68
1:M:197:THR:HG22	1:M:204:PRO:HG3	1.74	0.68
2:N:156:SER:HA	2:N:197:ASN:ND2	2.08	0.68
2:H:67:VAL:HG22	2:H:68:THR:N	2.09	0.68
1:A:158:ASN:HA	1:M:24:ARG:HH21	1.57	0.68
2:B:51:ILE:HG12	2:B:52:ILE:H	1.58	0.68
1:I:32:TYR:CB	1:I:92:TYR:H	2.07	0.68
2:N:28:THR:HA	3:N:217:HOH:O	1.93	0.68
2:P:53:VAL:HG12	2:P:54:PHE:HD2	1.59	0.68
1:A:124:GLN:CD	1:A:130:ALA:HA	2.18	0.67
2:F:5:LEU:HB2	2:F:23:LYS:HB2	1.75	0.67
2:F:57:ALA:HB1	2:F:59:TYR:CE2	2.28	0.67
2:L:62:LYS:HG3	2:L:63:PHE:N	2.10	0.67
2:N:36:TRP:HE1	2:N:78:THR:HG21	1.58	0.67
2:H:154:TRP:CH2	2:H:196:CYS:HB3	2.29	0.67
1:M:17:ASP:O	1:M:78:LEU:HD22	1.94	0.67
2:N:94:LYS:HB3	2:N:102:VAL:CG1	2.24	0.67
1:I:114:SER:HB2	1:I:137:ASN:HB3	1.76	0.67
1:I:210:ASN:N	1:I:210:ASN:ND2	2.42	0.67
1:K:164:THR:HG22	1:K:174:SER:H	1.59	0.67
2:N:47:TRP:CH2	2:N:49:GLY:HA2	2.29	0.67
1:O:169:LYS:HG3	1:O:170:ASP:OD1	1.94	0.67
1:A:108:ARG:HD3	1:A:171:SER:O	1.94	0.67
1:A:124:GLN:HE22	1:A:131:SER:N	1.92	0.67
1:E:39:LYS:HG2	1:E:84:ALA:CB	2.23	0.67
2:J:171:GLN:NE2	2:J:177:SER:CB	2.58	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:LEU:HD21	1:A:88:CYS:HB2	1.77	0.67
2:J:119:PRO:HB3	2:J:145:TYR:HB3	1.76	0.67
2:B:199:ASN:C	2:B:199:ASN:ND2	2.52	0.67
1:E:93:SER:OG	1:E:94:THR:N	2.25	0.67
2:J:62:LYS:C	2:J:64:GLN:H	2.02	0.67
1:M:29:ILE:O	1:M:30:SER:HB3	1.94	0.67
2:P:6:GLN:NE2	2:P:106:GLY:HA2	2.09	0.67
2:B:119:PRO:HB3	2:B:145:TYR:HB3	1.76	0.67
1:E:18:ARG:NH1	1:E:76:SER:HA	2.09	0.67
1:K:19:VAL:O	1:K:74:THR:HG23	1.95	0.67
1:A:48:ILE:HG22	1:A:49:TYR:N	2.10	0.67
2:B:54:PHE:N	2:B:54:PHE:HD1	1.92	0.67
2:J:11:VAL:CG2	2:J:147:PRO:HG3	2.25	0.67
1:K:201:LEU:HD13	1:K:205:VAL:CG2	2.25	0.67
2:L:85:GLU:CD	2:L:85:GLU:H	2.03	0.67
1:M:3:GLN:HB3	1:M:26:SER:HB3	1.75	0.67
2:F:94:LYS:HZ3	2:F:95:GLY:HA2	1.60	0.67
1:K:142:ARG:O	1:K:142:ARG:HG2	1.95	0.67
1:O:195:GLU:HA	1:O:206:THR:HA	1.77	0.67
2:B:29:PHE:O	2:B:31:SER:N	2.28	0.67
2:B:59:TYR:HE2	2:B:69:ILE:H	1.42	0.67
2:B:4:LEU:HD12	2:B:103:TRP:C	2.21	0.66
2:B:19:LYS:HE2	2:B:79:TYR:CD2	2.30	0.66
2:H:29:PHE:CB	2:H:76:SER:HB2	2.25	0.66
1:I:193:ALA:CB	1:I:208:SER:HB3	2.24	0.66
2:P:145:TYR:O	2:P:146:PHE:HB2	1.94	0.66
1:A:32:TYR:HB2	1:A:92:TYR:HB2	1.76	0.66
2:F:105:GLN:HG2	2:F:106:GLY:H	1.60	0.66
2:F:185:PRO:HB2	2:F:188:SER:HB3	1.77	0.66
2:B:2:VAL:HA	2:B:26:GLY:CA	2.24	0.66
1:I:110:VAL:HG12	1:I:111:ALA:N	2.11	0.66
1:I:126:LYS:HD2	1:I:126:LYS:H	1.59	0.66
1:K:124:GLN:O	1:K:126:LYS:N	2.28	0.66
2:N:184:VAL:HG21	2:N:194:TYR:OH	1.95	0.66
1:G:139:PHE:HB2	1:G:198:HIS:CE1	2.30	0.66
1:M:193:ALA:HB2	1:M:208:SER:CB	2.25	0.66
2:J:12:LYS:NZ	2:J:18:VAL:HA	2.11	0.66
1:C:161:GLU:HB2	1:C:176:SER:O	1.96	0.66
2:F:5:LEU:HB2	2:F:23:LYS:CB	2.25	0.66
2:J:51:ILE:HD12	2:J:57:ALA:HB2	1.76	0.66
1:M:4:MET:HB3	1:M:99:GLY:HA2	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:38:GLN:O	1:M:84:ALA:HB1	1.96	0.66
2:P:2:VAL:HG21	2:P:32:TYR:HE1	1.60	0.66
1:A:8:PRO:HG3	1:A:100:GLN:OE1	1.94	0.66
1:C:90:GLN:NE2	1:C:97:THR:HB	2.11	0.66
1:E:54:LEU:HD21	1:E:59:PRO:O	1.94	0.66
2:H:48:MET:HE3	2:H:63:PHE:HE2	1.60	0.66
2:B:51:ILE:HB	2:B:57:ALA:HB2	1.78	0.66
1:G:35:TRP:CE2	1:G:73:LEU:HB2	2.31	0.66
2:H:61:GLN:O	2:H:64:GLN:HB2	1.96	0.66
2:H:84:SER:C	2:H:86:ASP:H	2.04	0.66
2:H:22:CYS:C	2:H:77:THR:HG23	2.21	0.66
1:I:6:GLN:HB3	1:I:99:GLY:HA3	1.76	0.66
1:G:134:CYS:HB2	1:G:148:TRP:CH2	2.31	0.66
1:K:143:GLU:N	1:K:143:GLU:OE2	2.29	0.66
2:N:30:SER:O	2:N:53:VAL:HG23	1.96	0.66
2:P:203:SER:O	2:P:205:THR:N	2.29	0.66
1:A:90:GLN:HE22	1:A:93:SER:H	1.44	0.65
1:G:175:LEU:HD23	1:G:176:SER:N	2.11	0.65
1:G:176:SER:HB3	2:H:166:PHE:CE1	2.31	0.65
2:H:124:LEU:HB2	2:H:139:GLY:C	2.21	0.65
1:M:122:ASP:O	1:M:126:LYS:HD3	1.96	0.65
1:C:154:LEU:HD23	1:O:18:ARG:O	1.96	0.65
1:A:46:LEU:HD23	1:A:55:GLN:NE2	2.07	0.65
1:A:158:ASN:HA	1:M:24:ARG:NH2	2.11	0.65
2:F:140:CYS:O	2:F:179:SER:HA	1.96	0.65
2:H:35:SER:O	2:H:92:CYS:HA	1.96	0.65
2:H:52(A):PRO:HG3	2:H:71:ALA:HB1	1.76	0.65
1:O:163:VAL:HG12	1:O:164:THR:O	1.96	0.65
1:C:113:PRO:HB3	1:C:139:PHE:HB3	1.78	0.65
2:D:210:LYS:HE2	2:D:212:GLU:CG	2.25	0.65
2:H:62:LYS:HE2	2:H:63:PHE:CE1	2.32	0.65
2:B:53:VAL:C	2:B:54:PHE:HD1	2.04	0.65
2:J:162:GLY:C	2:J:182:VAL:HG23	2.22	0.65
2:L:35:SER:OG	2:L:47:TRP:NE1	2.30	0.65
1:M:29:ILE:HG21	1:M:90:GLN:HG3	1.77	0.65
2:D:95:GLY:O	2:D:96:GLY:C	2.39	0.65
2:F:37:VAL:HG13	2:F:46:GLU:C	2.21	0.65
2:H:7:SER:HB3	2:H:21:SER:OG	1.96	0.65
2:J:41:PRO:HD3	2:J:87:THR:O	1.95	0.65
2:J:130:SER:HB3	2:J:137:ALA:O	1.96	0.65
2:L:73:GLU:C	2:L:75:THR:H	2.05	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:131:THR:HG22	2:B:136:ALA:HA	1.78	0.65
2:D:59:TYR:CD2	2:D:67:VAL:HG13	2.30	0.65
2:D:121:VAL:CG2	2:D:198:VAL:HG21	2.27	0.65
2:B:37:VAL:HG11	2:B:45:LEU:HB3	1.78	0.65
1:E:33:LEU:HD22	1:E:34:ASN:H	1.62	0.65
1:E:210:ASN:HD22	1:E:210:ASN:N	1.89	0.65
2:F:17:SER:HB3	2:F:82(A):SER:HA	1.79	0.65
2:H:36:TRP:CB	2:H:69:ILE:HD11	2.27	0.65
1:A:169:LYS:HG3	1:A:170:ASP:OD1	1.97	0.65
2:F:70:THR:OG1	2:F:79:TYR:HB2	1.97	0.65
2:F:158:ALA:O	2:F:160:THR:HG23	1.96	0.65
1:G:186:TYR:C	1:G:188:LYS:H	2.05	0.65
2:H:5:LEU:O	2:H:22:CYS:HA	1.95	0.65
1:I:50:ALA:O	1:I:51:ALA:HB3	1.96	0.65
2:L:71:ALA:O	2:L:72:ASP:HB2	1.97	0.65
2:L:155:ASN:HD21	2:L:194:TYR:HD1	1.43	0.65
1:O:11:LEU:O	1:O:104:LEU:HA	1.97	0.65
2:D:138:LEU:CD1	2:D:182:VAL:HG13	2.27	0.65
2:F:12:LYS:HG3	2:F:18:VAL:HB	1.78	0.65
2:J:13:LYS:HD2	2:J:113:SER:HA	1.79	0.65
2:J:19:LYS:HA	2:J:80:MET:O	1.96	0.65
1:K:100:GLN:HG2	1:K:101:GLY:N	2.12	0.65
2:N:32:TYR:CD2	2:N:94:LYS:HE3	2.32	0.65
1:I:197:THR:HG22	1:I:204:PRO:HB3	1.79	0.64
2:H:176:TYR:CD2	2:H:176:TYR:N	2.66	0.64
1:G:150:VAL:HG22	1:G:192:TYR:HD1	1.62	0.64
1:K:33:LEU:HG	1:K:71:PHE:CG	2.32	0.64
1:M:198:HIS:CD2	1:M:199:GLN:N	2.65	0.64
1:A:40:PRO:O	1:A:42:LYS:N	2.30	0.64
2:B:59:TYR:CD2	2:B:67:VAL:HG13	2.32	0.64
2:F:121:VAL:CG1	2:F:198:VAL:HG21	2.28	0.64
1:G:209:PHE:CD1	1:G:209:PHE:C	2.74	0.64
1:K:124:GLN:O	1:K:125:LEU:C	2.39	0.64
2:L:11:VAL:HG22	2:L:110:THR:HB	1.79	0.64
1:O:113:PRO:HB3	1:O:139:PHE:CB	2.18	0.64
2:B:54:PHE:N	2:B:54:PHE:CD1	2.63	0.64
1:G:148:TRP:CD1	1:G:159:SER:HG	2.15	0.64
1:K:147:GLN:O	1:K:194:CYS:HA	1.97	0.64
2:N:90:TYR:HE1	2:N:109:VAL:HB	1.63	0.64
2:P:2:VAL:HG22	2:P:3:GLN:N	2.12	0.64
2:P:176:TYR:O	2:P:177:SER:HB2	1.95	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:35:SER:OG	2:B:47:TRP:NE1	2.31	0.64
2:J:86:ASP:O	2:J:88:ALA:N	2.30	0.64
1:O:38:GLN:HA	3:O:217:HOH:O	1.98	0.64
2:J:4:LEU:HD21	2:J:102:VAL:HG13	1.79	0.64
2:L:138:LEU:HD12	2:L:139:GLY:N	2.11	0.64
2:L:164:HIS:HB2	2:L:181:VAL:CG2	2.28	0.64
2:P:201:LYS:HB3	2:P:202:PRO:CD	2.23	0.64
2:H:4:LEU:HD12	2:H:102:VAL:HG13	1.79	0.64
1:I:2:ILE:HB	1:I:90:GLN:NE2	2.11	0.64
1:K:96:HIS:O	2:L:47:TRP:HB3	1.98	0.64
1:O:46:LEU:HD23	1:O:55:GLN:OE1	1.98	0.64
2:P:30:SER:O	2:P:52(A):PRO:HB2	1.97	0.64
2:B:63:PHE:O	2:B:67:VAL:HG12	1.97	0.64
1:C:170:ASP:OD2	1:C:172:THR:HG23	1.98	0.64
1:E:175:LEU:HD23	1:E:176:SER:N	2.13	0.64
2:J:6:GLN:HE22	2:J:91:PHE:HA	1.63	0.64
2:J:161:SER:C	2:J:163:VAL:H	2.06	0.64
2:L:18:VAL:O	2:L:81:GLU:HA	1.98	0.64
2:L:159:LEU:HD12	2:L:160:THR:H	1.62	0.64
1:M:151:ASP:C	1:M:153:ALA:H	2.04	0.64
2:N:90:TYR:CE1	2:N:109:VAL:HB	2.32	0.64
1:G:121:SER:O	1:G:124:GLN:HB3	1.97	0.63
2:L:36:TRP:HE1	2:L:78:THR:HG21	1.64	0.63
2:L:115:SER:HB3	2:L:117:LYS:HE2	1.79	0.63
2:P:36:TRP:CG	2:P:80:MET:HG3	2.32	0.63
2:P:67:VAL:HG22	2:P:68:THR:H	1.63	0.63
2:B:188:SER:HA	2:B:191:THR:CG2	2.28	0.63
1:E:175:LEU:HD23	1:E:175:LEU:C	2.23	0.63
2:H:51:ILE:HB	2:H:57:ALA:CB	2.28	0.63
1:I:6:GLN:NE2	1:I:86:TYR:O	2.30	0.63
1:I:12:SER:O	1:I:13:ALA:HB2	1.97	0.63
2:J:19:LYS:HB2	2:J:81:GLU:OE1	1.98	0.63
2:J:171:GLN:NE2	2:J:177:SER:HB2	2.14	0.63
2:L:11:VAL:HG22	2:L:110:THR:CB	2.28	0.63
1:C:136:LEU:HD11	1:C:146:VAL:CG2	2.28	0.63
1:E:32:TYR:HD1	1:E:92:TYR:HD1	1.46	0.63
1:E:90:GLN:OE1	1:E:97:THR:N	2.25	0.63
2:H:120:SER:HB3	2:H:122:PHE:CE1	2.33	0.63
1:I:121:SER:O	1:I:124:GLN:N	2.31	0.63
2:N:1:GLN:HG3	2:N:2:VAL:N	2.09	0.63
1:O:8:PRO:CD	1:O:10:SER:H	2.11	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:111:ALA:O	1:G:139:PHE:HA	1.98	0.63
2:H:164:HIS:HB2	2:H:181:VAL:HG22	1.79	0.63
1:M:187:GLU:HG2	1:M:211:ARG:HD2	1.81	0.63
1:M:211:ARG:HG2	1:M:211:ARG:HH11	1.64	0.63
2:P:40:ALA:HA	2:P:88:ALA:HB2	1.80	0.63
2:D:34:ILE:HG21	2:D:78:THR:HG21	1.79	0.63
2:H:119:PRO:HD3	2:H:200:HIS:CD2	2.34	0.63
2:H:131:THR:HG22	2:H:136:ALA:HA	1.81	0.63
1:K:47:LEU:HD11	1:K:86:TYR:HE2	1.63	0.63
2:N:19:LYS:HA	2:N:80:MET:O	1.99	0.63
1:O:83:PHE:CE1	1:O:106:ILE:HD13	2.34	0.63
1:O:195:GLU:CD	1:O:204:PRO:HB3	2.23	0.63
2:L:126:PRO:HD2	2:L:213:PRO:HA	1.80	0.63
2:D:2:VAL:O	2:D:2:VAL:HG22	1.99	0.63
2:J:29:PHE:O	2:J:52(A):PRO:HG2	1.98	0.63
2:L:1:GLN:H3	2:L:1:GLN:CD	2.05	0.63
2:L:84:SER:HB2	2:L:85:GLU:OE2	1.99	0.63
1:E:54:LEU:HD11	1:E:58:VAL:HG11	1.81	0.63
2:H:199:ASN:HD22	2:H:200:HIS:H	1.43	0.63
1:I:32:TYR:HB3	1:I:91:SER:CB	2.18	0.63
1:K:96:HIS:HB2	2:L:47:TRP:CD2	2.34	0.63
2:N:55:GLY:O	2:N:56:SER:HB3	1.99	0.63
1:G:107:LYS:HA	1:G:140:TYR:HH	1.63	0.63
2:H:7:SER:OG	2:H:20:VAL:HG13	1.99	0.63
2:P:6:GLN:HE22	2:P:106:GLY:HA2	1.64	0.63
2:P:32:TYR:H	2:P:32:TYR:HD2	1.47	0.63
2:D:93:ALA:HB1	2:D:100(L):MET:HG2	1.81	0.62
2:D:108:THR:HG23	2:D:108:THR:O	1.99	0.62
2:H:121:VAL:HG21	2:H:207:VAL:HG11	1.81	0.62
1:O:35:TRP:CG	1:O:73:LEU:HD13	2.34	0.62
2:D:13:LYS:HA	2:D:112:ALA:O	1.99	0.62
2:D:138:LEU:C	2:D:138:LEU:HD12	2.24	0.62
2:J:171:GLN:C	2:J:173:SER:H	2.07	0.62
2:P:170:LEU:HD12	2:P:171:GLN:N	2.14	0.62
1:A:118:PHE:CD2	2:B:124:LEU:HB3	2.34	0.62
1:G:174:SER:O	2:H:166:PHE:HE2	1.82	0.62
1:I:139:PHE:CD2	1:I:198:HIS:NE2	2.66	0.62
1:O:210:ASN:O	1:O:213:GLU:HB3	1.99	0.62
1:A:54:LEU:HD12	1:A:54:LEU:N	2.14	0.62
2:B:50:GLY:O	2:B:57:ALA:HB1	1.98	0.62
1:C:125:LEU:HD21	1:C:130:ALA:HB2	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:54:LEU:HD11	1:E:58:VAL:CG1	2.30	0.62
1:G:47:LEU:CD2	1:G:48:ILE:HG13	2.28	0.62
2:H:138:LEU:HD11	2:H:154:TRP:CH2	2.34	0.62
2:J:148:GLU:HG2	2:J:149:PRO:HA	1.80	0.62
1:M:185:ASP:O	1:M:188:LYS:HB2	1.98	0.62
2:P:39:GLN:O	2:P:88:ALA:HB1	1.98	0.62
2:P:146:PHE:C	2:P:146:PHE:CD2	2.77	0.62
1:G:134:CYS:HB2	1:G:148:TRP:CZ2	2.35	0.62
2:J:150:VAL:HG23	2:J:200:HIS:CD2	2.35	0.62
1:K:151:ASP:OD2	1:K:189:HIS:HB3	2.00	0.62
1:E:110:VAL:HG22	1:E:141:PRO:CD	2.29	0.62
1:E:154:LEU:H	1:E:154:LEU:CD2	2.13	0.62
2:J:189:LEU:C	2:J:191:THR:H	2.08	0.62
1:O:146:VAL:HG13	1:O:196:VAL:HG22	1.82	0.62
2:P:47:TRP:CH2	2:P:49:GLY:HA2	2.34	0.62
2:P:82(A):SER:O	2:P:82(B):SER:C	2.42	0.62
1:A:11:LEU:HD23	1:A:104:LEU:HD23	1.75	0.62
1:G:176:SER:HB3	2:H:166:PHE:CZ	2.35	0.62
2:H:119:PRO:HB3	2:H:145:TYR:CB	2.29	0.62
2:H:138:LEU:HD11	2:H:154:TRP:CZ2	2.35	0.62
2:N:100(J):HIS:CG	2:N:100(K):GLY:H	2.18	0.62
2:P:94:LYS:HD3	2:P:94:LYS:C	2.25	0.62
2:D:121:VAL:HG21	2:D:198:VAL:HG21	1.81	0.62
2:F:93:ALA:HB3	2:F:100(L):MET:SD	2.39	0.62
1:G:164:THR:HG23	1:G:174:SER:O	1.99	0.62
2:J:93:ALA:HA	2:J:102:VAL:O	1.99	0.62
2:J:94:LYS:HE2	2:J:96:GLY:HA2	1.82	0.62
1:K:8:PRO:HA	1:K:101:GLY:O	2.00	0.62
2:N:52:ILE:HG22	2:N:52(A):PRO:O	2.00	0.62
1:E:11:LEU:HD21	1:I:154:LEU:HD12	1.82	0.62
2:F:121:VAL:HG21	2:F:198:VAL:HG21	1.81	0.62
1:G:164:THR:HG21	1:G:174:SER:HB2	1.82	0.62
1:G:186:TYR:CE1	1:G:192:TYR:HE2	2.18	0.62
2:H:54:PHE:N	2:H:54:PHE:CD1	2.68	0.62
2:J:87:THR:HG23	2:J:110:THR:HA	1.82	0.62
1:O:54:LEU:HD12	1:O:55:GLN:N	2.15	0.62
1:O:89:GLN:HG3	1:O:98:PHE:CE2	2.35	0.62
2:P:23:LYS:HB2	2:P:77:THR:OG1	2.00	0.62
2:B:126:PRO:HD3	2:B:211:VAL:HG12	1.82	0.61
2:D:12:LYS:HB3	2:D:16:SER:OG	1.99	0.61
1:E:151:ASP:O	1:E:152:ASN:CB	2.43	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:20:VAL:HG12	2:F:21:SER:H	1.65	0.61
2:F:105:GLN:OE1	2:F:105:GLN:N	2.28	0.61
2:H:32:TYR:CG	2:H:94:LYS:HE3	2.35	0.61
1:K:19:VAL:CG2	1:K:78:LEU:HD21	2.28	0.61
2:D:6:GLN:N	2:D:105:GLN:OE1	2.27	0.61
2:F:126:PRO:HG3	2:F:138:LEU:HB3	1.82	0.61
1:K:11:LEU:HB3	1:K:104:LEU:HD23	1.83	0.61
1:O:61:ARG:HG3	1:O:62:PHE:CE1	2.35	0.61
1:A:54:LEU:H	1:A:54:LEU:CD1	2.14	0.61
2:H:130:SER:O	2:H:137:ALA:N	2.31	0.61
1:K:136:LEU:HD21	1:K:196:VAL:CG1	2.30	0.61
1:O:7:SER:HB3	1:O:8:PRO:HD3	1.81	0.61
1:O:138:ASN:N	1:O:138:ASN:ND2	2.48	0.61
1:E:130:ALA:N	1:E:181:LEU:O	2.23	0.61
1:G:61:ARG:CZ	1:G:79:GLN:HG3	2.29	0.61
1:I:169:LYS:HE2	1:I:170:ASP:OD1	2.01	0.61
2:L:34:ILE:HD12	2:L:34:ILE:N	2.16	0.61
1:M:3:GLN:CB	1:M:26:SER:HB3	2.30	0.61
1:M:30:SER:O	1:M:71:PHE:HZ	1.84	0.61
1:O:210:ASN:HB2	1:O:213:GLU:OE1	2.00	0.61
1:G:118:PHE:CD2	1:G:118:PHE:N	2.67	0.61
1:A:33:LEU:HD13	1:A:34:ASN:N	2.16	0.61
2:B:126:PRO:HG3	2:B:138:LEU:CB	2.31	0.61
2:D:171:GLN:HB2	2:D:175:LEU:O	2.01	0.61
1:E:81:GLU:N	1:E:81:GLU:OE1	2.33	0.61
1:C:154:LEU:N	1:C:154:LEU:HD22	2.14	0.61
2:D:39:GLN:NE2	2:D:43:GLN:O	2.33	0.61
2:H:39:GLN:C	2:H:88:ALA:HB1	2.26	0.61
1:I:175:LEU:HD23	1:I:176:SER:N	2.16	0.61
2:J:136:ALA:O	2:J:183:THR:HA	2.01	0.61
2:L:55:GLY:O	2:L:56:SER:CB	2.48	0.61
1:M:61:ARG:NH2	3:M:228:HOH:O	2.33	0.61
1:M:113:PRO:HD3	1:M:198:HIS:ND1	2.09	0.61
2:N:109:VAL:O	2:N:109:VAL:HG12	2.00	0.61
1:A:20:THR:CG2	1:A:74:THR:HG23	2.29	0.61
2:B:34:ILE:HG21	2:B:78:THR:HG21	1.81	0.61
2:F:54:PHE:O	2:F:55:GLY:C	2.44	0.61
1:O:37:GLN:HG2	1:O:38:GLN:N	2.15	0.61
1:O:61:ARG:O	1:O:75:ILE:HA	2.01	0.61
1:O:155:GLN:OE1	1:O:158:ASN:ND2	2.34	0.61
1:E:33:LEU:HD13	1:E:34:ASN:N	2.16	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:143:LYS:HE2	2:F:171:GLN:OE1	2.01	0.61
1:I:143:GLU:O	1:I:198:HIS:CD2	2.54	0.61
1:K:59:PRO:HB3	1:K:61:ARG:NH1	2.16	0.61
1:K:201:LEU:HD13	1:K:205:VAL:HG21	1.81	0.61
2:F:94:LYS:HZ1	2:F:96:GLY:N	1.98	0.61
1:I:125:LEU:HD22	1:I:183:LYS:HG3	1.81	0.61
2:L:152:VAL:HG11	2:L:180:SER:OG	2.01	0.61
2:B:94:LYS:HD2	2:B:102:VAL:HG12	1.81	0.60
2:B:94:LYS:HE2	2:B:96:GLY:N	2.16	0.60
2:D:171:GLN:NE2	2:D:177:SER:HB2	2.14	0.60
1:E:11:LEU:CD2	1:I:156:SER:HB2	2.29	0.60
2:H:172:SER:O	1:K:26:SER:HA	2.01	0.60
1:I:184:ALA:HB1	1:I:188:LYS:HE3	1.83	0.60
2:J:94:LYS:HE2	2:J:96:GLY:CA	2.31	0.60
1:K:49:TYR:CD2	1:K:49:TYR:N	2.68	0.60
1:C:150:VAL:HG22	1:C:192:TYR:HD1	1.66	0.60
1:C:186:TYR:O	1:C:192:TYR:OH	2.19	0.60
1:E:192:TYR:O	1:E:208:SER:HB2	2.00	0.60
1:I:80:PRO:O	1:I:83:PHE:HD1	1.84	0.60
1:A:135:LEU:CD1	2:B:181:VAL:HG21	2.31	0.60
1:G:165:GLU:HB3	3:G:216:HOH:O	2.00	0.60
2:H:51:ILE:HD12	2:H:57:ALA:HB2	1.83	0.60
2:L:47:TRP:CH2	2:L:49:GLY:HA2	2.36	0.60
2:L:143:LYS:HA	2:L:177:SER:OG	2.01	0.60
2:H:2:VAL:O	2:H:2:VAL:HG22	1.99	0.60
1:I:33:LEU:HG	1:I:71:PHE:CD2	2.36	0.60
1:K:47:LEU:C	1:K:48:ILE:HG13	2.25	0.60
2:L:61:GLN:O	2:L:64:GLN:HB2	2.01	0.60
2:L:131:THR:HA	2:L:135:THR:O	2.01	0.60
1:M:161:GLU:HB2	1:M:175:LEU:HD21	1.83	0.60
1:O:191:VAL:HG22	1:O:210:ASN:OD1	2.02	0.60
2:B:39:GLN:HG3	2:B:43:GLN:O	2.01	0.60
2:J:2:VAL:HG13	2:J:2:VAL:O	2.01	0.60
1:K:195:GLU:HA	1:K:205:VAL:O	2.01	0.60
2:N:17:SER:HB3	2:N:82(A):SER:HA	1.83	0.60
2:P:29:PHE:HE1	2:P:73:GLU:HG3	1.66	0.60
2:P:67:VAL:HG22	2:P:68:THR:N	2.15	0.60
1:A:47:LEU:HD11	1:A:86:TYR:HE2	1.66	0.60
2:B:73:GLU:C	2:B:75:THR:H	2.10	0.60
2:B:163:VAL:HG22	2:B:182:VAL:HB	1.84	0.60
1:C:35:TRP:CE2	1:C:73:LEU:HB2	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:87:TYR:OH	2:D:44:GLY:HA2	2.02	0.60
2:H:61:GLN:HA	2:H:64:GLN:OE1	2.02	0.60
1:I:184:ALA:C	1:I:188:LYS:HE3	2.26	0.60
2:J:83:ARG:HB3	2:J:85:GLU:CG	2.25	0.60
2:H:102:VAL:HG23	3:H:221:HOH:O	2.02	0.60
2:J:30:SER:O	2:J:52(A):PRO:HB2	2.02	0.60
1:A:18:ARG:NH2	1:A:76:SER:HA	2.16	0.60
1:C:133:VAL:HG22	1:C:178:THR:HG23	1.83	0.60
2:J:109:VAL:HG12	2:J:109:VAL:O	2.01	0.60
2:J:201:LYS:HB2	2:J:202:PRO:HD3	1.83	0.60
2:D:18:VAL:CG2	2:D:19:LYS:N	2.65	0.60
2:F:37:VAL:HA	2:F:46:GLU:O	2.02	0.60
2:H:146:PHE:HB2	2:H:175:LEU:CD2	2.32	0.60
1:K:33:LEU:HD13	1:K:34:ASN:N	2.17	0.60
2:N:36:TRP:HE1	2:N:78:THR:CG2	2.14	0.60
2:F:89:VAL:CG2	2:F:108:THR:HG23	2.31	0.60
1:G:61:ARG:O	1:G:75:ILE:HA	2.02	0.60
1:I:83:PHE:CZ	1:I:106:ILE:HG12	2.37	0.60
2:N:30:SER:C	2:N:53:VAL:HG23	2.27	0.60
2:N:51:ILE:HG13	2:N:56:SER:O	2.02	0.60
2:N:115:SER:O	2:N:146:PHE:HB3	2.02	0.60
2:P:38:ARG:HG3	2:P:46:GLU:HB3	1.82	0.60
2:B:77:THR:HG22	2:B:78:THR:N	2.16	0.59
2:F:182:VAL:HG22	2:F:182:VAL:O	2.00	0.59
1:G:11:LEU:HD12	1:G:104:LEU:HD23	1.84	0.59
1:K:118:PHE:CB	2:L:124:LEU:HD22	2.31	0.59
1:A:211:ARG:HH11	1:A:211:ARG:CB	2.09	0.59
1:E:154:LEU:HD22	1:E:154:LEU:N	2.16	0.59
2:F:29:PHE:CD1	2:F:30:SER:N	2.70	0.59
2:H:29:PHE:HB2	2:H:76:SER:HB2	1.84	0.59
2:N:163:VAL:HG12	2:N:164:HIS:N	2.17	0.59
2:P:171:GLN:HG3	2:P:175:LEU:O	2.02	0.59
1:E:198:HIS:HB3	1:E:201:LEU:HD12	1.84	0.59
2:J:131:THR:HG22	2:J:136:ALA:CA	2.28	0.59
1:K:3:GLN:O	1:K:25:ALA:HA	2.02	0.59
2:L:30:SER:HA	2:L:52(A):PRO:HB2	1.83	0.59
2:L:82(A):SER:O	2:L:82(B):SER:HB2	2.01	0.59
1:E:2:ILE:N	1:E:26:SER:HG	1.99	0.59
2:F:199:ASN:HD22	2:F:200:HIS:N	2.01	0.59
1:G:180:THR:HG21	2:H:143:LYS:CE	2.32	0.59
2:H:36:TRP:CG	2:H:69:ILE:HD11	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:136:ALA:HB2	2:L:186:SER:HB3	1.82	0.59
2:P:2:VAL:HG21	2:P:32:TYR:CE1	2.36	0.59
2:P:21:SER:O	2:P:22:CYS:HB3	2.01	0.59
2:P:36:TRP:CE2	2:P:80:MET:HB2	2.37	0.59
1:C:150:VAL:HG22	1:C:192:TYR:CD1	2.38	0.59
2:D:111:VAL:O	2:D:111:VAL:HG12	2.01	0.59
2:F:32:TYR:HB3	2:F:94:LYS:CG	2.31	0.59
1:G:186:TYR:O	1:G:188:LYS:N	2.36	0.59
2:H:143:LYS:HA	2:H:177:SER:OG	2.02	0.59
2:J:53:VAL:O	2:J:53:VAL:HG12	2.02	0.59
1:K:182:SER:OG	1:K:184:ALA:HB3	2.02	0.59
2:P:10:GLU:O	2:P:109:VAL:HA	2.02	0.59
2:P:38:ARG:N	2:P:46:GLU:O	2.33	0.59
1:G:83:PHE:CD1	1:G:106:ILE:HG13	2.37	0.59
2:J:52:ILE:C	2:J:53:VAL:H	2.10	0.59
1:K:202:SER:O	1:K:203:SER:CB	2.51	0.59
2:L:162:GLY:O	2:L:182:VAL:HA	2.02	0.59
2:B:52(A):PRO:O	2:B:55:GLY:N	2.31	0.59
1:C:116:PHE:CD2	2:D:137:ALA:HB3	2.38	0.59
1:E:8:PRO:HA	1:E:102:THR:HA	1.85	0.59
1:I:117:ILE:CD1	1:I:207:LYS:O	2.51	0.59
1:I:139:PHE:HD2	1:I:198:HIS:CE1	2.20	0.59
2:L:202:PRO:O	2:L:203:SER:CB	2.48	0.59
1:A:119:PRO:HB3	1:A:209:PHE:CE2	2.37	0.59
2:H:134:GLY:O	2:H:185:PRO:HA	2.03	0.59
2:J:94:LYS:HB3	2:J:102:VAL:CG1	2.33	0.59
1:M:19:VAL:O	1:M:74:THR:HG23	2.02	0.59
1:M:136:LEU:HG	1:M:196:VAL:HG21	1.85	0.59
2:B:68:THR:HB	2:B:81:GLU:HB3	1.84	0.59
2:H:87:THR:HG23	2:H:109:VAL:O	2.03	0.59
2:H:94:LYS:HD3	2:H:94:LYS:C	2.27	0.59
1:M:136:LEU:N	1:M:136:LEU:HD12	2.17	0.59
2:N:192:GLN:HG2	2:N:194:TYR:CZ	2.38	0.59
2:P:53:VAL:HG12	2:P:53:VAL:O	2.02	0.59
2:P:195:ILE:HG12	2:P:210:LYS:HA	1.83	0.59
1:A:76:SER:OG	1:A:77:SER:N	2.35	0.59
2:B:36:TRP:HE1	2:B:78:THR:HG21	1.67	0.59
2:D:110:THR:O	2:D:110:THR:HG22	2.03	0.59
1:G:137:ASN:HD22	1:G:138:ASN:CG	2.11	0.59
1:I:88:CYS:O	1:I:98:PHE:HD2	1.85	0.59
2:J:17:SER:CB	2:J:82(A):SER:HA	2.28	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:18:VAL:HG22	2:L:19:LYS:N	2.17	0.59
1:M:210:ASN:ND2	1:M:210:ASN:N	2.51	0.59
2:N:83:ARG:O	2:N:111:VAL:HG11	2.02	0.59
1:A:123:GLU:OE2	1:A:123:GLU:N	2.36	0.58
2:B:36:TRP:HE1	2:B:78:THR:CG2	2.15	0.58
1:C:93:SER:C	1:C:95:SER:H	2.10	0.58
2:D:17:SER:HB2	2:D:82(A):SER:HA	1.84	0.58
1:G:137:ASN:ND2	1:G:138:ASN:CG	2.61	0.58
2:J:207:VAL:HG12	2:J:208:ASP:N	2.17	0.58
2:J:208:ASP:N	2:J:208:ASP:OD1	2.36	0.58
2:B:62:LYS:HA	2:N:83:ARG:NH2	2.17	0.58
1:C:11:LEU:C	1:C:11:LEU:HD22	2.28	0.58
1:E:18:ARG:HH12	1:E:76:SER:HB3	1.68	0.58
1:G:61:ARG:HE	1:G:82:ASP:CG	2.10	0.58
2:H:170:LEU:HD12	2:H:171:GLN:H	1.68	0.58
1:K:46:LEU:HB3	3:K:225:HOH:O	2.03	0.58
1:K:142:ARG:NH1	1:K:163:VAL:HG11	2.06	0.58
1:M:67:SER:HA	1:M:71:PHE:CZ	2.37	0.58
2:N:138:LEU:HD12	2:N:139:GLY:N	2.18	0.58
1:O:138:ASN:N	1:O:138:ASN:HD22	2.00	0.58
1:O:183:LYS:O	1:O:187:GLU:HG3	2.03	0.58
1:A:115:VAL:HG12	1:A:116:PHE:N	2.18	0.58
1:A:151:ASP:HB2	3:A:232:HOH:O	2.01	0.58
2:B:124:LEU:HD12	2:B:140:CYS:N	2.19	0.58
1:C:116:PHE:HD2	2:D:130:SER:CB	2.15	0.58
1:C:210:ASN:HD22	1:C:210:ASN:N	2.00	0.58
2:F:40:ALA:O	2:F:43:GLN:HB2	2.03	0.58
2:F:148:GLU:HG2	2:F:176:TYR:CD2	2.38	0.58
1:G:182:SER:O	1:G:183:LYS:C	2.46	0.58
1:K:79:GLN:HB3	1:K:80:PRO:HD2	1.84	0.58
1:K:152:ASN:N	1:K:152:ASN:ND2	2.51	0.58
1:M:24:ARG:NH1	3:M:221:HOH:O	2.36	0.58
1:O:161:GLU:HA	1:O:176:SER:O	2.03	0.58
1:O:183:LYS:HA	1:O:186:TYR:HB3	1.84	0.58
2:P:21:SER:O	2:P:22:CYS:CB	2.51	0.58
1:A:124:GLN:NE2	1:A:131:SER:N	2.51	0.58
1:I:122:ASP:HA	1:I:125:LEU:HD12	1.86	0.58
2:J:150:VAL:HG23	2:J:200:HIS:HD2	1.68	0.58
2:J:171:GLN:NE2	2:J:177:SER:HB3	2.18	0.58
1:M:181:LEU:N	1:M:181:LEU:HD12	2.18	0.58
1:G:154:LEU:HD22	1:G:154:LEU:H	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:19:LYS:CE	2:H:79:TYR:HB3	2.32	0.58
1:M:201:LEU:HD13	1:M:205:VAL:HG23	1.85	0.58
1:A:90:GLN:NE2	1:A:93:SER:HB3	2.18	0.58
1:K:11:LEU:HD12	1:K:104:LEU:CD2	2.31	0.58
1:A:34:ASN:ND2	1:A:91:SER:HB2	2.19	0.58
1:C:142:ARG:HG2	1:C:142:ARG:HH11	1.69	0.58
1:G:151:ASP:OD2	1:G:189:HIS:ND1	2.36	0.58
1:I:54:LEU:HD21	1:I:59:PRO:O	2.02	0.58
2:P:18:VAL:HG12	2:P:82(C):LEU:HD11	1.85	0.58
1:A:90:GLN:HE22	1:A:93:SER:HB3	1.68	0.58
1:G:83:PHE:CE1	1:G:106:ILE:HG13	2.38	0.58
1:I:142:ARG:HG2	1:I:142:ARG:O	2.03	0.58
2:P:131:THR:HG22	2:P:136:ALA:CB	2.32	0.58
1:A:142:ARG:HG3	1:A:142:ARG:O	2.02	0.58
1:E:65:SER:OG	1:E:72:THR:HG23	2.04	0.58
1:G:180:THR:HG21	2:H:143:LYS:HE2	1.85	0.58
1:K:27:GLN:O	1:K:69:THR:HG22	2.03	0.58
1:K:52:SER:HB3	1:K:64:GLY:O	2.04	0.58
2:P:119:PRO:HD3	2:P:200:HIS:ND1	2.19	0.58
2:B:68:THR:O	2:B:81:GLU:HB3	2.04	0.58
2:H:184:VAL:HG21	2:H:194:TYR:CZ	2.39	0.58
2:J:210:LYS:HZ2	2:J:212:GLU:CD	2.12	0.58
1:O:56:SER:C	1:O:58:VAL:H	2.12	0.58
1:O:138:ASN:HA	1:O:173:TYR:O	2.04	0.58
1:O:170:ASP:O	1:O:172:THR:N	2.37	0.58
1:A:18:ARG:HB2	1:A:18:ARG:NH1	2.19	0.57
2:B:52(A):PRO:O	2:B:54:PHE:N	2.37	0.57
2:D:197:ASN:ND2	2:D:208:ASP:OD1	2.37	0.57
1:E:4:MET:HE1	1:E:33:LEU:HD23	1.85	0.57
1:E:110:VAL:HG13	1:E:140:TYR:O	2.04	0.57
2:F:131:THR:HG22	2:F:136:ALA:HA	1.85	0.57
2:J:13:LYS:NZ	2:J:113:SER:O	2.35	0.57
1:M:79:GLN:HB3	1:M:81:GLU:OE2	2.04	0.57
1:M:197:THR:HG22	1:M:204:PRO:CG	2.33	0.57
2:B:184:VAL:HB	2:B:185:PRO:CD	2.34	0.57
2:F:182:VAL:O	2:F:184:VAL:HG13	2.04	0.57
2:H:67:VAL:HA	2:H:81:GLU:O	2.04	0.57
1:I:89:GLN:HB2	1:I:98:PHE:CE2	2.39	0.57
1:K:179:LEU:HD11	1:K:181:LEU:HD13	1.85	0.57
1:O:25:ALA:O	1:O:69:THR:HG22	2.04	0.57
1:O:83:PHE:CZ	1:O:106:ILE:HD13	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:39:LYS:HG2	1:C:84:ALA:HB2	1.87	0.57
1:C:75:ILE:CG2	1:C:78:LEU:HD12	2.34	0.57
2:H:170:LEU:HD12	2:H:171:GLN:N	2.19	0.57
1:K:149:LYS:HB2	1:K:149:LYS:HZ2	1.68	0.57
2:P:127:SER:O	2:P:131:THR:HG23	2.04	0.57
2:F:24:ALA:HB3	2:F:29:PHE:HB2	1.86	0.57
2:H:124:LEU:HD21	2:H:141:LEU:HB3	1.82	0.57
1:I:110:VAL:HG12	1:I:111:ALA:H	1.69	0.57
2:J:171:GLN:HE21	2:J:177:SER:HB3	1.69	0.57
1:K:136:LEU:HD21	1:K:196:VAL:HG11	1.85	0.57
2:L:63:PHE:HB3	2:L:67:VAL:CG1	2.34	0.57
2:B:69:ILE:HA	2:B:79:TYR:O	2.05	0.57
1:C:35:TRP:CZ3	1:C:88:CYS:HB3	2.39	0.57
2:D:18:VAL:HG12	2:D:82(C):LEU:CD1	2.29	0.57
2:F:155:ASN:HD22	2:F:159:LEU:HB2	1.70	0.57
2:H:69:ILE:HG13	2:H:80:MET:HG2	1.86	0.57
2:J:61:GLN:H	2:J:61:GLN:HE21	0.78	0.57
2:L:90:TYR:HE1	2:L:109:VAL:HB	1.70	0.57
2:N:28:THR:O	2:N:28:THR:HG22	2.03	0.57
1:O:135:LEU:HD13	2:P:181:VAL:HG21	1.84	0.57
2:P:146:PHE:H	2:P:200:HIS:HE1	1.52	0.57
1:C:32:TYR:HB3	1:C:91:SER:HB3	1.85	0.57
1:E:14:SER:HB2	1:E:17:ASP:OD1	2.04	0.57
2:H:73:GLU:CD	2:H:73:GLU:N	2.56	0.57
2:N:150:VAL:HG23	2:N:199:ASN:O	2.04	0.57
2:D:145:TYR:CD1	2:D:145:TYR:C	2.82	0.57
2:F:185:PRO:HB2	2:F:188:SER:CB	2.34	0.57
2:H:138:LEU:CD1	2:H:139:GLY:N	2.68	0.57
2:J:201:LYS:C	2:J:203:SER:H	2.13	0.57
1:K:156:SER:C	1:K:158:ASN:H	2.13	0.57
1:M:112:ALA:HB2	1:M:200:GLY:O	2.03	0.57
2:P:199:ASN:HD22	2:P:200:HIS:N	2.02	0.57
2:B:169:VAL:O	2:B:176:TYR:HA	2.05	0.57
1:C:45:LYS:HG2	1:C:47:LEU:HD23	1.86	0.57
2:D:17:SER:HB2	2:D:82:LEU:O	2.05	0.57
2:D:178:LEU:HD12	2:D:178:LEU:C	2.30	0.57
1:G:6:GLN:C	1:G:7:SER:O	2.44	0.57
1:K:55:GLN:O	1:K:58:VAL:HG23	2.05	0.57
2:L:40:ALA:HA	2:L:88:ALA:HB2	1.86	0.57
2:L:193:THR:HG22	2:L:194:TYR:N	2.20	0.57
1:O:27:GLN:O	1:O:29:ILE:HG23	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:39:GLN:C	2:P:88:ALA:HB1	2.29	0.57
2:B:141:LEU:C	2:B:141:LEU:HD12	2.30	0.57
1:C:199:GLN:HA	1:O:199:GLN:NE2	2.19	0.57
2:D:165:THR:HG23	2:D:180:SER:CB	2.31	0.57
2:H:193:THR:HG22	2:H:194:TYR:N	2.20	0.57
1:I:27:GLN:O	1:I:29:ILE:HG23	2.05	0.57
1:K:26:SER:HG	1:K:27:GLN:CD	2.11	0.57
1:O:94:THR:CG2	1:O:95:SER:N	2.68	0.57
1:A:3:GLN:O	1:A:4:MET:SD	2.62	0.57
1:C:145:LYS:HD3	1:C:197:THR:CG2	2.35	0.57
2:H:84:SER:C	2:H:86:ASP:N	2.62	0.57
1:M:26:SER:HB2	1:M:27:GLN:NE2	2.20	0.57
2:B:131:THR:HG22	2:B:136:ALA:CA	2.35	0.56
1:C:161:GLU:HA	3:C:214:HOH:O	2.03	0.56
1:C:168:SER:OG	1:C:169:LYS:N	2.38	0.56
1:C:199:GLN:NE2	1:O:199:GLN:HA	2.20	0.56
1:E:66:GLY:O	1:E:67:SER:HB3	2.04	0.56
2:F:30:SER:HA	2:F:52(A):PRO:CB	2.35	0.56
1:G:164:THR:CG2	1:G:174:SER:HB2	2.35	0.56
2:H:84:SER:O	2:H:86:ASP:N	2.38	0.56
1:K:47:LEU:O	1:K:55:GLN:HB3	2.05	0.56
2:N:201:LYS:C	2:N:203:SER:H	2.13	0.56
2:B:146:PHE:HB2	2:B:175:LEU:HD23	1.86	0.56
1:C:61:ARG:HD3	1:C:79:GLN:HE21	1.69	0.56
2:F:168:ALA:HA	2:F:178:LEU:HB3	1.88	0.56
1:I:6:GLN:HE22	1:I:87:TYR:CA	2.18	0.56
1:K:164:THR:HG22	1:K:174:SER:O	2.05	0.56
1:K:164:THR:HG21	1:K:174:SER:HB2	1.87	0.56
2:P:145:TYR:O	2:P:146:PHE:CB	2.52	0.56
2:B:51:ILE:HD11	2:B:55:GLY:O	2.04	0.56
1:C:45:LYS:HG2	1:C:47:LEU:CD2	2.35	0.56
1:C:90:GLN:OE1	1:C:93:SER:HB3	2.06	0.56
1:E:116:PHE:HD2	2:F:130:SER:CA	2.19	0.56
1:G:48:ILE:HD12	1:G:64:GLY:HA3	1.86	0.56
1:G:162:SER:OG	2:H:167:PRO:HD2	2.05	0.56
2:H:75:THR:O	2:H:76:SER:C	2.49	0.56
1:I:201:LEU:O	1:I:202:SER:C	2.48	0.56
2:J:145:TYR:O	2:J:146:PHE:HB2	2.05	0.56
1:K:6:GLN:C	1:K:100:GLN:NE2	2.64	0.56
1:K:55:GLN:HB3	1:K:58:VAL:HG21	1.87	0.56
2:L:154:TRP:CZ3	2:L:196:CYS:HB3	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:170:LEU:HD12	2:L:171:GLN:N	2.20	0.56
1:M:62:PHE:HE2	1:M:86:TYR:HE2	1.53	0.56
1:M:124:GLN:HE22	1:M:131:SER:HB2	1.69	0.56
1:M:192:TYR:O	1:M:208:SER:HB2	2.06	0.56
2:P:89:VAL:HA	2:P:107:THR:O	2.05	0.56
1:A:191:VAL:HG12	1:A:192:TYR:N	2.20	0.56
1:C:130:ALA:N	1:C:181:LEU:O	2.31	0.56
2:D:48:MET:HE3	2:D:63:PHE:CE2	2.40	0.56
1:G:11:LEU:HD12	1:G:104:LEU:HD21	1.87	0.56
1:G:96:HIS:HB2	2:H:47:TRP:CE2	2.40	0.56
2:H:1:GLN:O	2:H:26:GLY:HA3	2.06	0.56
2:H:30:SER:O	2:H:53:VAL:HG23	2.06	0.56
1:I:175:LEU:HD23	1:I:175:LEU:C	2.30	0.56
2:J:171:GLN:HE21	2:J:177:SER:CB	2.18	0.56
2:J:178:LEU:C	2:J:178:LEU:HD12	2.30	0.56
2:N:40:ALA:O	2:N:41:PRO:C	2.49	0.56
1:O:142:ARG:HG2	1:O:142:ARG:O	2.06	0.56
1:C:167:ASP:HA	3:C:221:HOH:O	2.05	0.56
2:D:84:SER:HB2	2:D:85:GLU:OE2	2.05	0.56
2:F:4:LEU:HA	2:F:23:LYS:O	2.05	0.56
2:F:4:LEU:HD22	2:F:22:CYS:SG	2.46	0.56
2:F:100(J):HIS:N	3:F:225:HOH:O	2.39	0.56
1:G:14:SER:HB2	1:G:17:ASP:OD1	2.04	0.56
2:H:111:VAL:O	2:H:112:ALA:HB2	2.05	0.56
1:M:164:THR:HB	1:M:174:SER:H	1.70	0.56
1:A:117:ILE:HG22	2:B:129:LYS:HB3	1.88	0.56
1:E:47:LEU:O	1:E:48:ILE:HG13	2.05	0.56
2:F:11:VAL:HA	2:F:110:THR:O	2.05	0.56
1:K:122:ASP:C	1:K:124:GLN:N	2.58	0.56
2:L:37:VAL:HG12	2:L:38:ARG:N	2.19	0.56
1:C:128:GLY:C	1:C:129:THR:HG22	2.30	0.56
2:D:63:PHE:HB3	2:D:67:VAL:HG12	1.86	0.56
2:D:145:TYR:CE1	2:D:176:TYR:HB2	2.41	0.56
2:F:201:LYS:N	2:F:202:PRO:CD	2.68	0.56
1:G:48:ILE:CD1	1:G:64:GLY:HA3	2.35	0.56
1:G:143:GLU:H	1:G:143:GLU:CD	2.14	0.56
2:J:91:PHE:CD1	2:J:91:PHE:N	2.74	0.56
1:K:6:GLN:O	1:K:100:GLN:NE2	2.39	0.56
2:L:141:LEU:C	2:L:141:LEU:HD12	2.31	0.56
1:A:147:GLN:OE1	1:A:147:GLN:HA	2.06	0.56
1:C:142:ARG:NH2	1:C:163:VAL:HG21	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:19:LYS:HE2	2:H:79:TYR:HD2	1.70	0.56
2:L:19:LYS:HG2	3:L:215:HOH:O	2.05	0.56
1:O:119:PRO:HB3	1:O:209:PHE:CZ	2.41	0.56
2:P:2:VAL:O	2:P:3:GLN:HB2	2.06	0.56
2:P:28:THR:N	2:P:32:TYR:OH	2.38	0.56
1:A:90:GLN:HG3	1:A:97:THR:N	2.20	0.56
1:C:28:SER:HA	1:C:68:GLY:O	2.06	0.56
1:C:195:GLU:HA	1:C:205:VAL:O	2.06	0.56
2:D:10:GLU:O	2:D:109:VAL:HA	2.05	0.56
2:F:7:SER:N	2:F:21:SER:OG	2.38	0.56
2:F:52:ILE:O	2:F:52(A):PRO:C	2.48	0.56
2:F:94:LYS:C	2:F:94:LYS:CD	2.78	0.56
2:P:73:GLU:H	2:P:73:GLU:CD	2.12	0.56
2:B:82(A):SER:O	2:B:82(B):SER:C	2.50	0.56
2:B:192:GLN:HG3	2:B:193:THR:N	2.20	0.56
1:C:153:ALA:HA	1:O:18:ARG:HB3	1.88	0.56
1:E:55:GLN:OE1	1:E:56:SER:N	2.37	0.56
1:G:61:ARG:NE	1:G:82:ASP:OD2	2.38	0.56
1:G:150:VAL:HG22	1:G:192:TYR:CD1	2.41	0.56
1:G:151:ASP:O	1:G:152:ASN:HB2	2.05	0.56
2:H:1:GLN:O	2:H:25:SER:O	2.24	0.56
1:O:182:SER:O	1:O:183:LYS:C	2.49	0.56
2:D:201:LYS:C	2:D:203:SER:H	2.14	0.55
1:G:11:LEU:HB3	1:G:104:LEU:HD23	1.88	0.55
2:H:7:SER:CB	2:H:21:SER:H	2.19	0.55
1:I:13:ALA:N	1:I:107:LYS:HB2	2.21	0.55
1:I:120:PRO:HD3	1:I:132:VAL:HG22	1.88	0.55
1:O:133:VAL:HG22	1:O:178:THR:HG23	1.87	0.55
1:A:167:ASP:O	1:A:171:SER:HA	2.06	0.55
1:A:169:LYS:HG3	1:A:170:ASP:H	1.71	0.55
1:C:83:PHE:HA	1:C:104:LEU:HB3	1.87	0.55
1:E:154:LEU:HD23	1:I:18:ARG:O	2.05	0.55
1:G:136:LEU:HD11	1:G:196:VAL:CG2	2.34	0.55
1:I:83:PHE:CE1	1:I:106:ILE:HG12	2.40	0.55
2:J:30:SER:O	2:J:53:VAL:HG23	2.06	0.55
1:K:30:SER:O	1:K:71:PHE:HZ	1.89	0.55
1:K:128:GLY:HA2	3:K:218:HOH:O	2.06	0.55
1:M:18:ARG:HB2	1:M:18:ARG:NH1	2.15	0.55
1:C:52:SER:HB2	3:C:220:HOH:O	2.06	0.55
1:E:26:SER:HB2	1:E:27:GLN:NE2	2.21	0.55
2:H:37:VAL:HG13	2:H:47:TRP:HA	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:168:ALA:HA	2:H:178:LEU:HB3	1.88	0.55
1:M:125:LEU:HD22	1:M:183:LYS:HG3	1.87	0.55
1:M:186:TYR:CE1	1:M:192:TYR:CE2	2.95	0.55
1:O:158:ASN:OD1	1:O:158:ASN:N	2.33	0.55
2:P:70:THR:O	2:P:78:THR:HG23	2.07	0.55
2:B:73:GLU:C	2:B:75:THR:N	2.62	0.55
2:D:33:ALA:HB3	2:D:95:GLY:HA3	1.87	0.55
1:E:42:LYS:O	1:E:43:VAL:C	2.48	0.55
1:E:210:ASN:O	1:E:211:ARG:C	2.50	0.55
1:G:110:VAL:CG1	1:G:111:ALA:N	2.69	0.55
2:H:124:LEU:HG	2:H:141:LEU:N	2.19	0.55
1:I:11:LEU:O	1:I:104:LEU:HA	2.06	0.55
1:K:118:PHE:CD1	2:L:124:LEU:HB3	2.41	0.55
2:L:6:GLN:NE2	2:L:90:TYR:O	2.40	0.55
2:L:115:SER:O	2:L:117:LYS:HG2	2.06	0.55
2:L:165:THR:O	2:L:165:THR:HG22	2.05	0.55
1:O:61:ARG:NE	1:O:79:GLN:HG3	2.21	0.55
2:B:94:LYS:C	2:B:94:LYS:HD3	2.31	0.55
2:D:39:GLN:NE2	2:D:44:GLY:HA2	2.21	0.55
2:D:138:LEU:CD1	2:D:138:LEU:C	2.80	0.55
1:E:38:GLN:HB3	1:E:85:THR:HG22	1.89	0.55
2:J:123:PRO:HG3	2:J:209:LYS:HZ1	1.70	0.55
1:K:4:MET:CB	1:K:98:PHE:O	2.53	0.55
1:K:170:ASP:OD1	1:K:170:ASP:N	2.40	0.55
2:N:20:VAL:HG12	2:N:36:TRP:CH2	2.42	0.55
1:A:135:LEU:HD13	2:B:181:VAL:HG11	1.89	0.55
2:B:53:VAL:C	2:B:54:PHE:CD1	2.85	0.55
2:F:85:GLU:CD	2:F:85:GLU:N	2.64	0.55
2:H:164:HIS:O	2:H:180:SER:HA	2.07	0.55
1:I:13:ALA:H	1:I:107:LYS:HB2	1.71	0.55
2:J:155:ASN:O	2:J:158:ALA:HB3	2.06	0.55
1:E:119:PRO:HB3	1:E:209:PHE:CE1	2.42	0.55
1:E:205:VAL:HG12	1:E:206:THR:N	2.22	0.55
1:G:142:ARG:O	1:G:144:ALA:N	2.40	0.55
1:G:158:ASN:HD22	1:K:22:THR:HG21	1.71	0.55
2:H:10:GLU:O	2:H:109:VAL:HA	2.06	0.55
2:J:82:LEU:HD23	2:J:82(C):LEU:CD2	2.37	0.55
1:O:48:ILE:HD13	1:O:64:GLY:HA3	1.88	0.55
1:C:62:PHE:CD1	1:C:62:PHE:N	2.73	0.55
1:C:124:GLN:HB2	3:C:223:HOH:O	2.07	0.55
1:G:110:VAL:HG12	1:G:111:ALA:N	2.20	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:118:PHE:CE2	2:H:130:SER:HB3	2.42	0.55
2:H:119:PRO:HD3	2:H:200:HIS:HD2	1.72	0.55
1:I:79:GLN:HB2	1:I:82:ASP:OD2	2.06	0.55
1:I:150:VAL:HG23	1:I:155:GLN:HG3	1.89	0.55
2:B:14:PRO:HG2	2:B:113:SER:N	2.22	0.55
2:D:32:TYR:HB2	2:D:34:ILE:CD1	2.37	0.55
2:D:192:GLN:HG2	2:D:194:TYR:CZ	2.41	0.55
2:F:71:ALA:HB2	2:F:78:THR:HG23	1.87	0.55
1:M:29:ILE:CG2	1:M:90:GLN:HG3	2.37	0.55
1:M:43:VAL:HG11	2:N:103:TRP:HB2	1.88	0.55
2:P:155:ASN:HB2	2:P:158:ALA:HB3	1.89	0.55
2:B:51:ILE:CG1	2:B:52:ILE:H	2.20	0.55
2:D:61:GLN:O	2:D:64:GLN:HB2	2.07	0.55
1:E:199:GLN:OE1	1:I:199:GLN:HA	2.06	0.55
1:G:132:VAL:HG12	1:G:148:TRP:CH2	2.42	0.55
1:I:20:THR:HG23	1:I:74:THR:OG1	2.07	0.55
1:I:142:ARG:HB2	1:I:173:TYR:CE2	2.42	0.55
2:N:30:SER:HB2	2:N:53:VAL:HG23	1.89	0.55
2:P:29:PHE:HB3	2:P:76:SER:CB	2.32	0.55
2:P:185:PRO:O	2:P:186:SER:C	2.50	0.55
1:I:195:GLU:HA	1:I:205:VAL:O	2.07	0.54
2:J:4:LEU:HD13	2:J:22:CYS:SG	2.47	0.54
2:J:48:MET:O	2:J:60:ALA:HB2	2.06	0.54
2:J:170:LEU:HD12	2:J:171:GLN:N	2.22	0.54
1:K:179:LEU:HD12	1:K:180:THR:H	1.71	0.54
2:N:121:VAL:HA	2:N:141:LEU:O	2.06	0.54
1:O:203:SER:O	1:O:204:PRO:O	2.24	0.54
2:P:19:LYS:HA	2:P:81:GLU:HA	1.87	0.54
2:B:19:LYS:HE2	2:B:79:TYR:CG	2.41	0.54
2:B:87:THR:O	2:B:88:ALA:HB2	2.08	0.54
2:D:122:PHE:HB2	2:D:141:LEU:HB3	1.89	0.54
2:D:184:VAL:HB	2:D:185:PRO:CD	2.37	0.54
2:F:18:VAL:HG22	2:F:19:LYS:N	2.22	0.54
1:K:54:LEU:HD12	1:K:55:GLN:H	1.72	0.54
2:L:6:GLN:N	2:L:105:GLN:HE22	2.05	0.54
1:M:159:SER:HA	1:M:178:THR:O	2.08	0.54
2:N:117:LYS:NZ	2:N:144:ASP:HB2	2.22	0.54
2:F:94:LYS:HE2	2:F:95:GLY:CA	2.37	0.54
1:G:35:TRP:HB2	1:G:48:ILE:HB	1.89	0.54
1:I:95:SER:O	1:I:96:HIS:HD2	1.91	0.54
1:K:12:SER:HA	1:K:105:GLU:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:8:GLY:O	2:L:9:ALA:C	2.51	0.54
2:L:163:VAL:CG2	2:L:182:VAL:HB	2.30	0.54
2:N:163:VAL:HG12	2:N:164:HIS:H	1.72	0.54
1:E:124:GLN:HE22	1:E:131:SER:HB2	1.73	0.54
1:E:168:SER:OG	1:E:169:LYS:N	2.40	0.54
2:F:52(A):PRO:O	2:F:53:VAL:C	2.50	0.54
1:I:86:TYR:O	1:I:101:GLY:HA2	2.07	0.54
1:K:11:LEU:HB3	1:K:104:LEU:CD2	2.38	0.54
2:N:64:GLN:N	3:N:229:HOH:O	2.40	0.54
2:B:150:VAL:HG13	2:B:150:VAL:O	2.06	0.54
1:E:12:SER:HA	1:E:105:GLU:HG3	1.89	0.54
1:G:175:LEU:C	1:G:175:LEU:CD2	2.78	0.54
1:I:4:MET:SD	1:I:90:GLN:HB2	2.48	0.54
2:L:1:GLN:CD	2:L:1:GLN:N	2.66	0.54
2:L:29:PHE:HA	2:L:32:TYR:CD1	2.42	0.54
2:N:201:LYS:O	2:N:203:SER:N	2.41	0.54
1:A:119:PRO:HB3	1:A:209:PHE:CZ	2.43	0.54
2:D:52(A):PRO:O	2:D:53:VAL:C	2.50	0.54
2:J:105:GLN:HA	3:J:219:HOH:O	2.08	0.54
2:L:7:SER:OG	2:L:20:VAL:HG13	2.08	0.54
2:P:51:ILE:CB	2:P:57:ALA:HB2	2.29	0.54
2:B:19:LYS:HE2	2:B:79:TYR:HB3	1.90	0.54
2:B:194:TYR:C	2:B:195:ILE:HD12	2.33	0.54
2:D:29:PHE:CD1	2:D:30:SER:N	2.76	0.54
1:E:124:GLN:HB2	3:E:216:HOH:O	2.07	0.54
2:H:191:THR:OG1	2:H:192:GLN:N	2.41	0.54
1:K:37:GLN:HG3	1:K:86:TYR:CE2	2.43	0.54
1:M:28:SER:HA	1:M:69:THR:HG22	1.90	0.54
2:H:119:PRO:CB	2:H:145:TYR:HB3	2.33	0.54
2:H:141:LEU:HD11	2:H:143:LYS:HB2	1.90	0.54
1:I:32:TYR:CD1	1:I:92:TYR:HD1	2.25	0.54
1:K:34:ASN:HD22	1:K:89:GLN:HE22	1.55	0.54
1:K:52:SER:O	1:K:54:LEU:N	2.40	0.54
1:M:24:ARG:HA	1:M:69:THR:O	2.08	0.54
2:N:201:LYS:C	2:N:203:SER:N	2.65	0.54
1:A:136:LEU:HD13	1:A:175:LEU:HD22	1.90	0.54
1:E:61:ARG:O	1:E:75:ILE:HA	2.07	0.54
1:E:179:LEU:HD11	1:E:181:LEU:HD21	1.89	0.54
2:F:201:LYS:H	2:F:202:PRO:CD	2.21	0.54
1:G:32:TYR:HB3	1:G:91:SER:HB2	1.90	0.54
1:G:118:PHE:N	1:G:118:PHE:HD2	2.04	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:158:ASN:O	1:G:179:LEU:HD12	2.07	0.54
2:J:77:THR:HB	2:J:79:TYR:HE1	1.73	0.54
1:M:19:VAL:CG1	1:M:20:THR:H	2.20	0.54
2:P:141:LEU:CD1	2:P:179:SER:HB3	2.38	0.54
1:C:148:TRP:CG	1:C:179:LEU:HD12	2.43	0.54
2:D:210:LYS:HE2	2:D:212:GLU:OE2	2.08	0.54
2:F:105:GLN:CG	2:F:106:GLY:H	2.21	0.54
1:G:136:LEU:HB3	1:G:139:PHE:CE1	2.43	0.54
2:H:3:GLN:OE1	2:H:5:LEU:HG	2.08	0.54
2:J:39:GLN:NE2	2:J:45:LEU:HD23	2.22	0.54
2:J:39:GLN:HE21	2:J:45:LEU:HD23	1.72	0.54
1:K:164:THR:CG2	1:K:174:SER:N	2.67	0.54
2:N:171:GLN:NE2	2:N:177:SER:HB2	2.23	0.54
1:C:140:TYR:CD2	1:C:173:TYR:HE2	2.26	0.53
1:I:151:ASP:O	1:I:152:ASN:C	2.51	0.53
1:I:185:ASP:O	1:I:188:LYS:HB2	2.08	0.53
2:J:94:LYS:CG	2:J:95:GLY:N	2.71	0.53
1:K:126:LYS:HA	1:K:126:LYS:HE3	1.90	0.53
2:L:87:THR:HG23	2:L:109:VAL:O	2.08	0.53
1:M:112:ALA:HB2	1:M:200:GLY:C	2.33	0.53
2:N:31:SER:O	2:N:32:TYR:C	2.51	0.53
2:N:143:LYS:HA	2:N:177:SER:OG	2.08	0.53
1:C:125:LEU:CD2	1:C:130:ALA:HB2	2.38	0.53
1:C:140:TYR:HD2	1:C:173:TYR:HE2	1.55	0.53
1:G:2:ILE:HD13	3:H:236:HOH:O	2.07	0.53
2:J:113:SER:O	2:J:114:ALA:C	2.51	0.53
2:L:73:GLU:OE2	2:L:73:GLU:N	2.36	0.53
2:P:29:PHE:CE1	2:P:52(A):PRO:HB3	2.43	0.53
2:B:154:TRP:O	2:B:155:ASN:C	2.51	0.53
2:D:52:ILE:O	2:D:53:VAL:N	2.41	0.53
1:G:55:GLN:CD	1:G:56:SER:N	2.66	0.53
1:G:124:GLN:O	1:G:127:SER:N	2.40	0.53
2:H:145:TYR:CE2	2:H:177:SER:HA	2.43	0.53
2:N:158:ALA:O	2:N:160:THR:HG23	2.09	0.53
1:A:125:LEU:HD23	1:A:130:ALA:HB2	1.89	0.53
1:E:150:VAL:C	1:E:152:ASN:H	2.15	0.53
2:J:83:ARG:CB	2:J:85:GLU:HG3	2.28	0.53
2:N:30:SER:HB2	2:N:53:VAL:CG2	2.38	0.53
1:O:18:ARG:NH2	1:O:76:SER:HB2	2.23	0.53
2:P:134:GLY:O	2:P:186:SER:N	2.40	0.53
1:A:120:PRO:HD3	1:A:132:VAL:HG22	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1:GLN:O	2:F:2:VAL:C	2.51	0.53
1:G:142:ARG:HG3	1:G:143:GLU:N	2.24	0.53
1:K:146:VAL:HG11	1:K:177:SER:CB	2.38	0.53
1:M:151:ASP:OD2	1:M:189:HIS:HB3	2.08	0.53
2:B:137:ALA:CB	2:B:183:THR:HA	2.38	0.53
2:D:197:ASN:ND2	2:D:208:ASP:CG	2.66	0.53
1:E:4:MET:HE3	1:E:23:CYS:SG	2.49	0.53
1:G:148:TRP:CE3	1:G:194:CYS:HB3	2.44	0.53
2:H:176:TYR:N	2:H:176:TYR:HD2	2.07	0.53
1:I:50:ALA:O	1:I:51:ALA:CB	2.57	0.53
2:J:156:SER:C	2:J:158:ALA:H	2.16	0.53
2:L:155:ASN:OD1	2:L:194:TYR:HA	2.09	0.53
1:M:26:SER:HB2	1:M:27:GLN:HE22	1.72	0.53
2:N:194:TYR:C	2:N:195:ILE:HG13	2.33	0.53
1:A:90:GLN:C	1:A:90:GLN:OE1	2.52	0.53
1:A:198:HIS:O	1:M:199:GLN:NE2	2.26	0.53
2:B:40:ALA:HA	2:B:88:ALA:HB2	1.90	0.53
2:B:138:LEU:H	2:B:138:LEU:CD2	2.16	0.53
2:D:71:ALA:HA	2:D:77:THR:O	2.09	0.53
2:F:24:ALA:O	2:F:26:GLY:N	2.38	0.53
2:H:51:ILE:HG23	2:H:51:ILE:O	2.09	0.53
2:H:131:THR:HB	2:H:135:THR:O	2.09	0.53
1:I:185:ASP:HA	1:I:188:LYS:CD	2.33	0.53
2:J:64:GLN:O	2:J:66:ARG:N	2.42	0.53
2:J:67:VAL:CG2	2:J:80:MET:SD	2.97	0.53
2:J:152:VAL:HG22	2:J:198:VAL:HG22	1.91	0.53
2:L:145:TYR:O	2:L:176:TYR:HB2	2.08	0.53
2:P:29:PHE:CE1	2:P:73:GLU:HG3	2.44	0.53
1:C:142:ARG:HD2	3:C:225:HOH:O	2.09	0.53
1:C:145:LYS:NZ	1:C:147:GLN:HE21	2.06	0.53
2:D:201:LYS:O	2:D:203:SER:N	2.42	0.53
1:E:122:ASP:O	1:E:126:LYS:HD2	2.09	0.53
1:G:130:ALA:O	1:G:180:THR:HA	2.08	0.53
2:H:7:SER:O	2:H:107:THR:HG23	2.08	0.53
1:I:54:LEU:HD11	1:I:58:VAL:CB	2.39	0.53
2:J:153:SER:OG	2:J:197:ASN:HB2	2.09	0.53
2:L:93:ALA:HB1	2:L:100(L):MET:HB3	1.91	0.53
1:C:12:SER:OG	1:C:105:GLU:OE1	2.22	0.53
1:C:170:ASP:OD2	1:C:172:THR:OG1	2.24	0.53
2:F:30:SER:HA	2:F:52(A):PRO:HB2	1.91	0.53
2:H:38:ARG:HB3	2:H:90:TYR:CE2	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:36:TRP:CD1	2:L:69:ILE:HD13	2.43	0.53
1:A:61:ARG:HA	1:A:76:SER:HB3	1.91	0.53
1:A:124:GLN:OE1	1:A:130:ALA:HA	2.09	0.53
1:A:143:GLU:OE2	1:A:143:GLU:N	2.41	0.53
2:B:119:PRO:HB3	2:B:145:TYR:HD2	1.74	0.53
1:C:135:LEU:HD12	1:C:175:LEU:O	2.09	0.53
1:E:170:ASP:C	1:E:170:ASP:OD2	2.51	0.53
1:G:39:LYS:HD3	1:G:84:ALA:CB	2.39	0.53
2:H:138:LEU:HD12	2:H:138:LEU:C	2.34	0.53
2:J:207:VAL:CG1	2:J:208:ASP:N	2.72	0.53
1:M:158:ASN:OD1	1:M:158:ASN:N	2.42	0.53
2:N:206:LYS:C	2:N:207:VAL:CG2	2.82	0.53
1:O:61:ARG:HG3	1:O:62:PHE:CD1	2.44	0.53
1:O:67:SER:N	1:O:70:ASP:O	2.41	0.53
1:O:108:ARG:HH11	1:O:172:THR:HG22	1.74	0.53
2:P:203:SER:C	2:P:205:THR:N	2.67	0.53
2:B:53:VAL:HG23	2:B:54:PHE:CD1	2.43	0.52
2:B:186:SER:O	2:B:189:LEU:HG	2.09	0.52
1:C:164:THR:HG22	1:C:173:TYR:HA	1.92	0.52
2:F:145:TYR:HD2	2:F:145:TYR:N	2.07	0.52
2:H:53:VAL:HB	2:H:54:PHE:CD1	2.44	0.52
2:H:208:ASP:O	2:H:209:LYS:HB2	2.08	0.52
1:K:202:SER:O	1:K:203:SER:HB3	2.08	0.52
2:N:116:THR:HG22	2:N:116:THR:O	2.09	0.52
2:P:40:ALA:HB3	2:P:43:GLN:CG	2.40	0.52
1:A:90:GLN:HE22	1:A:93:SER:CB	2.22	0.52
1:A:124:GLN:CD	1:A:131:SER:H	2.18	0.52
2:D:83:ARG:HD2	2:P:61:GLN:OE1	2.08	0.52
2:F:34:ILE:HG21	2:F:78:THR:HG21	1.92	0.52
1:I:12:SER:HB3	1:I:107:LYS:HG3	1.90	0.52
2:J:35:SER:OG	2:J:47:TRP:NE1	2.42	0.52
2:J:141:LEU:C	2:J:141:LEU:HD12	2.34	0.52
2:J:199:ASN:HD22	2:J:200:HIS:N	2.08	0.52
1:K:145:LYS:HD3	1:K:197:THR:HG21	1.90	0.52
2:L:193:THR:CG2	2:L:195:ILE:HD11	2.40	0.52
2:N:159:LEU:CD2	2:N:182:VAL:HG21	2.39	0.52
1:A:199:GLN:HB2	3:A:219:HOH:O	2.08	0.52
2:B:52(A):PRO:C	2:B:54:PHE:H	2.16	0.52
1:C:163:VAL:HG12	1:C:164:THR:H	1.75	0.52
1:E:49:TYR:H	1:E:49:TYR:HD2	1.57	0.52
2:F:62:LYS:HG3	2:F:63:PHE:CD1	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:105:GLN:CG	2:F:106:GLY:N	2.72	0.52
1:G:124:GLN:OE1	1:G:131:SER:HB2	2.09	0.52
1:G:180:THR:C	1:G:181:LEU:HD12	2.34	0.52
1:K:212:GLY:C	1:K:213:GLU:HG3	2.35	0.52
2:L:66:ARG:HG3	2:L:82:LEU:HD12	1.90	0.52
1:M:93:SER:OG	1:M:94:THR:N	2.36	0.52
2:N:6:GLN:OE1	2:N:91:PHE:HA	2.09	0.52
2:P:17:SER:O	2:P:18:VAL:HB	2.09	0.52
1:A:164:THR:HG21	2:B:164:HIS:CD2	2.45	0.52
2:B:2:VAL:HG23	2:B:26:GLY:HA3	1.91	0.52
2:B:51:ILE:CG1	2:B:52:ILE:N	2.72	0.52
1:E:110:VAL:CG1	1:E:111:ALA:N	2.73	0.52
2:F:1:GLN:HG2	2:N:3:GLN:NE2	2.24	0.52
2:F:13:LYS:CD	2:F:113:SER:HA	2.35	0.52
2:H:124:LEU:CD2	2:H:141:LEU:HB2	2.24	0.52
2:J:163:VAL:HG12	2:J:164:HIS:N	2.24	0.52
1:K:195:GLU:CG	1:K:204:PRO:HB3	2.39	0.52
2:N:4:LEU:HD23	2:N:4:LEU:N	2.24	0.52
1:E:199:GLN:N	1:I:199:GLN:HE22	2.07	0.52
2:F:51:ILE:O	2:F:52(A):PRO:HD3	2.09	0.52
2:F:184:VAL:HB	2:F:185:PRO:CD	2.39	0.52
1:G:185:ASP:O	1:G:188:LYS:HB2	2.09	0.52
1:I:32:TYR:CB	1:I:91:SER:HB2	2.20	0.52
1:I:49:TYR:O	1:I:50:ALA:HB3	2.10	0.52
2:J:62:LYS:O	2:J:64:GLN:N	2.43	0.52
1:K:136:LEU:HD11	1:K:196:VAL:CG2	2.40	0.52
1:K:190:LYS:HG2	1:K:210:ASN:CB	2.27	0.52
2:N:20:VAL:HG12	2:N:36:TRP:HH2	1.75	0.52
1:A:210:ASN:O	1:A:213:GLU:HG3	2.10	0.52
1:C:12:SER:HA	1:C:105:GLU:CG	2.37	0.52
2:D:12:LYS:CG	2:D:18:VAL:HB	2.30	0.52
1:E:116:PHE:HD2	2:F:130:SER:HA	1.73	0.52
1:E:143:GLU:H	1:E:143:GLU:CD	2.18	0.52
1:G:124:GLN:HE22	1:G:131:SER:CB	2.22	0.52
2:J:3:GLN:HB2	3:J:224:HOH:O	2.10	0.52
2:J:64:GLN:C	2:J:66:ARG:H	2.18	0.52
1:K:185:ASP:O	1:K:188:LYS:HB2	2.09	0.52
1:M:66:GLY:O	1:M:71:PHE:CE2	2.63	0.52
1:M:95:SER:HA	2:N:47:TRP:CZ3	2.45	0.52
2:P:93:ALA:HB1	2:P:100(L):MET:HB3	1.91	0.52
1:A:150:VAL:HG23	1:A:155:GLN:CG	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2:ILE:HG22	1:C:3:GLN:N	2.25	0.52
2:F:103:TRP:N	2:F:103:TRP:CD1	2.78	0.52
1:G:154:LEU:C	1:G:155:GLN:HE21	2.16	0.52
1:G:159:SER:HB3	1:G:179:LEU:HD13	1.92	0.52
1:G:181:LEU:HD12	1:G:181:LEU:N	2.25	0.52
2:H:123:PRO:HD3	2:H:209:LYS:HE2	1.91	0.52
2:H:192:GLN:NE2	2:H:193:THR:N	2.58	0.52
2:J:12:LYS:HZ2	2:J:18:VAL:HA	1.73	0.52
1:M:110:VAL:HG22	1:M:141:PRO:HD3	1.90	0.52
1:M:151:ASP:C	1:M:153:ALA:N	2.68	0.52
1:A:39:LYS:HE3	1:A:81:GLU:O	2.10	0.52
1:A:40:PRO:C	1:A:42:LYS:H	2.18	0.52
1:A:71:PHE:N	1:A:71:PHE:CD1	2.78	0.52
1:A:151:ASP:OD2	1:A:189:HIS:HA	2.10	0.52
2:F:145:TYR:CE2	2:F:176:TYR:HB2	2.45	0.52
1:G:39:LYS:NZ	1:G:81:GLU:O	2.42	0.52
1:G:162:SER:OG	2:H:166:PHE:HB3	2.10	0.52
2:H:112:ALA:C	2:H:114:ALA:H	2.18	0.52
1:M:89:GLN:HE21	1:M:96:HIS:HB3	1.75	0.52
1:O:14:SER:O	1:O:15:VAL:O	2.27	0.52
1:O:93:SER:OG	1:O:94:THR:N	2.40	0.52
1:A:135:LEU:HD13	2:B:181:VAL:HG21	1.91	0.52
1:A:182:SER:O	1:A:183:LYS:C	2.52	0.52
2:B:201:LYS:N	2:B:202:PRO:CD	2.73	0.52
1:C:17:ASP:O	1:C:77:SER:HA	2.10	0.52
2:D:62:LYS:HE2	2:D:63:PHE:CE1	2.45	0.52
2:F:121:VAL:CG2	2:F:198:VAL:HG11	2.40	0.52
2:F:163:VAL:HG12	2:F:164:HIS:N	2.25	0.52
1:I:37:GLN:HG2	1:I:38:GLN:N	2.25	0.52
2:J:64:GLN:CB	2:L:204:ASN:OD1	2.55	0.52
1:K:34:ASN:HD22	1:K:89:GLN:NE2	2.08	0.52
1:O:138:ASN:HD22	1:O:138:ASN:H	1.57	0.52
2:P:31:SER:O	2:P:32:TYR:C	2.52	0.52
1:A:61:ARG:CB	1:A:76:SER:OG	2.58	0.52
1:A:116:PHE:HD1	1:A:135:LEU:HD23	1.70	0.52
1:A:211:ARG:HB2	1:A:211:ARG:NH1	2.10	0.52
2:D:36:TRP:CD2	2:D:80:MET:HB2	2.45	0.52
2:H:23:LYS:N	2:H:77:THR:HG23	2.25	0.52
2:H:59:TYR:O	2:H:64:GLN:NE2	2.43	0.52
1:O:108:ARG:NH1	1:O:172:THR:HG22	2.24	0.52
1:A:18:ARG:NH1	1:A:76:SER:O	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:52(A):PRO:C	2:B:54:PHE:N	2.67	0.51
2:B:137:ALA:HB2	2:B:183:THR:HA	1.92	0.51
2:D:113:SER:O	2:D:114:ALA:C	2.53	0.51
2:D:188:SER:O	2:D:189:LEU:C	2.53	0.51
1:E:18:ARG:NH1	1:E:76:SER:CA	2.72	0.51
2:F:125:ALA:HB1	2:F:213:PRO:O	2.10	0.51
1:I:195:GLU:HG2	1:I:196:VAL:N	2.23	0.51
2:J:145:TYR:O	2:J:146:PHE:CB	2.57	0.51
1:K:33:LEU:HG	1:K:71:PHE:CB	2.39	0.51
1:M:39:LYS:HG2	1:M:84:ALA:CB	2.38	0.51
1:O:15:VAL:HG13	1:O:78:LEU:O	2.09	0.51
1:O:209:PHE:C	1:O:209:PHE:CD2	2.87	0.51
1:A:164:THR:HG21	2:B:164:HIS:HD2	1.75	0.51
1:G:138:ASN:HB3	1:G:172:THR:HG21	1.92	0.51
1:G:211:ARG:HG2	1:G:211:ARG:HH11	1.74	0.51
1:E:30:SER:OG	1:E:31:SER:N	2.38	0.51
1:G:113:PRO:HD3	1:G:198:HIS:ND1	2.25	0.51
1:G:169:LYS:HG3	1:G:170:ASP:H	1.76	0.51
2:H:14:PRO:HA	2:H:82(C):LEU:O	2.11	0.51
2:H:95:GLY:HA2	2:H:101:ASP:OD2	2.09	0.51
1:I:90:GLN:OE1	1:I:90:GLN:O	2.28	0.51
1:I:184:ALA:HB1	1:I:188:LYS:CE	2.40	0.51
2:J:119:PRO:HB2	2:J:142:VAL:HG13	1.92	0.51
2:L:40:ALA:HA	2:L:88:ALA:CB	2.40	0.51
2:N:165:THR:HG23	2:N:180:SER:HB2	1.92	0.51
1:A:208:SER:O	2:B:129:LYS:HD3	2.11	0.51
2:B:131:THR:HG22	2:B:136:ALA:HB2	1.90	0.51
2:F:18:VAL:HG12	2:F:82(C):LEU:HD11	1.92	0.51
2:H:32:TYR:CD2	2:H:94:LYS:HE3	2.46	0.51
1:K:182:SER:O	1:K:183:LYS:C	2.52	0.51
2:L:18:VAL:O	2:L:81:GLU:HG3	2.11	0.51
2:L:127:SER:OG	2:L:129:LYS:HB2	2.10	0.51
2:L:164:HIS:HB2	2:L:181:VAL:HG23	1.92	0.51
2:N:94:LYS:HG2	2:N:95:GLY:N	2.26	0.51
2:N:94:LYS:O	2:N:100(L):MET:HA	2.11	0.51
1:O:36:TYR:CE2	1:O:46:LEU:HD13	2.45	0.51
1:A:117:ILE:O	1:A:117:ILE:CG2	2.57	0.51
1:C:90:GLN:HE22	1:C:97:THR:HB	1.75	0.51
1:C:136:LEU:HD12	1:C:136:LEU:N	2.25	0.51
1:E:24:ARG:HH12	1:I:158:ASN:HA	1.75	0.51
2:F:94:LYS:NZ	2:F:96:GLY:N	2.59	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:171:GLN:HE21	2:F:177:SER:HB2	1.74	0.51
1:I:15:VAL:C	1:I:17:ASP:H	2.18	0.51
2:J:34:ILE:HG22	2:J:35:SER:N	2.24	0.51
2:B:77:THR:CG2	2:B:78:THR:N	2.74	0.51
2:H:116:THR:CG2	2:H:117:LYS:N	2.73	0.51
1:K:62:PHE:CE2	1:K:75:ILE:HG12	2.46	0.51
1:K:122:ASP:O	1:K:126:LYS:HD2	2.11	0.51
2:L:11:VAL:HA	2:L:110:THR:O	2.11	0.51
2:L:40:ALA:O	2:L:43:GLN:HB2	2.11	0.51
2:L:145:TYR:HD1	2:L:200:HIS:CD2	2.29	0.51
1:O:130:ALA:O	1:O:180:THR:HG23	2.10	0.51
1:O:150:VAL:O	1:O:151:ASP:C	2.53	0.51
2:P:53:VAL:HG12	2:P:54:PHE:CD2	2.44	0.51
2:B:20:VAL:O	2:B:79:TYR:HA	2.11	0.51
2:D:63:PHE:HB3	2:D:67:VAL:CG1	2.41	0.51
1:G:32:TYR:CD1	1:G:32:TYR:N	2.79	0.51
1:I:61:ARG:NE	1:I:82:ASP:OD2	2.38	0.51
2:J:139:GLY:HA3	2:J:180:SER:O	2.11	0.51
1:O:33:LEU:HD22	1:O:34:ASN:H	1.75	0.51
1:O:205:VAL:O	1:O:205:VAL:HG12	2.09	0.51
1:A:39:LYS:CE	1:A:81:GLU:O	2.59	0.51
2:B:107:THR:HG22	2:B:109:VAL:HG23	1.92	0.51
2:F:4:LEU:HD13	2:F:92:CYS:O	2.10	0.51
1:G:117:ILE:HG21	1:G:207:LYS:HG3	1.93	0.51
2:H:193:THR:HG22	2:H:194:TYR:H	1.76	0.51
1:I:2:ILE:N	3:I:220:HOH:O	2.42	0.51
1:I:32:TYR:HB2	1:I:92:TYR:H	1.73	0.51
1:K:29:ILE:O	1:K:30:SER:CB	2.59	0.51
2:L:63:PHE:O	2:L:67:VAL:HG12	2.10	0.51
1:M:124:GLN:CD	1:M:131:SER:H	2.18	0.51
2:N:94:LYS:HG2	2:N:95:GLY:H	1.74	0.51
2:D:3:GLN:HG2	2:D:4:LEU:N	2.26	0.51
2:H:51:ILE:CB	2:H:57:ALA:HB2	2.37	0.51
1:I:48:ILE:HG21	1:I:64:GLY:HA3	1.91	0.51
1:I:136:LEU:HD12	1:I:136:LEU:N	2.26	0.51
1:M:19:VAL:CG1	1:M:20:THR:N	2.72	0.51
1:O:20:THR:HG23	1:O:72:THR:CG2	2.41	0.51
1:O:124:GLN:HG2	1:O:129:THR:O	2.11	0.51
1:A:184:ALA:HB1	1:A:188:LYS:HE3	1.92	0.51
2:B:19:LYS:HA	2:B:80:MET:O	2.11	0.51
1:I:81:GLU:OE1	1:I:81:GLU:N	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:90:TYR:CD1	2:J:90:TYR:N	2.79	0.51
2:L:123:PRO:HB2	2:L:211:VAL:HG22	1.92	0.51
1:O:112:ALA:HB1	1:O:201:LEU:HD21	1.92	0.51
1:C:78:LEU:HD21	1:C:104:LEU:HD11	1.92	0.50
1:C:154:LEU:H	1:C:154:LEU:CD2	2.23	0.50
1:G:186:TYR:C	1:G:188:LYS:N	2.64	0.50
2:D:42:GLY:C	2:D:43:GLN:OE1	2.54	0.50
2:F:35:SER:O	2:F:92:CYS:HA	2.10	0.50
2:H:12:LYS:HE3	2:H:18:VAL:HG23	1.93	0.50
2:H:162:GLY:O	2:H:182:VAL:HA	2.11	0.50
2:L:141:LEU:HD12	2:L:142:VAL:N	2.26	0.50
2:P:28:THR:O	2:P:30:SER:N	2.44	0.50
2:P:29:PHE:O	2:P:52(A):PRO:HG2	2.11	0.50
1:A:188:LYS:O	1:A:189:HIS:CG	2.64	0.50
1:G:63:SER:OG	1:G:74:THR:HB	2.10	0.50
1:G:197:THR:HG22	1:G:204:PRO:HG3	1.94	0.50
2:H:36:TRP:HB2	2:H:69:ILE:CD1	2.38	0.50
2:H:67:VAL:CG2	2:H:68:THR:N	2.74	0.50
2:L:24:ALA:HB3	2:L:76:SER:HB3	1.94	0.50
2:P:159:LEU:HD12	2:P:160:THR:N	2.26	0.50
1:C:136:LEU:HD11	1:C:146:VAL:HG21	1.92	0.50
1:C:145:LYS:HD3	1:C:197:THR:HG23	1.94	0.50
1:C:162:SER:OG	2:D:167:PRO:HD2	2.11	0.50
1:C:167:ASP:OD1	1:C:169:LYS:HG2	2.11	0.50
2:D:73:GLU:CD	2:D:73:GLU:H	2.19	0.50
2:D:159:LEU:HD12	2:D:160:THR:N	2.27	0.50
1:E:3:GLN:N	1:E:26:SER:OG	2.44	0.50
1:E:90:GLN:NE2	1:E:97:THR:OG1	2.43	0.50
1:G:91:SER:O	1:G:92:TYR:C	2.54	0.50
1:K:50:ALA:HB3	1:K:53:SER:OG	2.12	0.50
1:K:79:GLN:O	1:K:82:ASP:HB2	2.12	0.50
1:M:75:ILE:HD11	1:M:86:TYR:CE2	2.46	0.50
1:O:148:TRP:CE3	1:O:194:CYS:HB3	2.46	0.50
2:B:51:ILE:CG1	2:B:57:ALA:HB2	2.41	0.50
1:C:154:LEU:N	1:C:154:LEU:CD2	2.75	0.50
2:D:82:LEU:HG	2:D:82(C):LEU:CD2	2.41	0.50
1:E:154:LEU:HD21	1:I:17:ASP:HB3	1.93	0.50
1:G:161:GLU:HA	1:G:176:SER:O	2.11	0.50
2:H:62:LYS:HG3	2:H:63:PHE:HD1	1.76	0.50
1:K:169:LYS:HG3	1:K:170:ASP:OD1	2.12	0.50
1:O:11:LEU:HB3	1:O:104:LEU:CD2	2.38	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:94:THR:CG2	1:O:95:SER:H	2.25	0.50
1:A:158:ASN:CA	1:M:24:ARG:HH21	2.24	0.50
1:C:192:TYR:O	1:C:208:SER:HB2	2.11	0.50
1:E:36:TYR:CE2	1:E:46:LEU:HD13	2.47	0.50
1:G:154:LEU:HD22	1:G:154:LEU:N	2.27	0.50
2:J:73:GLU:O	2:J:76:SER:N	2.44	0.50
1:M:150:VAL:HG11	1:M:189:HIS:CD2	2.46	0.50
1:O:48:ILE:HD12	1:O:73:LEU:HD12	1.94	0.50
1:O:95:SER:HA	2:P:47:TRP:CZ3	2.47	0.50
1:A:118:PHE:HZ	2:B:137:ALA:O	1.95	0.50
2:D:27:GLY:O	2:D:29:PHE:N	2.45	0.50
2:F:24:ALA:HB2	2:F:29:PHE:HD2	1.76	0.50
2:F:145:TYR:N	2:F:145:TYR:CD2	2.77	0.50
2:F:201:LYS:H	2:F:202:PRO:HD3	1.76	0.50
1:G:35:TRP:CZ3	1:G:88:CYS:HB3	2.47	0.50
1:G:89:GLN:HG3	1:G:98:PHE:CE2	2.46	0.50
2:H:48:MET:HE1	2:H:90:TYR:HE2	1.76	0.50
1:I:32:TYR:HB3	1:I:92:TYR:H	1.74	0.50
1:K:161:GLU:HA	1:K:177:SER:HA	1.93	0.50
2:L:11:VAL:HG22	2:L:110:THR:OG1	2.11	0.50
2:N:89:VAL:HG12	2:N:91:PHE:CE1	2.46	0.50
1:A:142:ARG:O	1:A:142:ARG:CG	2.60	0.50
2:B:2:VAL:HG21	2:B:32:TYR:CE1	2.47	0.50
1:E:113:PRO:HB3	1:E:139:PHE:CD1	2.47	0.50
2:F:11:VAL:HG22	2:F:110:THR:HB	1.94	0.50
2:F:34:ILE:HD12	2:F:94:LYS:HB2	1.94	0.50
1:I:119:PRO:HB3	1:I:209:PHE:CZ	2.47	0.50
2:N:119:PRO:HB2	2:N:142:VAL:CG1	2.36	0.50
1:C:212:GLY:O	1:C:213:GLU:CG	2.54	0.50
2:F:117:LYS:HE3	2:F:144:ASP:HB3	1.94	0.50
1:G:52:SER:HB3	1:G:65:SER:HA	1.94	0.50
2:H:150:VAL:HA	2:H:199:ASN:O	2.12	0.50
1:I:61:ARG:HH21	1:I:82:ASP:CG	2.19	0.50
1:K:96:HIS:HB2	2:L:47:TRP:CE2	2.47	0.50
1:O:86:TYR:O	1:O:101:GLY:HA2	2.12	0.50
2:P:19:LYS:HA	2:P:80:MET:O	2.12	0.50
2:P:38:ARG:CG	2:P:46:GLU:HB3	2.42	0.50
2:P:134:GLY:O	2:P:185:PRO:HA	2.12	0.50
2:P:189:LEU:HD13	2:P:213:PRO:CG	2.39	0.50
1:A:118:PHE:HE1	2:B:130:SER:OG	1.95	0.49
1:A:174:SER:O	2:B:166:PHE:HE2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:23:LYS:HD3	2:B:24:ALA:H	1.76	0.49
2:B:153:SER:O	2:B:197:ASN:HB2	2.12	0.49
1:E:190:LYS:O	1:E:210:ASN:HA	2.11	0.49
2:F:126:PRO:HB2	2:F:189:LEU:HD13	1.94	0.49
2:H:68:THR:HB	2:H:81:GLU:CB	2.21	0.49
1:I:140:TYR:O	1:I:198:HIS:HE1	1.94	0.49
2:J:72:ASP:O	2:J:76:SER:N	2.45	0.49
2:J:178:LEU:HD12	2:J:178:LEU:O	2.12	0.49
2:L:181:VAL:C	2:L:182:VAL:HG12	2.36	0.49
2:N:154:TRP:CZ3	2:N:196:CYS:CB	2.91	0.49
2:P:36:TRP:CD2	2:P:80:MET:HG3	2.47	0.49
1:A:164:THR:HG22	1:A:174:SER:H	1.77	0.49
2:B:124:LEU:HD21	2:B:141:LEU:HB2	1.94	0.49
1:E:15:VAL:HG11	1:E:80:PRO:HD3	1.94	0.49
2:F:68:THR:HB	2:F:81:GLU:CG	2.43	0.49
1:G:115:VAL:HG12	1:G:116:PHE:N	2.28	0.49
2:H:199:ASN:C	2:H:199:ASN:ND2	2.66	0.49
2:H:201:LYS:C	2:H:204:ASN:H	2.20	0.49
1:C:26:SER:O	1:C:27:GLN:NE2	2.46	0.49
2:D:48:MET:HE3	2:D:63:PHE:HE2	1.77	0.49
2:D:82:LEU:HG	2:D:82(C):LEU:HD23	1.93	0.49
1:G:14:SER:HB2	1:G:17:ASP:CG	2.37	0.49
2:J:168:ALA:HA	2:J:178:LEU:HB3	1.95	0.49
1:K:126:LYS:C	1:K:128:GLY:N	2.68	0.49
1:K:179:LEU:HD11	1:K:181:LEU:CD1	2.42	0.49
1:O:145:LYS:HB3	1:O:197:THR:OG1	2.13	0.49
1:A:87:TYR:CE2	2:B:44:GLY:HA2	2.47	0.49
2:B:89:VAL:HA	2:B:107:THR:O	2.12	0.49
1:C:29:ILE:O	1:C:31:SER:N	2.46	0.49
1:C:48:ILE:HD12	1:C:73:LEU:CD1	2.43	0.49
1:C:90:GLN:HE22	1:C:97:THR:N	2.11	0.49
2:D:6:GLN:CA	2:D:21:SER:O	2.57	0.49
2:D:24:ALA:HB3	2:D:76:SER:HB3	1.94	0.49
2:D:201:LYS:N	2:D:202:PRO:CD	2.75	0.49
1:E:34:ASN:OD1	1:E:49:TYR:CB	2.61	0.49
1:E:116:PHE:CD2	2:F:130:SER:HA	2.46	0.49
1:G:83:PHE:CE2	1:G:105:GLU:C	2.90	0.49
2:L:86:ASP:HB2	2:L:111:VAL:HG21	1.94	0.49
2:L:138:LEU:C	2:L:138:LEU:CD1	2.71	0.49
2:L:186:SER:C	2:L:188:SER:H	2.20	0.49
1:M:66:GLY:O	1:M:71:PHE:CD2	2.65	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:100(K):GLY:HA2	2:P:100(L):MET:HE3	1.93	0.49
2:P:159:LEU:HD12	2:P:160:THR:H	1.77	0.49
1:C:39:LYS:HG2	1:C:84:ALA:CB	2.42	0.49
2:D:119:PRO:HB3	2:D:145:TYR:CD2	2.47	0.49
2:H:6:GLN:OE1	2:H:104:GLY:HA3	2.13	0.49
1:K:33:LEU:HD13	1:K:33:LEU:C	2.37	0.49
1:K:48:ILE:HG12	1:K:54:LEU:HD13	1.94	0.49
2:L:34:ILE:N	2:L:34:ILE:CD1	2.76	0.49
2:N:3:GLN:O	2:N:4:LEU:HD23	2.13	0.49
2:N:85:GLU:O	2:N:87:THR:N	2.45	0.49
2:N:87:THR:HG23	2:N:110:THR:HA	1.93	0.49
2:N:171:GLN:HE21	2:N:177:SER:HB2	1.77	0.49
2:P:29:PHE:O	2:P:29:PHE:CG	2.66	0.49
2:P:53:VAL:C	2:P:54:PHE:CD2	2.90	0.49
1:A:48:ILE:HG22	1:A:49:TYR:H	1.78	0.49
1:C:155:GLN:O	1:C:156:SER:HB2	2.13	0.49
2:D:154:TRP:CZ2	2:D:196:CYS:HB3	2.47	0.49
1:K:126:LYS:C	1:K:128:GLY:H	2.21	0.49
1:C:54:LEU:HD23	1:C:55:GLN:N	2.28	0.49
2:F:131:THR:HG22	2:F:136:ALA:CB	2.42	0.49
2:F:163:VAL:CG1	2:F:164:HIS:N	2.75	0.49
1:G:79:GLN:HB3	1:G:81:GLU:OE1	2.13	0.49
1:G:130:ALA:N	1:G:181:LEU:O	2.46	0.49
1:I:148:TRP:CE3	1:I:194:CYS:HB3	2.47	0.49
2:J:22:CYS:HB3	2:J:78:THR:HB	1.94	0.49
1:K:118:PHE:HB3	2:L:124:LEU:HD22	1.95	0.49
2:L:112:ALA:HB3	2:L:146:PHE:HZ	1.77	0.49
2:L:152:VAL:HB	2:L:165:THR:OG1	2.13	0.49
2:B:2:VAL:CA	2:B:26:GLY:HA3	2.36	0.49
2:B:158:ALA:O	2:B:160:THR:HG23	2.13	0.49
2:D:152:VAL:HG12	2:D:153:SER:N	2.28	0.49
1:E:11:LEU:O	1:E:104:LEU:HA	2.12	0.49
1:E:123:GLU:OE2	1:E:123:GLU:N	2.28	0.49
1:E:143:GLU:CD	1:E:143:GLU:N	2.70	0.49
1:G:19:VAL:HG12	1:G:20:THR:N	2.28	0.49
2:H:176:TYR:HD2	2:H:176:TYR:H	1.60	0.49
1:I:83:PHE:CE2	1:I:106:ILE:HG12	2.47	0.49
2:J:18:VAL:HG12	2:J:82(C):LEU:HD11	1.94	0.49
2:P:72:ASP:C	2:P:74:ALA:H	2.20	0.49
1:A:48:ILE:CG2	1:A:49:TYR:N	2.75	0.49
1:A:65:SER:OG	3:A:214:HOH:O	1.96	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:ASN:O	1:A:211:ARG:O	2.31	0.49
2:B:82(A):SER:O	2:B:82(C):LEU:N	2.45	0.49
1:C:45:LYS:HD3	1:C:47:LEU:HD21	1.95	0.49
1:C:167:ASP:OD1	1:C:169:LYS:CG	2.61	0.49
1:E:75:ILE:HG21	1:E:78:LEU:HD12	1.93	0.49
2:F:37:VAL:HG13	2:F:46:GLU:O	2.13	0.49
1:G:206:THR:HG22	1:G:207:LYS:N	2.27	0.49
2:H:72:ASP:O	2:H:76:SER:N	2.46	0.49
2:H:112:ALA:C	2:H:114:ALA:N	2.70	0.49
2:J:38:ARG:NH1	2:J:86:ASP:HA	2.26	0.49
2:J:62:LYS:C	2:J:64:GLN:N	2.70	0.49
2:J:64:GLN:HB3	2:L:204:ASN:CG	2.38	0.49
2:J:199:ASN:C	2:J:199:ASN:ND2	2.68	0.49
1:K:107:LYS:O	1:K:108:ARG:HB3	2.12	0.49
1:K:145:LYS:HB3	1:K:197:THR:OG1	2.13	0.49
1:M:179:LEU:HD12	1:M:179:LEU:C	2.38	0.49
1:A:70:ASP:C	1:A:71:PHE:CD1	2.91	0.49
1:A:115:VAL:CG1	1:A:116:PHE:N	2.76	0.49
1:C:184:ALA:O	1:C:187:GLU:N	2.46	0.49
2:D:154:TRP:CH2	2:D:196:CYS:HB3	2.48	0.49
1:E:18:ARG:HH12	1:E:76:SER:CB	2.26	0.49
2:H:20:VAL:HG12	2:H:36:TRP:HH2	1.77	0.49
2:H:62:LYS:HG3	2:H:63:PHE:CD1	2.48	0.49
1:I:18:ARG:NH1	1:I:76:SER:OG	2.45	0.49
1:I:97:THR:CG2	1:I:98:PHE:N	2.75	0.49
2:J:94:LYS:HD3	2:J:102:VAL:HG11	1.94	0.49
2:J:163:VAL:N	2:J:182:VAL:HG23	2.28	0.49
2:L:205:THR:HG22	2:L:205:THR:O	2.13	0.49
1:M:40:PRO:C	1:M:42:LYS:H	2.21	0.49
2:N:206:LYS:O	2:N:207:VAL:HG22	2.13	0.49
1:O:33:LEU:O	1:O:51:ALA:N	2.32	0.49
2:B:48:MET:SD	2:B:80:MET:HE2	2.53	0.48
2:B:61:GLN:O	2:B:63:PHE:N	2.46	0.48
1:C:170:ASP:OD2	1:C:172:THR:CG2	2.60	0.48
2:D:29:PHE:C	2:D:31:SER:H	2.21	0.48
1:E:150:VAL:C	1:E:152:ASN:N	2.70	0.48
2:F:20:VAL:HG12	2:F:21:SER:N	2.28	0.48
2:J:188:SER:O	2:J:192:GLN:HB3	2.13	0.48
1:K:182:SER:O	1:K:185:ASP:N	2.46	0.48
2:L:80:MET:HE1	2:L:90:TYR:CD2	2.48	0.48
2:L:154:TRP:HB2	2:L:159:LEU:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:33:LEU:HD22	1:M:33:LEU:C	2.37	0.48
2:N:184:VAL:HG21	2:N:194:TYR:CZ	2.48	0.48
2:P:7:SER:HB3	2:P:20:VAL:HG13	1.93	0.48
2:P:178:LEU:C	2:P:178:LEU:HD12	2.38	0.48
1:A:135:LEU:HD11	2:B:181:VAL:HG21	1.94	0.48
2:B:51:ILE:CB	2:B:57:ALA:HB2	2.43	0.48
1:C:36:TYR:CE1	1:C:89:GLN:NE2	2.81	0.48
2:D:20:VAL:HB	2:D:36:TRP:CZ3	2.49	0.48
2:D:29:PHE:CE1	2:D:76:SER:HA	2.47	0.48
1:G:162:SER:O	1:G:175:LEU:HA	2.14	0.48
2:H:40:ALA:HB3	2:H:43:GLN:HB2	1.95	0.48
2:H:87:THR:O	2:H:88:ALA:HB2	2.12	0.48
2:H:195:ILE:O	2:H:196:CYS:C	2.56	0.48
1:I:148:TRP:CZ3	1:I:194:CYS:HB3	2.48	0.48
1:K:142:ARG:HH12	1:K:163:VAL:CG1	2.10	0.48
1:K:153:ALA:O	1:K:155:GLN:NE2	2.46	0.48
2:L:126:PRO:HG3	2:L:138:LEU:CB	2.36	0.48
2:L:130:SER:HB2	2:L:137:ALA:O	2.12	0.48
2:L:197:ASN:ND2	2:L:208:ASP:OD2	2.45	0.48
1:M:77:SER:O	1:M:78:LEU:C	2.55	0.48
1:O:94:THR:HG23	1:O:95:SER:H	1.77	0.48
2:B:35:SER:HG	2:B:47:TRP:CD1	2.31	0.48
1:C:124:GLN:CB	3:C:223:HOH:O	2.61	0.48
2:D:84:SER:C	2:D:86:ASP:H	2.22	0.48
2:L:6:GLN:CD	2:L:106:GLY:HA2	2.38	0.48
2:L:7:SER:HG	2:L:20:VAL:HG13	1.78	0.48
1:M:124:GLN:HG2	1:M:129:THR:O	2.12	0.48
1:O:4:MET:HE3	1:O:23:CYS:SG	2.52	0.48
1:O:8:PRO:O	1:O:102:THR:HA	2.12	0.48
2:P:155:ASN:CB	2:P:158:ALA:HB3	2.44	0.48
2:B:10:GLU:O	2:B:109:VAL:HA	2.14	0.48
2:D:210:LYS:CD	2:D:212:GLU:OE2	2.60	0.48
1:E:19:VAL:HG22	1:I:154:LEU:CB	2.43	0.48
1:E:90:GLN:NE2	1:E:95:SER:O	2.46	0.48
1:E:113:PRO:CA	1:E:139:PHE:HB3	2.44	0.48
2:F:121:VAL:HG11	2:F:198:VAL:CG2	2.36	0.48
2:F:121:VAL:HG21	2:F:198:VAL:HG11	1.95	0.48
1:G:29:ILE:O	1:G:30:SER:HB3	2.14	0.48
2:H:163:VAL:HA	2:H:181:VAL:O	2.13	0.48
2:L:117:LYS:O	2:L:145:TYR:HA	2.12	0.48
1:O:61:ARG:C	1:O:62:PHE:HD1	2.21	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:61:GLN:HA	2:P:64:GLN:CD	2.38	0.48
1:A:43:VAL:HG13	1:A:44:PRO:HD2	1.94	0.48
1:A:131:SER:OG	1:A:180:THR:HG23	2.13	0.48
2:B:17:SER:OG	2:B:18:VAL:N	2.44	0.48
2:B:200:HIS:CG	2:B:202:PRO:HD2	2.48	0.48
1:C:31:SER:O	1:C:33:LEU:N	2.43	0.48
1:C:74:THR:CG2	1:C:75:ILE:N	2.76	0.48
1:E:13:ALA:O	1:E:107:LYS:HB3	2.13	0.48
1:M:163:VAL:HG12	1:M:164:THR:H	1.79	0.48
2:N:203:SER:C	2:N:205:THR:H	2.22	0.48
1:A:193:ALA:HA	1:A:207:LYS:O	2.14	0.48
1:A:193:ALA:CB	1:A:208:SER:HB3	2.39	0.48
1:C:16:GLY:HA2	1:C:77:SER:OG	2.13	0.48
2:D:83:ARG:N	2:D:86:ASP:OD2	2.35	0.48
1:E:85:THR:HG21	1:E:87:TYR:CE1	2.48	0.48
2:F:1:GLN:HG2	2:N:3:GLN:HE22	1.78	0.48
2:H:18:VAL:HG12	2:H:82:LEU:HB3	1.96	0.48
2:H:127:SER:O	2:H:128:SER:C	2.56	0.48
1:I:85:THR:HA	1:I:102:THR:O	2.14	0.48
2:J:19:LYS:HE2	2:J:79:TYR:HB3	1.96	0.48
1:K:136:LEU:HD11	1:K:196:VAL:HG21	1.95	0.48
1:K:140:TYR:CD1	1:K:140:TYR:C	2.92	0.48
2:L:73:GLU:C	2:L:75:THR:N	2.69	0.48
2:N:52:ILE:C	2:N:52(A):PRO:O	2.51	0.48
2:P:51:ILE:HG12	2:P:52:ILE:N	2.28	0.48
2:B:73:GLU:OE1	2:B:73:GLU:N	2.46	0.48
2:B:192:GLN:CG	2:B:193:THR:N	2.77	0.48
1:C:49:TYR:CD2	1:C:53:SER:O	2.66	0.48
2:D:2:VAL:CG2	2:D:27:GLY:N	2.76	0.48
2:D:14:PRO:HD3	2:D:112:ALA:C	2.39	0.48
2:D:93:ALA:CB	2:D:100(L):MET:HG2	2.42	0.48
2:D:210:LYS:HD3	2:D:212:GLU:OE2	2.14	0.48
1:E:116:PHE:CD2	2:F:137:ALA:HB3	2.49	0.48
1:I:120:PRO:HG3	1:I:186:TYR:CZ	2.49	0.48
1:I:121:SER:O	1:I:122:ASP:C	2.55	0.48
2:J:6:GLN:NE2	2:J:91:PHE:HA	2.27	0.48
2:J:51:ILE:CG1	2:J:57:ALA:HB2	2.43	0.48
2:J:201:LYS:C	2:J:203:SER:N	2.72	0.48
2:L:83:ARG:HB3	2:L:85:GLU:OE1	2.13	0.48
2:L:185:PRO:O	2:L:188:SER:OG	2.31	0.48
1:M:117:ILE:HD12	1:M:208:SER:HA	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:204:ASN:OD1	2:P:64:GLN:CB	2.62	0.48
1:A:210:ASN:O	1:A:211:ARG:C	2.57	0.48
2:B:101:ASP:OD2	2:B:101:ASP:N	2.30	0.48
2:D:90:TYR:O	2:D:106:GLY:HA2	2.14	0.48
2:D:138:LEU:O	2:D:181:VAL:HB	2.14	0.48
1:E:25:ALA:O	1:E:26:SER:C	2.57	0.48
1:E:39:LYS:HB3	1:E:40:PRO:HD2	1.96	0.48
1:E:96:HIS:O	2:F:47:TRP:CG	2.66	0.48
2:F:111:VAL:O	2:F:111:VAL:CG1	2.56	0.48
2:F:153:SER:O	2:F:196:CYS:HA	2.14	0.48
2:F:188:SER:C	2:F:190:GLY:H	2.21	0.48
1:G:170:ASP:OD2	1:G:172:THR:HG23	2.13	0.48
2:H:187:SER:O	2:H:191:THR:HG21	2.14	0.48
2:H:199:ASN:ND2	2:H:200:HIS:N	2.41	0.48
1:I:203:SER:OG	1:I:204:PRO:HD2	2.14	0.48
1:K:195:GLU:HG3	1:K:204:PRO:HB3	1.96	0.48
2:L:13:LYS:O	2:L:14:PRO:O	2.32	0.48
2:L:67:VAL:HA	2:L:81:GLU:O	2.13	0.48
2:L:125:ALA:HA	2:L:126:PRO:HD3	1.79	0.48
2:L:164:HIS:HB2	2:L:181:VAL:HG22	1.95	0.48
1:M:81:GLU:H	1:M:81:GLU:CD	2.21	0.48
1:M:163:VAL:HG12	1:M:164:THR:N	2.28	0.48
1:O:188:LYS:O	1:O:189:HIS:CG	2.66	0.48
2:B:182:VAL:HG22	2:B:184:VAL:CG1	2.44	0.48
1:C:184:ALA:O	1:C:186:TYR:N	2.47	0.48
1:C:193:ALA:HB2	1:C:208:SER:CB	2.43	0.48
2:D:52:ILE:HG22	2:D:53:VAL:HG23	1.96	0.48
1:E:115:VAL:O	1:E:207:LYS:NZ	2.40	0.48
2:H:18:VAL:HB	2:H:82(C):LEU:HD11	1.96	0.48
2:H:116:THR:HG22	2:H:117:LYS:N	2.27	0.48
1:I:36:TYR:OH	2:J:100(L):MET:N	2.36	0.48
2:J:73:GLU:O	2:J:74:ALA:C	2.56	0.48
1:M:140:TYR:CD1	1:M:141:PRO:HA	2.48	0.48
2:N:123:PRO:HB3	2:N:211:VAL:HG22	1.96	0.48
1:O:40:PRO:O	1:O:41:GLY:C	2.57	0.48
1:A:55:GLN:OE1	1:A:55:GLN:HA	2.13	0.48
2:B:120:SER:O	2:B:121:VAL:CG2	2.62	0.48
2:B:141:LEU:HA	2:B:179:SER:HB3	1.96	0.48
1:C:30:SER:O	1:C:68:GLY:N	2.36	0.48
1:E:136:LEU:HD11	1:E:196:VAL:HG22	1.96	0.48
2:F:2:VAL:HA	2:F:26:GLY:HA3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:56:SER:O	2:F:57:ALA:C	2.55	0.48
1:G:147:GLN:CG	1:G:154:LEU:HD12	2.44	0.48
2:J:67:VAL:CG2	2:J:68:THR:N	2.77	0.48
2:L:82(A):SER:O	2:L:82(B):SER:CB	2.62	0.48
2:N:156:SER:CA	2:N:197:ASN:HD21	2.26	0.48
1:O:62:PHE:CD1	1:O:62:PHE:N	2.81	0.48
2:P:14:PRO:HD3	2:P:112:ALA:O	2.14	0.48
2:B:37:VAL:CG1	2:B:45:LEU:HB3	2.42	0.47
1:C:152:ASN:O	1:C:154:LEU:HD22	2.14	0.47
2:F:83:ARG:O	2:F:111:VAL:HG11	2.13	0.47
1:I:4:MET:HE3	1:I:23:CYS:SG	2.54	0.47
2:J:18:VAL:O	2:J:81:GLU:HA	2.14	0.47
1:K:32:TYR:N	1:K:32:TYR:CD1	2.81	0.47
1:K:195:GLU:O	1:K:195:GLU:HG2	2.12	0.47
2:L:85:GLU:CD	2:L:85:GLU:N	2.71	0.47
2:L:105:GLN:OE1	2:L:105:GLN:N	2.47	0.47
1:M:113:PRO:CD	1:M:198:HIS:HD1	2.13	0.47
2:B:95:GLY:HA2	2:B:101:ASP:OD2	2.14	0.47
2:B:203:SER:O	2:B:204:ASN:C	2.56	0.47
1:C:6:GLN:OE1	1:C:99:GLY:HA3	2.13	0.47
2:D:71:ALA:HB2	2:D:78:THR:CG2	2.41	0.47
2:F:143:LYS:HG2	2:F:144:ASP:OD2	2.14	0.47
1:G:55:GLN:CD	1:G:56:SER:H	2.22	0.47
2:H:201:LYS:H	2:H:202:PRO:CD	2.26	0.47
1:I:79:GLN:O	1:I:82:ASP:HB2	2.13	0.47
2:J:70:THR:O	2:J:78:THR:HA	2.13	0.47
2:J:101:ASP:C	2:J:101:ASP:OD1	2.55	0.47
1:K:32:TYR:N	1:K:32:TYR:HD1	2.12	0.47
1:K:62:PHE:CD2	1:K:75:ILE:HG23	2.50	0.47
1:K:197:THR:HG22	1:K:204:PRO:HG3	1.97	0.47
2:L:184:VAL:HB	2:L:185:PRO:HD2	1.96	0.47
2:N:122:PHE:HB2	2:N:141:LEU:HB3	1.97	0.47
1:O:29:ILE:HD11	1:O:71:PHE:CE1	2.49	0.47
2:P:6:GLN:NE2	2:P:106:GLY:CA	2.76	0.47
1:A:125:LEU:CD2	1:A:130:ALA:HB2	2.44	0.47
1:A:191:VAL:CG1	1:A:192:TYR:N	2.77	0.47
1:E:128:GLY:O	1:E:129:THR:HG23	2.14	0.47
2:J:60:ALA:O	2:J:61:GLN:C	2.57	0.47
1:K:4:MET:SD	1:K:25:ALA:HB2	2.54	0.47
1:K:62:PHE:CE2	1:K:75:ILE:HG23	2.49	0.47
1:K:183:LYS:HA	1:K:186:TYR:HB3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:18:VAL:CG2	2:L:19:LYS:N	2.77	0.47
1:M:108:ARG:HD2	1:M:171:SER:HB2	1.96	0.47
2:B:19:LYS:HE2	2:B:79:TYR:CB	2.44	0.47
2:B:40:ALA:HB3	2:B:43:GLN:NE2	2.20	0.47
1:C:151:ASP:OD2	1:C:189:HIS:HB3	2.14	0.47
1:E:26:SER:HB2	1:E:27:GLN:CD	2.39	0.47
1:E:123:GLU:H	1:E:123:GLU:CD	2.21	0.47
2:F:40:ALA:HB3	2:F:43:GLN:HG3	1.96	0.47
2:F:145:TYR:CE2	2:F:176:TYR:CB	2.97	0.47
1:G:29:ILE:HG12	1:G:68:GLY:O	2.15	0.47
1:G:34:ASN:N	1:G:34:ASN:ND2	2.62	0.47
1:I:49:TYR:C	1:I:51:ALA:H	2.20	0.47
1:I:96:HIS:HB2	2:J:47:TRP:CD1	2.50	0.47
1:M:4:MET:CB	1:M:99:GLY:CA	2.87	0.47
2:N:206:LYS:C	2:N:207:VAL:HG23	2.39	0.47
2:P:32:TYR:N	2:P:32:TYR:CD2	2.78	0.47
1:A:198:HIS:C	1:A:200:GLY:N	2.72	0.47
1:C:23:CYS:HB3	1:C:35:TRP:CH2	2.50	0.47
2:F:5:LEU:HB2	2:F:23:LYS:HB3	1.95	0.47
1:G:118:PHE:HE1	2:H:138:LEU:O	1.97	0.47
1:K:201:LEU:HD13	1:K:205:VAL:HG23	1.95	0.47
1:M:96:HIS:N	1:M:96:HIS:CD2	2.81	0.47
1:M:165:GLU:O	1:M:166:GLN:C	2.57	0.47
1:O:179:LEU:O	1:O:179:LEU:HG	2.14	0.47
1:O:187:GLU:HA	1:O:211:ARG:CZ	2.45	0.47
1:A:85:THR:OG1	1:A:103:LYS:HG3	2.14	0.47
1:A:175:LEU:HD23	1:A:176:SER:N	2.29	0.47
2:B:35:SER:O	2:B:92:CYS:HA	2.14	0.47
1:C:48:ILE:HD12	1:C:73:LEU:HD12	1.96	0.47
1:C:154:LEU:HD22	1:C:154:LEU:H	1.79	0.47
2:F:18:VAL:CG2	2:F:19:LYS:N	2.77	0.47
2:F:121:VAL:CG2	2:F:198:VAL:HG21	2.44	0.47
1:G:69:THR:O	1:G:71:PHE:HD1	1.98	0.47
1:G:83:PHE:HD2	1:G:104:LEU:O	1.97	0.47
2:J:51:ILE:HG13	2:J:57:ALA:HB2	1.95	0.47
2:J:151:THR:O	2:J:198:VAL:HG13	2.15	0.47
1:K:122:ASP:C	1:K:124:GLN:H	2.22	0.47
1:K:135:LEU:HD12	1:K:136:LEU:O	2.14	0.47
1:K:165:GLU:O	1:K:166:GLN:C	2.58	0.47
1:K:174:SER:O	2:L:166:PHE:HE2	1.98	0.47
1:K:210:ASN:HD22	1:K:210:ASN:H	1.52	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:89:GLN:NE2	1:M:96:HIS:HB3	2.28	0.47
2:P:16:SER:OG	2:P:17:SER:N	2.45	0.47
2:P:119:PRO:HD2	2:P:205:THR:HG21	1.96	0.47
2:P:203:SER:C	2:P:205:THR:H	2.22	0.47
1:A:6:GLN:HE22	1:A:101:GLY:HA2	1.80	0.47
1:A:135:LEU:HG	1:A:136:LEU:H	1.79	0.47
2:B:63:PHE:O	2:B:67:VAL:CG1	2.62	0.47
2:B:83:ARG:NH2	3:B:222:HOH:O	2.47	0.47
2:D:85:GLU:CD	2:D:85:GLU:N	2.70	0.47
1:E:187:GLU:HA	1:E:211:ARG:NE	2.29	0.47
2:F:29:PHE:HD1	2:F:30:SER:N	2.12	0.47
2:F:71:ALA:CA	2:F:77:THR:O	2.61	0.47
1:G:18:ARG:HD3	1:K:153:ALA:HB2	1.97	0.47
1:G:191:VAL:HG22	1:G:210:ASN:HD21	1.80	0.47
2:H:141:LEU:HD12	2:H:142:VAL:H	1.80	0.47
1:I:6:GLN:HB2	1:I:88:CYS:SG	2.55	0.47
2:J:203:SER:O	2:J:205:THR:N	2.48	0.47
2:L:136:ALA:HB1	2:L:189:LEU:HD11	1.97	0.47
1:M:142:ARG:NH1	1:M:163:VAL:HG11	2.29	0.47
1:O:103:LYS:C	1:O:104:LEU:HD23	2.40	0.47
1:O:140:TYR:O	1:O:198:HIS:CE1	2.68	0.47
1:O:184:ALA:O	1:O:188:LYS:HG3	2.15	0.47
2:D:5:LEU:O	2:D:22:CYS:HA	2.15	0.47
2:D:52:ILE:O	2:D:52(A):PRO:C	2.58	0.47
2:F:24:ALA:C	2:F:26:GLY:H	2.22	0.47
2:F:64:GLN:C	2:F:66:ARG:H	2.23	0.47
1:G:208:SER:OG	1:G:209:PHE:N	2.48	0.47
2:H:187:SER:O	2:H:191:THR:CG2	2.62	0.47
1:I:192:TYR:O	1:I:208:SER:HA	2.15	0.47
1:M:92:TYR:O	1:M:93:SER:O	2.33	0.47
1:M:186:TYR:CD1	1:M:192:TYR:CZ	3.02	0.47
2:N:166:PHE:HA	2:N:167:PRO:HD3	1.80	0.47
2:P:84:SER:C	2:P:86:ASP:H	2.22	0.47
1:A:131:SER:HA	1:A:180:THR:HA	1.95	0.47
1:A:147:GLN:HG3	1:A:154:LEU:HD11	1.97	0.47
1:E:186:TYR:O	1:E:192:TYR:OH	2.29	0.47
1:G:182:SER:O	1:G:184:ALA:N	2.48	0.47
2:N:96:GLY:CA	2:N:101:ASP:HB2	2.45	0.47
1:O:32:TYR:HB2	1:O:92:TYR:HB2	1.96	0.47
1:O:50:ALA:C	1:O:52:SER:H	2.23	0.47
1:A:124:GLN:NE2	1:A:131:SER:OG	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:124:GLN:HE22	1:C:131:SER:HB2	1.79	0.47
2:D:46:GLU:O	2:D:47:TRP:C	2.58	0.47
2:H:160:THR:HA	2:H:163:VAL:HG21	1.96	0.47
1:K:120:PRO:HD3	1:K:132:VAL:HG22	1.97	0.47
2:L:14:PRO:C	2:L:16:SER:H	2.23	0.47
1:M:55:GLN:NE2	1:M:56:SER:H	2.12	0.47
1:M:207:LYS:HD3	2:N:129:LYS:O	2.15	0.47
2:N:1:GLN:O	2:N:3:GLN:HG3	2.15	0.47
1:O:62:PHE:HD1	1:O:62:PHE:N	2.12	0.47
1:A:113:PRO:HD3	1:A:198:HIS:CD2	2.49	0.46
2:B:14:PRO:CG	2:B:113:SER:N	2.79	0.46
2:B:117:LYS:NZ	2:B:144:ASP:HB3	2.31	0.46
1:C:74:THR:HG22	1:C:75:ILE:N	2.30	0.46
1:C:142:ARG:HG2	1:C:142:ARG:NH1	2.29	0.46
1:G:79:GLN:O	1:G:80:PRO:C	2.58	0.46
1:G:117:ILE:HG23	1:G:117:ILE:O	2.15	0.46
1:I:48:ILE:HD13	1:I:64:GLY:H	1.79	0.46
1:I:122:ASP:O	1:I:123:GLU:C	2.57	0.46
2:J:192:GLN:NE2	2:J:193:THR:O	2.38	0.46
2:L:30:SER:C	2:L:53:VAL:HG23	2.40	0.46
2:L:83:ARG:N	2:L:86:ASP:OD2	2.47	0.46
1:M:147:GLN:CG	1:M:154:LEU:HD12	2.45	0.46
1:M:165:GLU:HA	1:M:165:GLU:OE2	2.16	0.46
2:P:146:PHE:CD2	2:P:147:PRO:N	2.84	0.46
2:B:199:ASN:ND2	2:B:205:THR:O	2.49	0.46
1:C:29:ILE:HG12	1:C:71:PHE:CE1	2.50	0.46
1:C:38:GLN:HE21	1:C:44:PRO:HG3	1.80	0.46
1:C:180:THR:HG22	1:O:24:ARG:HH22	1.79	0.46
2:H:3:GLN:CD	2:H:5:LEU:HD21	2.40	0.46
2:H:51:ILE:CG1	2:H:57:ALA:HB2	2.46	0.46
1:I:183:LYS:O	1:I:187:GLU:HG3	2.14	0.46
1:K:79:GLN:HB3	1:K:81:GLU:OE2	2.15	0.46
2:L:186:SER:O	2:L:188:SER:N	2.48	0.46
1:M:58:VAL:O	1:M:59:PRO:C	2.57	0.46
2:N:145:TYR:CE1	2:N:150:VAL:HG12	2.51	0.46
2:P:32:TYR:HD2	2:P:32:TYR:N	2.13	0.46
1:A:61:ARG:HB3	1:A:76:SER:OG	2.15	0.46
1:E:110:VAL:HG12	1:E:111:ALA:N	2.30	0.46
1:E:126:LYS:N	1:E:126:LYS:HE3	2.31	0.46
2:F:52(A):PRO:O	2:F:54:PHE:N	2.48	0.46
1:I:55:GLN:HG3	1:I:56:SER:N	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:140:TYR:C	1:I:198:HIS:HE1	2.23	0.46
1:K:100:GLN:HG2	1:K:101:GLY:H	1.81	0.46
1:K:185:ASP:O	1:K:188:LYS:N	2.44	0.46
2:L:186:SER:HA	2:L:189:LEU:HG	1.97	0.46
1:M:4:MET:HB2	1:M:99:GLY:CA	2.39	0.46
1:M:4:MET:HB2	1:M:98:PHE:O	2.14	0.46
1:A:198:HIS:C	1:A:200:GLY:H	2.23	0.46
2:B:37:VAL:HG13	2:B:46:GLU:C	2.40	0.46
2:B:100(J):HIS:HB3	2:B:100(K):GLY:H	1.52	0.46
2:D:18:VAL:H	2:D:82(C):LEU:HD11	1.79	0.46
1:E:34:ASN:OD1	1:E:49:TYR:HA	2.16	0.46
2:F:142:VAL:HB	2:F:178:LEU:HD12	1.98	0.46
2:H:68:THR:N	2:H:81:GLU:O	2.48	0.46
1:M:124:GLN:O	1:M:127:SER:N	2.45	0.46
2:N:193:THR:HG22	2:N:194:TYR:N	2.31	0.46
1:O:61:ARG:NE	1:O:79:GLN:CG	2.78	0.46
2:P:29:PHE:CD1	2:P:76:SER:HA	2.49	0.46
1:A:64:GLY:O	3:A:233:HOH:O	2.21	0.46
1:C:90:GLN:NE2	1:C:90:GLN:O	2.49	0.46
2:F:20:VAL:HG11	2:F:36:TRP:HZ3	1.81	0.46
2:F:94:LYS:CE	2:F:95:GLY:CA	2.94	0.46
1:G:147:GLN:HG3	1:G:154:LEU:HD12	1.98	0.46
1:I:35:TRP:CE2	1:I:73:LEU:HB2	2.51	0.46
1:I:110:VAL:CG1	1:I:111:ALA:N	2.78	0.46
1:I:182:SER:C	1:I:184:ALA:N	2.71	0.46
1:K:62:PHE:HE2	1:K:75:ILE:HG12	1.81	0.46
2:D:52(A):PRO:O	2:D:53:VAL:O	2.34	0.46
1:E:8:PRO:HG3	1:E:100:GLN:OE1	2.15	0.46
1:E:154:LEU:HB2	1:I:19:VAL:HG22	1.97	0.46
2:F:2:VAL:CB	2:F:27:GLY:H	2.27	0.46
2:H:84:SER:HA	2:H:111:VAL:HB	1.96	0.46
1:M:47:LEU:HD13	1:M:62:PHE:CD2	2.51	0.46
2:N:125:ALA:HA	2:N:126:PRO:HD3	1.81	0.46
2:N:203:SER:OG	2:N:205:THR:HG23	2.16	0.46
1:O:83:PHE:CZ	1:O:106:ILE:HG23	2.51	0.46
1:O:144:ALA:HB3	1:O:175:LEU:HD13	1.98	0.46
1:O:203:SER:C	1:O:204:PRO:O	2.59	0.46
2:P:41:PRO:HD3	2:P:87:THR:O	2.14	0.46
1:C:146:VAL:HG22	1:C:196:VAL:HG22	1.98	0.46
1:E:107:LYS:CG	1:E:108:ARG:N	2.79	0.46
2:F:112:ALA:HB3	2:F:146:PHE:CZ	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:2:ILE:N	1:G:26:SER:HG	2.14	0.46
2:H:32:TYR:HB3	2:H:94:LYS:CG	2.46	0.46
2:H:115:SER:OG	2:H:116:THR:N	2.49	0.46
2:H:207:VAL:HG12	2:H:208:ASP:N	2.30	0.46
1:I:155:GLN:HB3	1:I:158:ASN:HD21	1.81	0.46
1:K:7:SER:HA	1:K:100:GLN:NE2	2.31	0.46
1:M:36:TYR:CE2	2:N:103:TRP:HZ2	2.34	0.46
1:O:108:ARG:HE	1:O:108:ARG:C	2.23	0.46
1:A:47:LEU:HD11	1:A:86:TYR:CE2	2.49	0.46
1:A:183:LYS:NZ	1:A:187:GLU:OE2	2.48	0.46
2:B:36:TRP:CD1	2:B:69:ILE:HD13	2.51	0.46
2:B:123:PRO:C	2:B:125:ALA:H	2.23	0.46
2:D:18:VAL:CG2	2:D:19:LYS:H	2.27	0.46
1:E:107:LYS:HG2	1:E:108:ARG:N	2.31	0.46
1:G:182:SER:C	1:G:184:ALA:N	2.72	0.46
1:G:188:LYS:O	1:G:189:HIS:CG	2.68	0.46
2:J:131:THR:HG22	2:J:135:THR:O	2.16	0.46
1:K:19:VAL:HG23	1:K:78:LEU:CD2	2.40	0.46
2:L:35:SER:O	2:L:92:CYS:HA	2.16	0.46
1:M:3:GLN:HB3	1:M:26:SER:CB	2.44	0.46
1:O:38:GLN:HE22	2:P:39:GLN:HE22	1.64	0.46
2:P:90:TYR:N	2:P:90:TYR:CD1	2.84	0.46
2:B:120:SER:C	2:B:121:VAL:HG23	2.40	0.46
1:C:167:ASP:O	1:C:171:SER:HA	2.16	0.46
2:D:30:SER:HA	2:D:52(A):PRO:HB2	1.98	0.46
2:F:70:THR:O	2:F:71:ALA:HB2	2.16	0.46
1:G:95:SER:O	1:G:96:HIS:C	2.58	0.46
2:H:137:ALA:HA	2:H:182:VAL:O	2.15	0.46
2:H:155:ASN:O	2:H:156:SER:HB2	2.15	0.46
1:I:7:SER:OG	1:I:100:GLN:NE2	2.49	0.46
2:J:39:GLN:NE2	2:J:45:LEU:CD2	2.79	0.46
1:K:124:GLN:C	1:K:126:LYS:N	2.73	0.46
1:K:136:LEU:HD21	1:K:196:VAL:HG13	1.98	0.46
2:L:115:SER:H	2:L:117:LYS:HE2	1.81	0.46
2:L:119:PRO:HD3	2:L:145:TYR:HB2	1.98	0.46
2:N:170:LEU:HD13	2:N:176:TYR:CE1	2.50	0.46
1:O:89:GLN:HG3	1:O:98:PHE:CD2	2.51	0.46
2:B:39:GLN:C	2:B:88:ALA:HB1	2.41	0.46
2:B:125:ALA:HA	2:B:126:PRO:HD3	1.65	0.46
1:C:62:PHE:O	1:C:63:SER:CB	2.60	0.46
1:C:190:LYS:O	1:C:210:ASN:HA	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:60:SER:HB3	1:M:81:GLU:OE1	2.16	0.46
1:E:212:GLY:O	1:E:213:GLU:HB2	2.16	0.46
2:F:62:LYS:HA	2:J:83:ARG:NH1	2.31	0.46
2:F:155:ASN:ND2	2:F:159:LEU:HB2	2.30	0.46
2:H:171:GLN:NE2	2:H:175:LEU:O	2.49	0.46
2:H:178:LEU:C	2:H:178:LEU:HD12	2.40	0.46
1:I:119:PRO:HB3	1:I:209:PHE:CE1	2.51	0.46
1:I:159:SER:C	1:I:160:GLN:HG2	2.41	0.46
2:J:12:LYS:HZ1	2:J:18:VAL:HA	1.80	0.46
2:N:31:SER:O	2:N:32:TYR:O	2.34	0.46
1:O:8:PRO:CD	1:O:10:SER:N	2.77	0.46
1:O:142:ARG:HB2	1:O:173:TYR:CE2	2.51	0.46
2:P:53:VAL:O	2:P:53:VAL:CG1	2.63	0.46
2:D:35:SER:CB	2:D:49:GLY:O	2.65	0.45
1:E:20:THR:CG2	1:E:72:THR:OG1	2.64	0.45
2:H:119:PRO:HB2	2:H:142:VAL:CG1	2.46	0.45
2:H:144:ASP:HB3	2:H:175:LEU:HD12	1.98	0.45
1:I:193:ALA:HB1	1:I:206:THR:HG23	1.98	0.45
1:K:37:GLN:HB2	1:K:47:LEU:HD11	1.98	0.45
1:K:126:LYS:HE3	1:K:126:LYS:CA	2.46	0.45
1:K:198:HIS:C	1:K:200:GLY:H	2.25	0.45
1:K:203:SER:O	1:K:204:PRO:C	2.59	0.45
2:L:171:GLN:NE2	2:L:173:SER:OG	2.49	0.45
1:M:79:GLN:O	1:M:82:ASP:HB2	2.16	0.45
1:M:135:LEU:HD12	1:M:175:LEU:O	2.16	0.45
1:O:83:PHE:CE2	1:O:106:ILE:HG23	2.51	0.45
1:A:138:ASN:HA	1:A:173:TYR:O	2.16	0.45
2:B:183:THR:HG23	2:B:183:THR:O	2.16	0.45
2:B:184:VAL:CB	2:B:185:PRO:CD	2.94	0.45
1:E:4:MET:CE	1:E:33:LEU:HD23	2.46	0.45
1:E:32:TYR:CD1	1:E:92:TYR:CD1	2.98	0.45
1:E:98:PHE:CZ	2:F:37:VAL:HG11	2.50	0.45
1:E:125:LEU:O	1:E:183:LYS:HD2	2.16	0.45
2:F:145:TYR:HE1	2:F:150:VAL:CB	2.13	0.45
1:I:182:SER:O	1:I:183:LYS:C	2.59	0.45
1:K:47:LEU:HD11	1:K:86:TYR:CE2	2.46	0.45
1:K:146:VAL:HG11	1:K:177:SER:OG	2.16	0.45
2:L:193:THR:CG2	2:L:194:TYR:N	2.79	0.45
1:M:89:GLN:HG2	1:M:90:GLN:N	2.31	0.45
2:N:63:PHE:HB3	2:N:67:VAL:HG12	1.98	0.45
2:N:85:GLU:C	2:N:87:THR:H	2.24	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:95:GLY:HA2	2:N:100(L):MET:HA	1.98	0.45
1:O:61:ARG:HG3	1:O:62:PHE:HE1	1.80	0.45
2:P:52:ILE:O	2:P:53:VAL:N	2.49	0.45
1:A:151:ASP:O	1:A:152:ASN:HB2	2.16	0.45
1:A:210:ASN:O	1:A:213:GLU:CG	2.64	0.45
2:D:36:TRP:CZ2	2:D:80:MET:HB2	2.51	0.45
2:D:126:PRO:HD2	2:D:213:PRO:HA	1.98	0.45
1:E:24:ARG:NH1	1:I:158:ASN:HA	2.31	0.45
1:E:55:GLN:O	1:E:58:VAL:HG23	2.16	0.45
1:E:170:ASP:O	1:E:172:THR:HG23	2.15	0.45
2:F:94:LYS:CE	2:F:95:GLY:C	2.86	0.45
2:H:32:TYR:HB3	2:H:94:LYS:HG2	1.99	0.45
2:J:201:LYS:O	2:J:203:SER:N	2.49	0.45
1:M:62:PHE:HE2	1:M:86:TYR:CE2	2.35	0.45
2:P:70:THR:HG1	2:P:79:TYR:HB2	1.77	0.45
2:D:191:THR:O	2:D:192:GLN:C	2.59	0.45
1:E:98:PHE:CE1	2:F:37:VAL:HG11	2.52	0.45
2:F:115:SER:O	2:F:116:THR:C	2.58	0.45
1:G:32:TYR:HB3	1:G:92:TYR:H	1.82	0.45
2:H:112:ALA:O	2:H:114:ALA:N	2.50	0.45
2:J:20:VAL:O	2:J:79:TYR:HA	2.16	0.45
1:K:60:SER:C	1:K:62:PHE:H	2.23	0.45
1:K:156:SER:C	1:K:158:ASN:N	2.74	0.45
1:K:183:LYS:HD2	3:K:218:HOH:O	2.16	0.45
1:O:79:GLN:HB3	1:O:81:GLU:HG2	1.99	0.45
1:O:120:PRO:HB3	1:O:131:SER:H	1.82	0.45
1:O:183:LYS:O	1:O:184:ALA:C	2.59	0.45
1:A:201:LEU:HD13	1:A:205:VAL:CG2	2.38	0.45
2:B:38:ARG:CZ	2:B:63:PHE:HZ	2.30	0.45
2:B:162:GLY:O	2:B:182:VAL:HA	2.16	0.45
1:C:4:MET:CE	1:C:33:LEU:HD23	2.47	0.45
1:C:185:ASP:HA	1:C:188:LYS:HD2	1.98	0.45
2:D:12:LYS:O	2:D:13:LYS:C	2.59	0.45
2:D:39:GLN:HE22	2:D:44:GLY:HA2	1.81	0.45
2:D:73:GLU:C	2:D:75:THR:N	2.74	0.45
1:E:66:GLY:O	1:E:67:SER:CB	2.64	0.45
1:E:140:TYR:CG	1:E:141:PRO:HA	2.52	0.45
2:F:94:LYS:NZ	2:F:95:GLY:HA2	2.31	0.45
2:F:214:LYS:CG	2:F:214:LYS:OXT	2.65	0.45
1:G:184:ALA:O	1:G:185:ASP:C	2.60	0.45
2:J:171:GLN:C	2:J:173:SER:N	2.72	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:203:SER:O	2:J:204:ASN:C	2.59	0.45
1:K:7:SER:O	1:K:7:SER:OG	2.29	0.45
1:M:180:THR:C	1:M:181:LEU:HD12	2.42	0.45
2:N:178:LEU:C	2:N:178:LEU:CD1	2.85	0.45
2:P:12:LYS:HE3	2:P:18:VAL:CG2	2.47	0.45
1:A:72:THR:O	1:A:72:THR:HG22	2.14	0.45
1:A:90:GLN:HE22	1:A:93:SER:N	2.13	0.45
1:E:26:SER:C	1:E:27:GLN:NE2	2.75	0.45
1:G:64:GLY:O	1:G:65:SER:HB3	2.16	0.45
1:G:73:LEU:C	1:G:73:LEU:CD2	2.82	0.45
1:G:74:THR:HG22	1:G:75:ILE:N	2.31	0.45
1:G:90:GLN:OE1	1:G:90:GLN:C	2.60	0.45
2:H:145:TYR:HE2	2:H:177:SER:HA	1.82	0.45
1:I:197:THR:HG22	1:I:204:PRO:CB	2.46	0.45
2:J:28:THR:C	2:J:30:SER:H	2.23	0.45
1:K:210:ASN:O	1:K:211:ARG:C	2.60	0.45
2:L:8:GLY:C	2:L:107:THR:CG2	2.90	0.45
2:L:20:VAL:C	3:L:215:HOH:O	2.60	0.45
2:L:51:ILE:O	2:L:51:ILE:HG23	2.17	0.45
2:L:145:TYR:HE2	2:L:177:SER:HA	1.81	0.45
2:L:186:SER:C	2:L:188:SER:N	2.75	0.45
1:M:146:VAL:HG22	1:M:196:VAL:HG22	1.98	0.45
2:N:203:SER:C	2:N:205:THR:N	2.75	0.45
1:O:175:LEU:C	1:O:175:LEU:HD23	2.42	0.45
1:A:90:GLN:HG3	1:A:90:GLN:O	2.16	0.45
1:A:143:GLU:N	1:A:143:GLU:CD	2.75	0.45
2:B:94:LYS:HB3	2:B:102:VAL:HG13	1.98	0.45
1:C:61:ARG:HG3	1:C:62:PHE:CD1	2.52	0.45
1:C:67:SER:HA	1:C:71:PHE:CE2	2.51	0.45
2:D:73:GLU:C	2:D:75:THR:H	2.23	0.45
2:F:11:VAL:HG11	2:F:146:PHE:HZ	1.82	0.45
1:G:7:SER:HA	1:G:8:PRO:HD3	1.50	0.45
1:G:92:TYR:O	1:G:93:SER:C	2.60	0.45
1:G:191:VAL:CG2	1:G:210:ASN:HD21	2.29	0.45
2:J:161:SER:C	2:J:163:VAL:N	2.72	0.45
2:J:163:VAL:HG12	2:J:164:HIS:H	1.80	0.45
2:L:87:THR:O	2:L:88:ALA:HB2	2.16	0.45
1:M:28:SER:HA	1:M:69:THR:CG2	2.46	0.45
1:M:162:SER:OG	2:N:167:PRO:HD2	2.17	0.45
1:M:211:ARG:HG2	1:M:211:ARG:NH1	2.28	0.45
2:N:138:LEU:HD13	2:N:211:VAL:HG11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:16:SER:O	2:F:82(C):LEU:HG	2.16	0.45
2:F:32:TYR:CD2	2:F:94:LYS:HE3	2.51	0.45
2:F:68:THR:HB	2:F:81:GLU:CB	2.42	0.45
1:G:17:ASP:OD1	1:G:17:ASP:N	2.49	0.45
2:H:89:VAL:HG13	2:H:107:THR:H	1.82	0.45
2:H:153:SER:HB2	2:H:197:ASN:CG	2.41	0.45
2:H:172:SER:C	2:H:174:GLY:H	2.24	0.45
2:J:181:VAL:O	2:J:182:VAL:HB	2.16	0.45
2:L:112:ALA:HB3	2:L:146:PHE:CZ	2.52	0.45
1:O:114:SER:HB2	1:O:137:ASN:HB3	1.98	0.45
2:P:141:LEU:HD12	2:P:179:SER:HB3	1.99	0.45
1:A:50:ALA:O	1:A:51:ALA:HB3	2.16	0.45
1:A:140:TYR:CG	1:A:141:PRO:HA	2.52	0.45
2:B:29:PHE:O	2:B:32:TYR:N	2.49	0.45
2:B:83:ARG:HD2	2:B:85:GLU:OE1	2.17	0.45
2:B:138:LEU:HD23	2:B:138:LEU:N	2.15	0.45
2:B:200:HIS:HE1	2:B:202:PRO:HB2	1.77	0.45
2:D:51:ILE:O	2:D:52:ILE:CG1	2.64	0.45
1:G:142:ARG:O	1:G:143:GLU:C	2.59	0.45
2:H:6:GLN:HA	2:H:21:SER:O	2.17	0.45
1:I:203:SER:OG	1:I:204:PRO:CD	2.65	0.45
1:M:29:ILE:O	1:M:30:SER:CB	2.63	0.45
2:N:40:ALA:O	2:N:43:GLN:HB2	2.16	0.45
1:O:13:ALA:O	1:O:107:LYS:N	2.34	0.45
1:O:70:ASP:C	1:O:71:PHE:CD1	2.95	0.45
1:O:148:TRP:CE3	1:O:193:ALA:O	2.70	0.45
1:O:199:GLN:CA	1:O:199:GLN:HE21	2.30	0.45
1:A:108:ARG:NH1	1:A:172:THR:CG2	2.80	0.45
1:A:114:SER:O	1:A:116:PHE:CE1	2.70	0.45
2:D:178:LEU:HD12	2:D:179:SER:N	2.32	0.45
1:G:60:SER:C	1:G:62:PHE:N	2.75	0.45
2:H:127:SER:C	2:H:129:LYS:N	2.75	0.45
2:H:138:LEU:CD1	2:H:154:TRP:CH2	2.98	0.45
1:I:32:TYR:CB	1:I:92:TYR:N	2.79	0.45
1:O:140:TYR:O	1:O:198:HIS:HE1	1.99	0.45
1:A:25:ALA:N	1:A:69:THR:O	2.49	0.44
1:A:119:PRO:HB3	1:A:209:PHE:CD2	2.53	0.44
2:D:17:SER:CB	2:D:82:LEU:O	2.65	0.44
2:H:1:GLN:CD	2:H:1:GLN:N	2.75	0.44
2:H:126:PRO:O	2:H:127:SER:C	2.59	0.44
1:I:106:ILE:N	1:I:166:GLN:OE1	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:154:TRP:CH2	2:L:196:CYS:HB3	2.53	0.44
1:M:29:ILE:CD1	1:M:33:LEU:HB2	2.46	0.44
2:N:32:TYR:O	2:N:52(A):PRO:HD2	2.17	0.44
2:N:47:TRP:CE3	2:N:60:ALA:HB2	2.52	0.44
2:P:12:LYS:HE3	2:P:18:VAL:HB	2.00	0.44
2:P:36:TRP:HD1	2:P:69:ILE:CD1	2.30	0.44
1:A:90:GLN:C	1:A:90:GLN:CD	2.85	0.44
1:A:145:LYS:HB3	1:A:197:THR:CG2	2.47	0.44
1:A:174:SER:HB2	2:B:164:HIS:CD2	2.52	0.44
2:B:72:ASP:OD2	2:B:72:ASP:C	2.59	0.44
2:B:210:LYS:HE2	2:B:212:GLU:CD	2.42	0.44
1:C:29:ILE:O	1:C:30:SER:C	2.60	0.44
2:F:24:ALA:C	2:F:26:GLY:N	2.75	0.44
2:F:184:VAL:CB	2:F:185:PRO:CD	2.96	0.44
1:G:169:LYS:HG3	1:G:170:ASP:N	2.32	0.44
2:H:172:SER:C	2:H:174:GLY:N	2.74	0.44
1:I:6:GLN:NE2	1:I:87:TYR:HA	2.28	0.44
1:I:121:SER:O	1:I:124:GLN:HB3	2.18	0.44
1:K:108:ARG:NH2	1:K:109:THR:OG1	2.51	0.44
1:K:119:PRO:HB3	1:K:209:PHE:CZ	2.52	0.44
1:K:185:ASP:O	1:K:186:TYR:C	2.60	0.44
2:L:37:VAL:HG21	2:L:103:TRP:CH2	2.52	0.44
2:L:193:THR:HG22	2:L:195:ILE:HD11	2.00	0.44
1:M:40:PRO:HD3	3:M:218:HOH:O	2.18	0.44
2:N:188:SER:O	2:N:189:LEU:C	2.59	0.44
2:N:203:SER:O	2:N:205:THR:N	2.50	0.44
2:P:22:CYS:O	2:P:22:CYS:SG	2.74	0.44
2:P:29:PHE:CZ	2:P:52(A):PRO:HB3	2.52	0.44
1:C:201:LEU:HD13	1:C:205:VAL:HG23	1.99	0.44
2:D:2:VAL:O	2:D:2:VAL:HG13	2.18	0.44
2:F:140:CYS:O	2:F:179:SER:CA	2.63	0.44
2:F:212:GLU:HA	2:F:213:PRO:HD3	1.77	0.44
1:G:14:SER:H	1:G:17:ASP:CG	2.25	0.44
2:H:184:VAL:HG21	2:H:194:TYR:CE1	2.53	0.44
2:H:199:ASN:ND2	2:H:200:HIS:O	2.50	0.44
2:J:30:SER:CA	2:J:52(A):PRO:HB2	2.44	0.44
2:J:64:GLN:HG2	2:L:204:ASN:OD1	2.18	0.44
2:J:189:LEU:C	2:J:191:THR:N	2.73	0.44
1:K:116:PHE:CD2	2:L:130:SER:HA	2.52	0.44
2:L:39:GLN:C	2:L:88:ALA:HB1	2.42	0.44
1:M:140:TYR:HA	1:M:141:PRO:C	2.40	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:183:LYS:O	1:M:184:ALA:C	2.60	0.44
2:N:90:TYR:O	2:N:106:GLY:HA2	2.18	0.44
2:P:199:ASN:C	2:P:199:ASN:ND2	2.75	0.44
2:B:48:MET:HE1	2:B:80:MET:HE1	2.00	0.44
2:B:150:VAL:O	2:B:150:VAL:CG1	2.65	0.44
1:C:93:SER:OG	1:C:94:THR:N	2.50	0.44
1:C:209:PHE:C	1:C:210:ASN:HD22	2.26	0.44
1:G:138:ASN:CA	1:G:172:THR:HB	2.47	0.44
1:G:150:VAL:O	1:G:151:ASP:HB2	2.16	0.44
1:G:206:THR:CG2	1:G:207:LYS:N	2.79	0.44
2:H:70:THR:O	2:H:78:THR:HA	2.17	0.44
2:H:128:SER:O	2:H:130:SER:N	2.44	0.44
1:I:12:SER:O	1:I:13:ALA:CB	2.63	0.44
2:J:14:PRO:HD3	2:J:112:ALA:C	2.43	0.44
2:J:170:LEU:HD12	2:J:170:LEU:C	2.43	0.44
1:K:210:ASN:ND2	1:K:210:ASN:H	2.09	0.44
2:L:11:VAL:HG13	2:L:110:THR:HB	1.99	0.44
2:L:28:THR:O	2:L:29:PHE:C	2.60	0.44
1:O:79:GLN:C	1:O:81:GLU:N	2.75	0.44
2:P:72:ASP:OD2	2:P:74:ALA:HB2	2.17	0.44
1:A:28:SER:HA	1:A:69:THR:CG2	2.45	0.44
1:A:145:LYS:HB3	1:A:197:THR:HG23	1.98	0.44
1:E:124:GLN:HG2	1:E:129:THR:O	2.17	0.44
1:E:207:LYS:O	1:E:208:SER:HB3	2.17	0.44
1:E:209:PHE:C	1:E:209:PHE:CD2	2.96	0.44
2:F:184:VAL:HB	2:F:185:PRO:HD2	1.99	0.44
1:G:31:SER:O	1:G:50:ALA:HA	2.18	0.44
1:G:32:TYR:N	1:G:32:TYR:HD1	2.16	0.44
1:G:148:TRP:HD1	1:G:159:SER:HG	1.62	0.44
2:J:12:LYS:CD	2:J:18:VAL:HB	2.44	0.44
2:J:47:TRP:CD1	2:J:100(L):MET:HE1	2.53	0.44
1:K:48:ILE:HD12	1:K:73:LEU:CD1	2.47	0.44
2:L:7:SER:HB2	2:L:10:GLU:OE2	2.16	0.44
2:N:94:LYS:HE2	2:N:95:GLY:O	2.17	0.44
2:N:96:GLY:HA2	2:N:101:ASP:HB2	2.00	0.44
2:P:69:ILE:HG12	2:P:80:MET:HG2	1.99	0.44
1:C:61:ARG:HG3	1:C:62:PHE:CE1	2.53	0.44
2:D:64:GLN:C	2:D:66:ARG:H	2.25	0.44
2:D:119:PRO:HB3	2:D:145:TYR:HD2	1.82	0.44
2:D:138:LEU:HD12	2:D:138:LEU:O	2.18	0.44
2:D:210:LYS:CE	2:D:212:GLU:OE2	2.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:138:ASN:HA	1:E:173:TYR:O	2.17	0.44
1:E:149:LYS:HG2	1:E:154:LEU:HD13	2.00	0.44
1:G:136:LEU:HD22	1:G:175:LEU:HD22	2.00	0.44
2:H:76:SER:O	2:H:76:SER:OG	2.29	0.44
1:I:91:SER:O	1:I:93:SER:O	2.35	0.44
1:K:55:GLN:CG	1:K:56:SER:N	2.80	0.44
1:K:90:GLN:NE2	1:K:97:THR:OG1	2.51	0.44
2:L:6:GLN:NE2	2:L:106:GLY:HA2	2.33	0.44
1:M:150:VAL:HG11	1:M:189:HIS:HD2	1.82	0.44
2:P:82(A):SER:OG	2:P:82(B):SER:N	2.49	0.44
2:P:146:PHE:C	2:P:146:PHE:HD2	2.23	0.44
2:B:126:PRO:CG	2:B:138:LEU:HB3	2.41	0.44
2:B:141:LEU:HG	2:B:141:LEU:O	2.18	0.44
2:D:47:TRP:CZ3	2:D:49:GLY:HA2	2.53	0.44
2:D:51:ILE:CG1	2:D:52:ILE:N	2.77	0.44
2:D:139:GLY:O	2:D:140:CYS:SG	2.76	0.44
1:E:124:GLN:HE22	1:E:131:SER:CB	2.31	0.44
1:E:183:LYS:O	1:E:187:GLU:HG2	2.18	0.44
2:F:17:SER:HB2	2:F:82:LEU:O	2.17	0.44
2:H:141:LEU:HD12	2:H:141:LEU:C	2.42	0.44
2:H:154:TRP:CZ3	2:H:196:CYS:HB3	2.53	0.44
1:I:48:ILE:HD13	1:I:64:GLY:CA	2.48	0.44
2:L:29:PHE:C	2:L:29:PHE:CD1	2.95	0.44
1:M:155:GLN:O	1:M:156:SER:HB2	2.17	0.44
2:N:20:VAL:HB	2:N:80:MET:HE3	2.00	0.44
1:O:107:LYS:HA	1:O:140:TYR:OH	2.17	0.44
2:P:37:VAL:HA	2:P:46:GLU:O	2.18	0.44
2:B:23:LYS:NZ	2:B:75:THR:O	2.50	0.44
1:C:165:GLU:O	1:C:166:GLN:C	2.60	0.44
1:E:11:LEU:C	1:E:11:LEU:HD13	2.42	0.44
1:E:96:HIS:N	1:E:96:HIS:CD2	2.86	0.44
1:G:106:ILE:HD12	1:G:166:GLN:OE1	2.17	0.44
2:J:36:TRP:CG	2:J:80:MET:HG2	2.52	0.44
1:K:55:GLN:HG3	1:K:56:SER:N	2.32	0.44
1:K:188:LYS:C	1:K:189:HIS:CG	2.95	0.44
2:L:55:GLY:O	2:L:56:SER:HB3	2.16	0.44
2:L:66:ARG:CG	2:L:67:VAL:H	2.31	0.44
2:N:100(J):HIS:CG	2:N:100(K):GLY:N	2.85	0.44
1:A:147:GLN:HE22	1:M:11:LEU:HD22	1.82	0.44
1:A:158:ASN:ND2	1:A:158:ASN:N	2.39	0.44
2:B:135:THR:O	2:B:135:THR:HG22	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:96:HIS:CD2	1:E:96:HIS:H	2.35	0.44
2:F:34:ILE:HA	2:F:94:LYS:HB2	1.99	0.44
2:F:62:LYS:O	2:F:64:GLN:N	2.44	0.44
1:G:180:THR:HG21	2:H:143:LYS:HE3	1.99	0.44
2:H:6:GLN:NE2	2:H:107:THR:OG1	2.48	0.44
1:I:210:ASN:HB2	1:I:213:GLU:CD	2.43	0.44
2:J:36:TRP:CE2	2:J:80:MET:HB2	2.53	0.44
1:K:126:LYS:O	1:K:128:GLY:N	2.50	0.44
1:K:153:ALA:O	1:K:154:LEU:C	2.59	0.44
2:L:36:TRP:HE1	2:L:78:THR:CG2	2.29	0.44
1:O:51:ALA:HB1	1:O:71:PHE:HD2	1.82	0.44
1:O:79:GLN:C	1:O:81:GLU:H	2.26	0.44
1:O:90:GLN:NE2	1:O:95:SER:O	2.50	0.44
2:P:168:ALA:HA	2:P:178:LEU:HB3	1.99	0.44
2:P:169:VAL:HG22	2:P:177:SER:O	2.17	0.44
1:A:49:TYR:O	1:A:50:ALA:HB3	2.18	0.43
1:A:167:ASP:OD2	1:A:169:LYS:HE2	2.17	0.43
2:B:22:CYS:SG	2:B:22:CYS:O	2.76	0.43
1:C:36:TYR:HA	1:C:45:LYS:O	2.18	0.43
1:C:193:ALA:CB	1:C:208:SER:HB3	2.48	0.43
1:C:199:GLN:HE22	1:O:198:HIS:C	2.26	0.43
2:D:35:SER:HB2	2:D:49:GLY:O	2.18	0.43
2:D:70:THR:O	2:D:78:THR:HA	2.18	0.43
1:E:113:PRO:HA	1:E:137:ASN:O	2.18	0.43
2:F:29:PHE:CD1	2:F:29:PHE:C	2.96	0.43
2:F:60:ALA:O	2:F:61:GLN:C	2.60	0.43
1:G:60:SER:C	1:G:62:PHE:H	2.25	0.43
1:G:210:ASN:HD22	1:G:210:ASN:HA	1.65	0.43
2:H:142:VAL:O	2:H:145:TYR:HD2	2.01	0.43
1:I:129:THR:HA	1:I:182:SER:HA	2.00	0.43
1:I:141:PRO:HD2	1:I:199:GLN:HB3	2.00	0.43
1:I:142:ARG:CZ	1:I:163:VAL:HG21	2.48	0.43
1:E:124:GLN:CB	3:E:216:HOH:O	2.64	0.43
1:E:167:ASP:HB3	1:E:170:ASP:OD2	2.18	0.43
2:F:210:LYS:HG2	2:F:212:GLU:HG2	2.00	0.43
1:G:33:LEU:HA	1:G:89:GLN:O	2.18	0.43
1:G:75:ILE:O	1:G:76:SER:C	2.60	0.43
1:G:113:PRO:HD3	1:G:198:HIS:CG	2.53	0.43
2:H:66:ARG:NH2	2:H:86:ASP:OD1	2.51	0.43
2:J:10:GLU:HB2	2:J:109:VAL:HG22	2.00	0.43
1:K:182:SER:C	1:K:184:ALA:N	2.75	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:198:HIS:ND1	1:K:199:GLN:N	2.65	0.43
2:L:71:ALA:O	2:L:72:ASP:CB	2.66	0.43
2:L:119:PRO:CG	2:L:145:TYR:HB3	2.48	0.43
1:M:186:TYR:C	1:M:188:LYS:H	2.26	0.43
2:N:85:GLU:C	2:N:87:THR:N	2.75	0.43
2:P:100(L):MET:O	2:P:103:TRP:NE1	2.51	0.43
2:B:51:ILE:HB	2:B:57:ALA:CB	2.47	0.43
2:B:59:TYR:CD2	2:B:67:VAL:CG1	3.02	0.43
2:B:73:GLU:C	2:B:76:SER:H	2.25	0.43
2:D:5:LEU:O	2:D:23:LYS:N	2.39	0.43
2:D:108:THR:O	2:D:108:THR:CG2	2.66	0.43
1:E:157:GLY:HA3	1:I:22:THR:HG23	2.01	0.43
2:F:30:SER:HA	2:F:52(A):PRO:HG2	2.00	0.43
2:F:171:GLN:HG3	2:F:175:LEU:O	2.18	0.43
1:G:69:THR:O	1:G:71:PHE:CD1	2.70	0.43
2:J:29:PHE:HA	2:J:32:TYR:HD1	1.83	0.43
2:J:64:GLN:CG	2:L:204:ASN:OD1	2.67	0.43
2:J:82(A):SER:O	2:J:82(B):SER:O	2.36	0.43
1:K:54:LEU:HD11	1:K:58:VAL:HG11	2.00	0.43
1:K:112:ALA:HB1	1:K:201:LEU:HG	2.00	0.43
1:K:186:TYR:O	1:K:192:TYR:OH	2.34	0.43
1:M:95:SER:HA	2:N:47:TRP:CH2	2.53	0.43
2:N:170:LEU:HD11	2:N:174:GLY:C	2.43	0.43
1:A:132:VAL:HG12	1:A:148:TRP:CH2	2.54	0.43
2:D:2:VAL:HG21	2:D:27:GLY:N	2.34	0.43
2:F:146:PHE:CD1	2:F:147:PRO:HA	2.54	0.43
1:G:14:SER:HB2	1:G:17:ASP:OD2	2.18	0.43
1:G:117:ILE:O	1:G:117:ILE:HG12	2.17	0.43
2:H:82:LEU:HD23	2:H:82(C):LEU:HD21	2.00	0.43
2:J:171:GLN:HB2	2:J:173:SER:OG	2.18	0.43
1:K:26:SER:HB2	1:K:27:GLN:HE22	1.83	0.43
1:K:43:VAL:CG1	2:L:103:TRP:HB2	2.48	0.43
1:K:96:HIS:O	2:L:47:TRP:CB	2.64	0.43
2:L:4:LEU:HA	2:L:23:LYS:O	2.18	0.43
1:M:175:LEU:HD23	1:M:176:SER:H	1.77	0.43
1:O:190:LYS:HE2	1:O:210:ASN:OD1	2.17	0.43
2:B:205:THR:O	2:B:206:LYS:HG3	2.18	0.43
2:D:153:SER:OG	2:D:197:ASN:HB2	2.18	0.43
2:F:67:VAL:CG2	2:F:68:THR:N	2.79	0.43
1:G:47:LEU:HD23	1:G:48:ILE:CG1	2.36	0.43
1:G:111:ALA:O	1:G:112:ALA:C	2.60	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:149:LYS:HB2	1:G:193:ALA:HB3	2.00	0.43
2:H:119:PRO:HB2	2:H:142:VAL:HG13	2.01	0.43
2:H:142:VAL:HG22	2:H:198:VAL:HG11	1.99	0.43
1:I:65:SER:HB2	1:I:72:THR:CG2	2.45	0.43
1:M:186:TYR:CE1	1:M:192:TYR:CZ	3.06	0.43
1:O:80:PRO:HA	1:O:83:PHE:CE1	2.53	0.43
1:O:148:TRP:HE3	1:O:193:ALA:O	2.00	0.43
2:B:182:VAL:HG13	2:B:182:VAL:O	2.19	0.43
1:C:31:SER:C	1:C:33:LEU:H	2.26	0.43
1:C:199:GLN:HA	1:O:199:GLN:HE22	1.84	0.43
2:D:75:THR:O	2:D:76:SER:HB2	2.19	0.43
2:D:189:LEU:O	2:D:190:GLY:C	2.60	0.43
1:E:142:ARG:HB2	1:E:173:TYR:CE2	2.54	0.43
1:G:11:LEU:C	1:G:11:LEU:HD13	2.44	0.43
2:H:121:VAL:HG12	2:H:121:VAL:O	2.18	0.43
1:I:2:ILE:HD12	1:I:93:SER:HB2	1.92	0.43
2:J:29:PHE:O	2:J:29:PHE:CG	2.72	0.43
2:J:53:VAL:O	2:J:54:PHE:CG	2.72	0.43
1:K:183:LYS:O	1:K:184:ALA:C	2.60	0.43
1:K:196:VAL:O	1:K:204:PRO:HA	2.18	0.43
2:L:23:LYS:O	2:L:24:ALA:O	2.37	0.43
2:N:30:SER:CB	2:N:53:VAL:HG23	2.49	0.43
1:O:14:SER:O	1:O:15:VAL:C	2.61	0.43
1:O:199:GLN:HA	1:O:199:GLN:HE21	1.83	0.43
2:P:100(L):MET:H	2:P:100(L):MET:CE	2.22	0.43
2:P:141:LEU:HD13	2:P:179:SER:HB3	2.00	0.43
2:B:61:GLN:C	2:B:63:PHE:N	2.77	0.43
2:B:120:SER:O	2:B:121:VAL:HG23	2.19	0.43
2:B:142:VAL:HG22	2:B:198:VAL:HG21	1.99	0.43
1:C:90:GLN:O	1:C:90:GLN:CD	2.62	0.43
2:F:117:LYS:HG2	2:F:118:GLY:O	2.18	0.43
2:J:6:GLN:OE1	2:J:106:GLY:N	2.50	0.43
2:J:70:THR:O	2:J:79:TYR:N	2.38	0.43
2:J:199:ASN:ND2	2:J:200:HIS:N	2.66	0.43
2:L:195:ILE:HG21	2:L:208:ASP:HB3	2.01	0.43
1:M:42:LYS:HB3	3:M:227:HOH:O	2.18	0.43
2:P:141:LEU:HA	2:P:179:SER:HB2	2.00	0.43
2:P:145:TYR:HB2	2:P:200:HIS:CE1	2.54	0.43
2:P:154:TRP:HB2	2:P:159:LEU:HB3	2.00	0.43
1:A:58:VAL:HA	1:A:59:PRO:HD3	1.88	0.43
1:A:154:LEU:HD13	1:A:154:LEU:HA	1.64	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:38:ARG:NH1	2:B:86:ASP:HA	2.34	0.43
2:B:105:GLN:HB2	3:B:232:HOH:O	2.19	0.43
2:B:138:LEU:HB2	2:B:211:VAL:HG11	2.00	0.43
1:C:62:PHE:H	1:C:62:PHE:HD1	1.67	0.43
1:C:116:PHE:CD2	2:D:137:ALA:CB	3.01	0.43
2:D:32:TYR:HB2	2:D:34:ILE:HD11	2.00	0.43
2:D:210:LYS:HE2	2:D:212:GLU:CD	2.44	0.43
1:E:19:VAL:HG12	1:E:20:THR:N	2.33	0.43
2:H:28:THR:O	2:H:29:PHE:C	2.62	0.43
2:H:146:PHE:HA	2:H:147:PRO:HA	1.80	0.43
2:J:48:MET:O	2:J:60:ALA:N	2.52	0.43
2:J:84:SER:HA	2:J:111:VAL:O	2.19	0.43
2:L:34:ILE:CD1	2:L:34:ILE:H	2.32	0.43
2:L:37:VAL:CG1	2:L:38:ARG:N	2.82	0.43
1:O:50:ALA:O	1:O:52:SER:N	2.52	0.43
1:O:148:TRP:CZ3	1:O:194:CYS:HB3	2.54	0.43
2:B:4:LEU:HB2	2:B:104:GLY:HA2	2.01	0.43
1:C:59:PRO:HG2	1:C:61:ARG:NH2	2.34	0.43
1:C:75:ILE:HG21	1:C:78:LEU:HD12	1.98	0.43
1:C:117:ILE:O	1:C:117:ILE:HG22	2.18	0.43
1:C:198:HIS:CE1	1:C:200:GLY:H	2.37	0.43
1:E:116:PHE:HD2	2:F:130:SER:HB2	1.83	0.43
2:F:62:LYS:HA	2:J:83:ARG:HH12	1.84	0.43
1:G:26:SER:HA	2:L:172:SER:O	2.19	0.43
1:G:112:ALA:HA	1:G:198:HIS:ND1	2.33	0.43
1:G:186:TYR:CE2	1:G:211:ARG:HD3	2.54	0.43
2:J:29:PHE:HA	2:J:32:TYR:CD1	2.54	0.43
1:K:94:THR:O	2:L:47:TRP:CH2	2.72	0.43
1:K:98:PHE:CE1	2:L:47:TRP:HB2	2.41	0.43
2:L:8:GLY:O	2:L:10:GLU:HG3	2.18	0.43
1:M:97:THR:HG22	1:M:98:PHE:N	2.34	0.43
2:N:55:GLY:O	2:N:56:SER:CB	2.65	0.43
1:O:43:VAL:HG13	2:P:103:TRP:HB2	1.99	0.43
1:O:55:GLN:HE21	1:O:56:SER:H	1.65	0.43
1:A:40:PRO:C	1:A:42:LYS:N	2.73	0.43
2:B:116:THR:HA	2:B:146:PHE:O	2.19	0.43
1:C:61:ARG:CZ	1:C:79:GLN:HG3	2.49	0.43
1:C:143:GLU:CD	1:C:143:GLU:H	2.26	0.43
1:C:173:TYR:CD2	1:C:173:TYR:N	2.87	0.43
2:D:4:LEU:HD12	2:D:103:TRP:C	2.44	0.43
1:E:136:LEU:HD22	1:E:175:LEU:HD22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:161:GLU:HA	1:E:176:SER:O	2.18	0.43
2:F:50:GLY:O	2:F:57:ALA:HA	2.19	0.43
2:F:126:PRO:CB	2:F:189:LEU:HD13	2.48	0.43
2:F:210:LYS:HE2	2:F:212:GLU:CD	2.43	0.43
2:F:210:LYS:HE2	2:F:212:GLU:OE1	2.19	0.43
1:G:49:TYR:O	1:G:50:ALA:HB3	2.19	0.43
1:G:54:LEU:HD11	1:G:62:PHE:O	2.19	0.43
2:H:48:MET:CE	2:H:90:TYR:HE2	2.31	0.43
2:J:136:ALA:N	2:J:184:VAL:O	2.51	0.43
2:L:8:GLY:C	2:L:107:THR:HG23	2.44	0.43
2:L:10:GLU:HG3	3:L:218:HOH:O	2.19	0.43
1:M:140:TYR:CD1	1:M:140:TYR:C	2.97	0.43
2:N:150:VAL:HG22	2:N:151:THR:N	2.33	0.43
1:A:33:LEU:C	1:A:33:LEU:CD1	2.84	0.42
1:A:75:ILE:CD1	1:A:78:LEU:HD23	2.49	0.42
1:A:132:VAL:HG12	1:A:132:VAL:O	2.19	0.42
1:C:193:ALA:HB2	1:C:208:SER:HB2	2.01	0.42
1:C:198:HIS:O	1:C:199:GLN:C	2.62	0.42
2:D:6:GLN:HE21	2:D:6:GLN:HB3	1.66	0.42
1:E:209:PHE:C	1:E:210:ASN:ND2	2.64	0.42
2:F:167:PRO:O	2:F:168:ALA:C	2.61	0.42
1:G:179:LEU:HG	1:G:181:LEU:CD1	2.45	0.42
2:H:178:LEU:C	2:H:178:LEU:CD1	2.92	0.42
1:I:120:PRO:HG3	1:I:186:TYR:CE1	2.54	0.42
2:J:103:TRP:CD1	2:J:103:TRP:N	2.87	0.42
1:K:49:TYR:O	1:K:50:ALA:HB3	2.18	0.42
1:K:164:THR:O	1:K:164:THR:HG23	2.18	0.42
2:L:75:THR:O	2:L:76:SER:HB2	2.19	0.42
2:L:136:ALA:HB3	2:L:184:VAL:O	2.18	0.42
2:P:12:LYS:HE3	2:P:18:VAL:HG23	2.01	0.42
1:A:189:HIS:O	1:A:211:ARG:CD	2.60	0.42
2:B:13:LYS:O	2:B:15:GLY:N	2.53	0.42
2:H:207:VAL:HG12	2:H:208:ASP:H	1.84	0.42
1:I:54:LEU:HD11	1:I:58:VAL:CG1	2.48	0.42
2:J:34:ILE:HA	2:J:93:ALA:O	2.19	0.42
2:J:160:THR:HA	2:J:163:VAL:HG21	2.01	0.42
2:L:94:LYS:HB3	2:L:102:VAL:CG1	2.37	0.42
1:M:4:MET:HB3	1:M:99:GLY:CA	2.46	0.42
1:M:39:LYS:O	1:M:42:LYS:HB2	2.19	0.42
1:M:129:THR:HA	1:M:182:SER:HA	2.01	0.42
1:M:136:LEU:HD21	1:M:196:VAL:CG2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:187:GLU:CG	1:M:211:ARG:HD2	2.49	0.42
1:O:8:PRO:HD2	1:O:10:SER:H	1.80	0.42
1:A:124:GLN:HG2	1:A:129:THR:O	2.19	0.42
2:B:51:ILE:HD12	2:B:57:ALA:HB2	2.00	0.42
2:B:85:GLU:H	2:B:85:GLU:HG3	1.58	0.42
2:F:124:LEU:HD21	2:F:141:LEU:HB2	2.01	0.42
1:G:37:GLN:HG2	1:G:84:ALA:CB	2.49	0.42
1:G:61:ARG:HB3	3:G:226:HOH:O	2.20	0.42
2:H:4:LEU:O	2:H:104:GLY:HA2	2.20	0.42
1:I:91:SER:HA	1:I:96:HIS:CD2	2.54	0.42
1:I:184:ALA:HB1	1:I:188:LYS:NZ	2.34	0.42
1:K:26:SER:HB2	1:K:27:GLN:NE2	2.34	0.42
1:K:60:SER:C	1:K:62:PHE:N	2.76	0.42
1:K:209:PHE:C	1:K:210:ASN:HD22	2.24	0.42
2:L:38:ARG:HH21	2:L:86:ASP:HA	1.71	0.42
2:L:90:TYR:O	2:L:106:GLY:HA2	2.18	0.42
1:O:195:GLU:CG	1:O:204:PRO:HB3	2.49	0.42
2:P:73:GLU:HA	2:P:76:SER:HA	2.01	0.42
2:P:197:ASN:CA	2:P:208:ASP:OD2	2.58	0.42
1:A:33:LEU:HD11	1:A:35:TRP:CD1	2.53	0.42
2:B:138:LEU:CD2	2:B:182:VAL:HG13	2.50	0.42
2:H:139:GLY:O	2:H:211:VAL:HG21	2.20	0.42
1:I:135:LEU:HD13	2:J:181:VAL:HG11	2.01	0.42
1:K:14:SER:O	1:K:15:VAL:C	2.62	0.42
1:K:136:LEU:CD2	1:K:196:VAL:HG11	2.50	0.42
2:L:12:LYS:N	2:L:110:THR:O	2.46	0.42
2:P:18:VAL:O	2:P:18:VAL:HG13	2.20	0.42
2:P:49:GLY:HA3	2:P:58:ASN:O	2.19	0.42
1:C:43:VAL:CG1	1:C:44:PRO:HD2	2.50	0.42
1:C:50:ALA:HB3	1:C:53:SER:CB	2.38	0.42
2:D:4:LEU:HB2	2:D:104:GLY:HA2	2.02	0.42
2:F:40:ALA:HA	2:F:88:ALA:CB	2.50	0.42
1:G:27:GLN:HB3	3:G:228:HOH:O	2.20	0.42
2:H:201:LYS:C	2:H:203:SER:N	2.77	0.42
2:H:201:LYS:O	2:H:204:ASN:N	2.46	0.42
2:L:150:VAL:HG23	2:L:200:HIS:HB2	2.00	0.42
1:O:186:TYR:CE2	1:O:211:ARG:HD2	2.54	0.42
1:A:116:PHE:HB2	1:A:135:LEU:HB3	2.01	0.42
1:A:144:ALA:HB2	1:A:198:HIS:HD2	1.83	0.42
1:C:49:TYR:HD1	2:D:100(J):HIS:O	2.02	0.42
1:C:134:CYS:HB2	1:C:148:TRP:CZ2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:151:THR:O	2:H:198:VAL:HA	2.19	0.42
2:H:188:SER:O	2:H:189:LEU:C	2.63	0.42
1:I:27:GLN:O	1:I:28:SER:C	2.62	0.42
1:I:33:LEU:HG	1:I:71:PHE:CG	2.54	0.42
2:J:47:TRP:CZ3	2:J:49:GLY:HA2	2.55	0.42
2:J:67:VAL:CG2	2:J:68:THR:H	2.27	0.42
2:J:123:PRO:HG3	2:J:209:LYS:NZ	2.34	0.42
2:J:192:GLN:NE2	2:J:193:THR:N	2.67	0.42
1:K:79:GLN:H	1:K:82:ASP:HB2	1.84	0.42
2:L:194:TYR:O	2:L:210:LYS:HA	2.20	0.42
1:M:3:GLN:CB	1:M:26:SER:CB	2.97	0.42
1:M:6:GLN:O	1:M:7:SER:C	2.62	0.42
1:M:186:TYR:O	1:M:192:TYR:OH	2.36	0.42
1:O:42:LYS:O	1:O:43:VAL:C	2.62	0.42
2:P:23:LYS:HG2	2:P:24:ALA:N	2.34	0.42
2:P:170:LEU:HD12	2:P:171:GLN:H	1.85	0.42
1:A:6:GLN:NE2	1:A:101:GLY:CA	2.83	0.42
1:C:64:GLY:HA2	1:C:72:THR:O	2.19	0.42
2:D:71:ALA:CA	2:D:77:THR:O	2.67	0.42
2:D:87:THR:O	2:D:88:ALA:HB2	2.18	0.42
2:D:126:PRO:HG3	2:D:138:LEU:CB	2.39	0.42
1:E:193:ALA:HB2	1:E:208:SER:HB2	2.02	0.42
2:F:100(J):HIS:HB3	2:F:100(K):GLY:H	1.65	0.42
2:F:131:THR:HG22	2:F:136:ALA:CA	2.49	0.42
1:G:28:SER:OG	1:G:68:GLY:HA2	2.19	0.42
2:H:2:VAL:O	2:H:3:GLN:C	2.63	0.42
2:H:32:TYR:CD1	2:H:94:LYS:HG3	2.54	0.42
1:I:97:THR:HG22	1:I:98:PHE:N	2.33	0.42
2:J:125:ALA:HA	2:J:126:PRO:HD3	1.76	0.42
1:K:189:HIS:O	1:K:211:ARG:NH2	2.53	0.42
1:M:47:LEU:C	1:M:48:ILE:HG13	2.45	0.42
2:N:204:ASN:OD1	2:P:64:GLN:HB3	2.19	0.42
1:O:163:VAL:HG22	1:O:175:LEU:HD12	2.02	0.42
2:P:42:GLY:C	2:P:43:GLN:OE1	2.62	0.42
1:C:145:LYS:HD3	1:C:197:THR:HG21	2.02	0.42
1:C:164:THR:HG22	1:C:164:THR:O	2.20	0.42
2:D:23:LYS:HD3	2:D:24:ALA:O	2.20	0.42
2:F:2:VAL:O	2:F:2:VAL:HG13	2.20	0.42
1:G:32:TYR:CD2	1:G:92:TYR:HA	2.55	0.42
1:G:165:GLU:O	1:G:166:GLN:C	2.62	0.42
2:H:1:GLN:CD	2:H:1:GLN:H3	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:72:ASP:O	2:J:76:SER:CA	2.67	0.42
2:J:151:THR:O	2:J:152:VAL:CG2	2.64	0.42
1:K:85:THR:OG1	1:K:103:LYS:HB2	2.19	0.42
1:K:89:GLN:HE21	1:K:89:GLN:HB3	1.50	0.42
1:K:135:LEU:HD12	1:K:136:LEU:N	2.35	0.42
1:K:212:GLY:O	1:K:213:GLU:HG3	2.19	0.42
1:O:72:THR:HG22	1:O:73:LEU:N	2.34	0.42
2:P:19:LYS:HB2	2:P:81:GLU:HB2	2.00	0.42
1:A:198:HIS:ND1	1:A:199:GLN:N	2.67	0.42
2:B:138:LEU:HD21	2:B:182:VAL:HG13	2.02	0.42
2:D:53:VAL:HG12	2:D:54:PHE:N	2.34	0.42
2:F:56:SER:O	2:F:57:ALA:O	2.38	0.42
2:H:34:ILE:N	2:H:34:ILE:HD12	2.34	0.42
1:I:83:PHE:CD1	1:I:106:ILE:HG12	2.54	0.42
1:I:183:LYS:NZ	1:I:187:GLU:CD	2.78	0.42
2:J:4:LEU:HA	2:J:24:ALA:CA	2.41	0.42
2:J:64:GLN:C	2:J:66:ARG:N	2.78	0.42
2:J:178:LEU:C	2:J:178:LEU:CD1	2.93	0.42
2:L:24:ALA:O	2:L:25:SER:HB2	2.20	0.42
2:N:204:ASN:OD1	2:P:64:GLN:HB2	2.19	0.42
1:O:175:LEU:HD23	1:O:176:SER:N	2.34	0.42
1:A:117:ILE:CG2	2:B:129:LYS:HB3	2.49	0.42
2:B:100(J):HIS:N	3:B:230:HOH:O	2.53	0.42
1:E:113:PRO:HB3	1:E:139:PHE:CG	2.54	0.42
2:F:146:PHE:CE1	2:F:147:PRO:HB3	2.55	0.42
2:H:72:ASP:O	2:H:76:SER:HA	2.20	0.42
1:K:48:ILE:CG2	1:K:52:SER:O	2.68	0.42
2:P:82(C):LEU:HB3	2:P:111:VAL:HG11	2.01	0.42
1:A:24:ARG:HG2	1:A:70:ASP:CG	2.44	0.41
1:A:149:LYS:HG3	1:A:154:LEU:HD13	2.02	0.41
2:B:170:LEU:HD13	2:B:176:TYR:CD1	2.55	0.41
1:E:14:SER:HB2	1:E:17:ASP:CG	2.45	0.41
1:G:39:LYS:CD	1:G:84:ALA:HB2	2.44	0.41
1:G:154:LEU:H	1:G:154:LEU:CD2	2.32	0.41
2:H:7:SER:HG	2:H:20:VAL:HG13	1.85	0.41
2:H:51:ILE:CD1	2:H:57:ALA:HB2	2.49	0.41
2:H:116:THR:O	2:H:117:LYS:HB2	2.19	0.41
2:H:140:CYS:SG	2:H:211:VAL:HG21	2.60	0.41
1:I:12:SER:HA	1:I:105:GLU:HG2	2.02	0.41
1:I:95:SER:O	1:I:96:HIS:CD2	2.72	0.41
1:I:144:ALA:CB	1:I:175:LEU:HD13	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:198:VAL:HG12	2:J:199:ASN:N	2.34	0.41
2:L:6:GLN:OE1	2:L:92:CYS:N	2.52	0.41
2:L:90:TYR:CE1	2:L:109:VAL:HB	2.54	0.41
1:M:19:VAL:CG2	1:M:78:LEU:HD21	2.50	0.41
1:O:203:SER:O	1:O:204:PRO:C	2.63	0.41
1:C:11:LEU:C	1:C:11:LEU:CD2	2.94	0.41
1:E:179:LEU:HD12	1:E:180:THR:N	2.35	0.41
2:F:39:GLN:HG3	2:F:43:GLN:O	2.20	0.41
1:G:132:VAL:CG1	1:G:148:TRP:CH2	3.02	0.41
2:J:67:VAL:HB	2:J:82:LEU:HD12	2.02	0.41
2:J:93:ALA:HB1	2:J:100(L):MET:HB3	2.02	0.41
1:K:48:ILE:HG23	1:K:52:SER:O	2.20	0.41
1:M:63:SER:O	1:M:73:LEU:HD12	2.20	0.41
1:M:102:THR:O	1:M:102:THR:HG22	2.20	0.41
1:A:33:LEU:CD1	1:A:35:TRP:NE1	2.75	0.41
2:D:47:TRP:CH2	2:D:49:GLY:HA2	2.55	0.41
1:E:30:SER:O	1:E:71:PHE:HZ	2.04	0.41
2:H:152:VAL:HG11	2:H:180:SER:HB3	2.01	0.41
1:I:193:ALA:CA	1:I:208:SER:HB3	2.50	0.41
2:J:17:SER:HB3	2:J:82(A):SER:OG	2.20	0.41
2:J:155:ASN:OD1	2:J:193:THR:O	2.38	0.41
2:J:189:LEU:HD23	2:J:194:TYR:HE2	1.85	0.41
2:L:150:VAL:HG22	2:L:151:THR:H	1.84	0.41
1:O:193:ALA:HB1	1:O:206:THR:HG22	2.02	0.41
2:P:94:LYS:C	2:P:94:LYS:CD	2.89	0.41
2:P:103:TRP:CD1	2:P:103:TRP:N	2.87	0.41
2:B:154:TRP:C	2:B:156:SER:N	2.78	0.41
2:D:152:VAL:CG1	2:D:153:SER:N	2.83	0.41
2:F:2:VAL:HA	2:F:26:GLY:CA	2.50	0.41
2:F:94:LYS:HE2	2:F:95:GLY:N	2.36	0.41
1:G:18:ARG:C	1:G:19:VAL:HG23	2.44	0.41
2:H:59:TYR:HH	2:H:69:ILE:H	1.64	0.41
2:H:72:ASP:O	2:H:76:SER:CA	2.68	0.41
2:H:155:ASN:HD22	2:H:159:LEU:HB3	1.85	0.41
2:J:52:ILE:O	2:J:53:VAL:N	2.40	0.41
2:J:154:TRP:O	2:J:155:ASN:C	2.61	0.41
1:K:6:GLN:HB2	1:K:100:GLN:HE21	1.85	0.41
1:K:195:GLU:CB	1:K:206:THR:HG23	2.44	0.41
2:L:13:LYS:O	2:L:14:PRO:C	2.63	0.41
2:L:55:GLY:O	2:L:56:SER:OG	2.35	0.41
2:L:116:THR:HG23	2:L:202:PRO:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:49:TYR:O	1:M:50:ALA:HB3	2.20	0.41
2:N:29:PHE:HB2	2:N:76:SER:HB2	2.03	0.41
2:N:52:ILE:O	2:N:52(A):PRO:C	2.61	0.41
2:N:52:ILE:HG21	2:N:54:PHE:CZ	2.54	0.41
1:O:80:PRO:HA	1:O:83:PHE:HE1	1.85	0.41
1:O:132:VAL:HG12	1:O:133:VAL:N	2.35	0.41
2:P:40:ALA:HB3	2:P:43:GLN:HG3	2.02	0.41
1:A:11:LEU:HD22	1:A:104:LEU:HD23	1.86	0.41
2:B:52:ILE:HG22	2:B:53:VAL:HG23	2.03	0.41
2:B:72:ASP:O	2:B:75:THR:OG1	2.37	0.41
2:B:145:TYR:O	2:B:175:LEU:HB3	2.20	0.41
1:C:36:TYR:HE1	1:C:89:GLN:NE2	2.19	0.41
1:C:70:ASP:OD2	1:C:70:ASP:N	2.52	0.41
2:H:28:THR:O	2:H:29:PHE:O	2.38	0.41
2:H:124:LEU:CG	2:H:141:LEU:H	2.28	0.41
1:I:33:LEU:HB3	1:I:51:ALA:HB2	2.02	0.41
2:L:39:GLN:O	2:L:89:VAL:HG23	2.20	0.41
2:L:170:LEU:CD1	2:L:174:GLY:O	2.68	0.41
1:M:43:VAL:HG13	1:M:44:PRO:HD2	2.02	0.41
1:M:48:ILE:HD12	1:M:73:LEU:HD13	2.02	0.41
1:M:136:LEU:CG	1:M:196:VAL:HG21	2.48	0.41
2:N:72:ASP:O	2:N:76:SER:N	2.52	0.41
2:N:186:SER:O	2:N:187:SER:C	2.63	0.41
2:P:29:PHE:HE2	2:P:78:THR:HG1	1.69	0.41
2:P:61:GLN:O	2:P:62:LYS:C	2.63	0.41
2:B:21:SER:O	2:B:22:CYS:CB	2.68	0.41
2:B:124:LEU:HB2	2:B:139:GLY:O	2.21	0.41
2:B:211:VAL:O	2:B:212:GLU:HG2	2.20	0.41
1:C:195:GLU:HB2	1:C:206:THR:OG1	2.19	0.41
2:D:29:PHE:CE1	2:D:73:GLU:HA	2.55	0.41
2:D:36:TRP:HZ2	2:D:78:THR:O	2.03	0.41
2:D:52:ILE:C	2:D:53:VAL:N	2.79	0.41
2:D:80:MET:HE2	2:D:90:TYR:CD2	2.56	0.41
1:E:136:LEU:HD11	1:E:146:VAL:HG22	2.03	0.41
1:E:147:GLN:NE2	1:I:11:LEU:CD2	2.68	0.41
1:G:47:LEU:O	1:G:48:ILE:HG12	2.21	0.41
1:G:148:TRP:CZ3	1:G:194:CYS:HB3	2.55	0.41
1:G:169:LYS:HG3	1:G:170:ASP:OD1	2.20	0.41
2:H:169:VAL:O	2:H:169:VAL:HG12	2.20	0.41
1:I:118:PHE:CE1	2:J:124:LEU:O	2.73	0.41
1:K:67:SER:HA	1:K:71:PHE:CZ	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:108:ARG:HD3	1:K:171:SER:O	2.20	0.41
1:O:49:TYR:CE1	1:O:53:SER:HB3	2.55	0.41
2:P:192:GLN:NE2	2:P:193:THR:H	2.03	0.41
1:A:113:PRO:HB3	1:A:139:PHE:HB3	2.02	0.41
2:B:35:SER:HG	2:B:47:TRP:NE1	2.19	0.41
2:B:178:LEU:C	2:B:178:LEU:HD12	2.44	0.41
1:C:33:LEU:HD21	1:C:88:CYS:HB2	2.03	0.41
2:D:27:GLY:O	2:D:28:THR:C	2.62	0.41
2:D:51:ILE:O	2:D:52:ILE:HG12	2.20	0.41
1:E:198:HIS:ND1	1:E:200:GLY:N	2.67	0.41
2:F:2:VAL:HB	2:F:27:GLY:N	2.36	0.41
1:G:186:TYR:CE1	1:G:192:TYR:CE2	3.04	0.41
2:H:36:TRP:CD2	2:H:80:MET:HG3	2.54	0.41
2:H:150:VAL:HG22	2:H:151:THR:O	2.20	0.41
2:H:201:LYS:C	2:H:203:SER:H	2.27	0.41
1:I:37:GLN:HB2	1:I:47:LEU:HD11	2.01	0.41
2:J:6:GLN:HG3	2:J:104:GLY:HA3	2.03	0.41
1:K:66:GLY:HA3	1:K:70:ASP:O	2.21	0.41
1:M:136:LEU:N	1:M:136:LEU:CD1	2.84	0.41
2:N:87:THR:O	2:N:88:ALA:HB2	2.20	0.41
1:O:83:PHE:CD1	1:O:106:ILE:HD13	2.56	0.41
1:A:198:HIS:ND1	1:A:198:HIS:C	2.78	0.41
2:B:29:PHE:O	2:B:30:SER:C	2.63	0.41
1:C:210:ASN:N	1:C:210:ASN:ND2	2.67	0.41
1:E:90:GLN:OE1	1:E:90:GLN:O	2.37	0.41
2:F:62:LYS:C	2:F:64:GLN:H	2.26	0.41
2:F:214:LYS:OXT	2:F:214:LYS:HG3	2.21	0.41
1:I:122:ASP:HA	1:I:125:LEU:HB2	2.03	0.41
2:J:52:ILE:C	2:J:53:VAL:N	2.77	0.41
2:J:154:TRP:HB3	2:J:159:LEU:HD23	2.03	0.41
1:K:195:GLU:HB2	1:K:206:THR:CG2	2.45	0.41
2:L:115:SER:O	2:L:146:PHE:HB3	2.19	0.41
1:A:55:GLN:O	1:A:58:VAL:HG23	2.21	0.41
1:A:184:ALA:O	1:A:185:ASP:C	2.64	0.41
2:B:72:ASP:OD2	2:B:74:ALA:HB3	2.21	0.41
1:C:120:PRO:HD3	1:C:132:VAL:HG22	2.03	0.41
2:D:143:LYS:HZ2	2:D:143:LYS:HG3	1.71	0.41
1:E:115:VAL:HG21	1:E:205:VAL:HG11	2.02	0.41
1:E:202:SER:OG	1:E:203:SER:N	2.54	0.41
2:F:87:THR:CG2	2:F:110:THR:HA	2.28	0.41
1:G:32:TYR:CB	1:G:92:TYR:H	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:39:LYS:HZ1	1:G:81:GLU:C	2.29	0.41
1:G:139:PHE:HZ	1:G:175:LEU:H	1.69	0.41
1:G:148:TRP:O	1:G:155:GLN:N	2.53	0.41
1:G:158:ASN:HD22	1:K:22:THR:CG2	2.34	0.41
1:I:89:GLN:HB2	1:I:98:PHE:HE2	1.85	0.41
1:I:195:GLU:CG	1:I:196:VAL:N	2.84	0.41
2:J:9:ALA:C	2:J:10:GLU:HG2	2.45	0.41
2:J:90:TYR:N	2:J:90:TYR:HD1	2.18	0.41
2:J:101:ASP:OD1	2:J:101:ASP:O	2.38	0.41
2:L:35:SER:N	2:L:93:ALA:O	2.53	0.41
2:L:115:SER:CB	2:L:117:LYS:HE2	2.48	0.41
2:L:195:ILE:N	2:L:195:ILE:HD12	2.36	0.41
1:M:80:PRO:C	1:M:82:ASP:H	2.28	0.41
1:M:96:HIS:O	2:N:47:TRP:CG	2.73	0.41
1:M:140:TYR:CA	1:M:141:PRO:O	2.67	0.41
2:N:117:LYS:HG2	2:N:118:GLY:O	2.21	0.41
1:O:37:GLN:CG	1:O:38:GLN:N	2.83	0.41
1:O:164:THR:HG22	1:O:174:SER:H	1.85	0.41
2:P:6:GLN:NE2	2:P:90:TYR:O	2.52	0.41
2:P:199:ASN:ND2	2:P:200:HIS:N	2.68	0.41
1:A:108:ARG:NH2	1:A:111:ALA:HB2	2.36	0.41
1:A:175:LEU:HD23	1:A:175:LEU:C	2.46	0.41
1:C:151:ASP:O	1:C:152:ASN:HB2	2.20	0.41
1:E:112:ALA:HB1	1:E:201:LEU:HD21	2.01	0.41
2:F:80:MET:SD	2:F:80:MET:O	2.79	0.41
2:F:168:ALA:HB2	2:F:178:LEU:HD23	2.02	0.41
2:H:29:PHE:O	2:H:30:SER:C	2.63	0.41
2:J:2:VAL:HG11	2:J:94:LYS:NZ	2.36	0.41
1:K:198:HIS:C	1:K:200:GLY:N	2.79	0.41
2:L:85:GLU:OE2	2:L:85:GLU:N	2.54	0.41
1:M:140:TYR:CD1	1:M:141:PRO:N	2.89	0.41
2:N:184:VAL:CG2	2:N:194:TYR:OH	2.68	0.41
1:O:20:THR:HG23	1:O:72:THR:HG23	2.03	0.41
1:O:117:ILE:HG22	2:P:129:LYS:HB3	2.03	0.41
1:A:95:SER:HA	2:B:47:TRP:CZ3	2.56	0.40
2:B:195:ILE:HD11	2:B:210:LYS:HD2	2.03	0.40
1:E:48:ILE:HD12	1:E:73:LEU:CD1	2.40	0.40
1:E:121:SER:HB2	1:E:123:GLU:OE2	2.21	0.40
2:F:20:VAL:O	2:F:21:SER:HB3	2.22	0.40
2:F:38:ARG:O	2:F:46:GLU:N	2.54	0.40
2:F:125:ALA:HA	2:F:126:PRO:HD3	1.81	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:52:ILE:O	2:H:52(A):PRO:C	2.64	0.40
2:H:52(A):PRO:C	2:H:54:PHE:N	2.78	0.40
2:J:160:THR:C	2:J:163:VAL:HG23	2.46	0.40
1:K:33:LEU:HB3	1:K:71:PHE:CD2	2.56	0.40
2:L:51:ILE:HG12	2:L:52:ILE:N	2.32	0.40
1:M:136:LEU:O	1:M:139:PHE:CE1	2.74	0.40
1:O:20:THR:HG1	1:O:74:THR:HG1	1.69	0.40
1:O:27:GLN:O	1:O:28:SER:C	2.65	0.40
1:O:108:ARG:NH1	1:O:172:THR:CG2	2.84	0.40
1:O:159:SER:HB2	1:O:178:THR:C	2.46	0.40
2:P:207:VAL:CG1	2:P:208:ASP:N	2.84	0.40
2:B:4:LEU:HD13	2:B:92:CYS:O	2.21	0.40
2:B:83:ARG:O	2:B:111:VAL:HG11	2.21	0.40
1:C:14:SER:HB2	1:C:17:ASP:CG	2.47	0.40
1:C:18:ARG:NH1	1:C:76:SER:O	2.54	0.40
1:C:61:ARG:HD3	1:C:79:GLN:NE2	2.36	0.40
2:D:32:TYR:HB2	2:D:34:ILE:HD12	2.03	0.40
1:E:96:HIS:O	1:E:97:THR:HG23	2.21	0.40
1:E:164:THR:CG2	1:E:174:SER:HB2	2.51	0.40
2:F:17:SER:HB2	2:F:82(A):SER:HA	1.99	0.40
2:F:29:PHE:CB	2:F:76:SER:HB2	2.51	0.40
2:F:142:VAL:HB	2:F:178:LEU:CD1	2.51	0.40
2:F:152:VAL:HG11	2:F:180:SER:CB	2.51	0.40
2:F:185:PRO:O	2:F:188:SER:OG	2.28	0.40
1:K:111:ALA:O	1:K:139:PHE:CA	2.66	0.40
1:K:125:LEU:O	1:K:128:GLY:N	2.48	0.40
2:L:200:HIS:C	2:L:202:PRO:CD	2.95	0.40
2:N:36:TRP:CZ2	2:N:80:MET:HB2	2.57	0.40
2:N:82(A):SER:O	2:N:82(B):SER:C	2.65	0.40
1:O:154:LEU:HD22	1:O:154:LEU:HA	1.88	0.40
1:A:117:ILE:HB	1:A:207:LYS:HG2	2.03	0.40
1:A:124:GLN:HE22	1:A:131:SER:CB	2.34	0.40
2:B:41:PRO:O	2:B:42:GLY:C	2.64	0.40
2:B:170:LEU:HD13	2:B:176:TYR:CZ	2.56	0.40
2:B:176:TYR:CD2	2:B:176:TYR:N	2.89	0.40
1:C:11:LEU:HD22	1:C:12:SER:N	2.37	0.40
1:C:34:ASN:OD1	1:C:49:TYR:HA	2.22	0.40
1:C:186:TYR:O	1:C:187:GLU:C	2.65	0.40
2:D:77:THR:CG2	2:D:78:THR:N	2.84	0.40
2:H:197:ASN:HA	2:H:208:ASP:OD2	2.21	0.40
1:I:141:PRO:C	1:I:143:GLU:H	2.30	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:51:ILE:HG23	2:J:52:ILE:N	2.37	0.40
2:J:62:LYS:HG3	2:J:63:PHE:N	2.36	0.40
2:L:128:SER:HA	2:L:131:THR:OG1	2.22	0.40
2:L:193:THR:HG22	2:L:195:ILE:CD1	2.51	0.40
1:M:136:LEU:HD21	1:M:196:VAL:HG22	2.03	0.40
1:O:115:VAL:O	1:O:116:PHE:CD2	2.75	0.40
1:O:122:ASP:HA	1:O:125:LEU:HD12	2.03	0.40
2:P:6:GLN:N	2:P:105:GLN:OE1	2.52	0.40
2:P:199:ASN:HD22	2:P:199:ASN:C	2.28	0.40
1:A:141:PRO:HB2	1:A:143:GLU:OE2	2.21	0.40
2:B:5:LEU:O	2:B:23:LYS:N	2.55	0.40
2:D:84:SER:O	2:D:86:ASP:N	2.49	0.40
2:F:11:VAL:HG11	2:F:146:PHE:CZ	2.57	0.40
2:F:48:MET:O	2:F:60:ALA:N	2.55	0.40
2:F:61:GLN:OE1	2:J:83:ARG:HD3	2.22	0.40
2:F:63:PHE:H	2:F:63:PHE:HD1	1.68	0.40
2:F:94:LYS:HZ1	2:F:96:GLY:H	1.69	0.40
1:G:124:GLN:C	1:G:126:LYS:N	2.78	0.40
2:H:63:PHE:O	2:H:64:GLN:C	2.64	0.40
2:H:131:THR:HA	2:H:135:THR:O	2.21	0.40
1:I:79:GLN:HB3	1:I:81:GLU:OE1	2.21	0.40
2:J:17:SER:HB3	2:J:82(A):SER:CB	2.51	0.40
2:J:166:PHE:HA	2:J:167:PRO:HD3	1.90	0.40
1:K:55:GLN:CD	1:K:56:SER:H	2.30	0.40
1:K:121:SER:HB2	1:K:123:GLU:OE1	2.21	0.40
1:O:14:SER:O	1:O:17:ASP:OD1	2.39	0.40
2:P:7:SER:OG	2:P:10:GLU:OE2	2.36	0.40
1:A:28:SER:CA	1:A:69:THR:HG22	2.47	0.40
1:A:48:ILE:CG2	1:A:49:TYR:H	2.34	0.40
2:D:34:ILE:HD12	2:D:34:ILE:H	1.87	0.40
2:D:54:PHE:O	2:D:55:GLY:C	2.64	0.40
2:D:171:GLN:C	2:D:173:SER:H	2.28	0.40
1:G:113:PRO:HA	1:G:137:ASN:O	2.22	0.40
2:H:164:HIS:ND1	2:H:164:HIS:N	2.69	0.40
1:I:6:GLN:OE1	1:I:101:GLY:N	2.44	0.40
1:I:36:TYR:HE2	2:J:100(L):MET:O	2.05	0.40
1:K:175:LEU:HD23	1:K:175:LEU:C	2.47	0.40
2:L:50:GLY:O	2:L:57:ALA:CB	2.65	0.40
1:M:26:SER:HG	1:M:27:GLN:CD	2.27	0.40
1:O:33:LEU:HD13	1:O:34:ASN:N	2.37	0.40
1:O:35:TRP:CB	1:O:73:LEU:HD13	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:134:CYS:HB3	1:O:177:SER:HB3	2.04	0.40
2:P:75:THR:OG1	2:P:77:THR:OG1	2.35	0.40
2:P:184:VAL:HG11	2:P:194:TYR:CZ	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	209/212 (99%)	170 (81%)	29 (14%)	10 (5%)	2	7
1	C	210/212 (99%)	171 (81%)	24 (11%)	15 (7%)	1	2
1	E	209/212 (99%)	168 (80%)	32 (15%)	9 (4%)	2	8
1	G	209/212 (99%)	167 (80%)	28 (13%)	14 (7%)	1	3
1	I	209/212 (99%)	160 (77%)	39 (19%)	10 (5%)	2	7
1	K	209/212 (99%)	160 (77%)	37 (18%)	12 (6%)	1	4
1	M	209/212 (99%)	166 (79%)	32 (15%)	11 (5%)	1	5
1	O	209/212 (99%)	164 (78%)	34 (16%)	11 (5%)	1	5
2	B	212/230 (92%)	153 (72%)	40 (19%)	19 (9%)	0	1
2	D	212/230 (92%)	152 (72%)	44 (21%)	16 (8%)	1	2
2	F	213/230 (93%)	153 (72%)	42 (20%)	18 (8%)	0	1
2	H	212/230 (92%)	146 (69%)	42 (20%)	24 (11%)	0	1
2	J	212/230 (92%)	151 (71%)	40 (19%)	21 (10%)	0	1
2	L	211/230 (92%)	152 (72%)	39 (18%)	20 (10%)	0	1
2	N	212/230 (92%)	164 (77%)	30 (14%)	18 (8%)	0	1
2	P	212/230 (92%)	152 (72%)	37 (18%)	23 (11%)	0	1
All	All	3369/3536 (95%)	2549 (76%)	569 (17%)	251 (8%)	1	2

All (251) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	11	LEU
1	A	211	ARG
2	B	22	CYS
2	B	30	SER
2	B	61	GLN
2	B	82(B)	SER
2	B	101	ASP
2	B	130	SER
1	C	7	SER
1	C	8	PRO
1	C	63	SER
1	C	78	LEU
1	C	184	ALA
2	D	53	VAL
2	D	100(L)	MET
1	E	8	PRO
1	E	67	SER
1	E	143	GLU
2	F	2	VAL
2	F	52(A)	PRO
2	F	53	VAL
2	F	57	ALA
2	F	61	GLN
2	F	158	ALA
2	F	182	VAL
2	F	213	PRO
1	G	8	PRO
1	G	117	ILE
1	G	143	GLU
2	H	29	PHE
2	H	30	SER
2	H	76	SER
2	H	149	PRO
2	H	189	LEU
1	I	8	PRO
1	I	92	TYR
1	I	184	ALA
2	J	63	PHE
2	J	74	ALA
2	J	87	THR
2	J	146	PHE
2	J	182	VAL

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Mol	Chain	Res	Type
2	J	204	ASN
1	K	8	PRO
1	K	157	GLY
1	K	203	SER
2	L	7	SER
2	L	24	ALA
2	L	56	SER
2	L	72	ASP
2	L	182	VAL
2	L	203	SER
1	M	8	PRO
1	M	93	SER
2	N	9	ALA
2	N	32	TYR
2	N	56	SER
2	N	61	GLN
2	N	144	ASP
1	O	8	PRO
1	O	15	VAL
1	O	59	PRO
1	O	113	PRO
1	O	171	SER
1	O	183	LYS
1	O	204	PRO
2	P	7	SER
2	P	16	SER
2	P	22	CYS
2	P	61	GLN
2	P	146	PHE
2	P	204	ASN
1	A	41	GLY
1	A	68	GLY
1	A	121	SER
2	B	16	SER
2	B	53	VAL
2	B	125	ALA
2	B	188	SER
2	B	204	ASN
1	C	30	SER
1	C	32	TYR
1	C	54	LEU
1	C	185	ASP

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Mol	Chain	Res	Type
2	D	28	THR
2	D	55	GLY
2	D	85	GLU
2	D	111	VAL
1	E	152	ASN
2	F	20	VAL
2	F	55	GLY
2	F	63	PHE
2	F	71	ALA
1	G	7	SER
1	G	92	TYR
1	G	96	HIS
1	G	187	GLU
2	H	82(C)	LEU
2	H	85	GLU
2	H	112	ALA
2	H	198	VAL
2	H	209	LYS
2	J	65	GLY
2	J	109	VAL
2	J	127	SER
2	J	164	HIS
1	K	30	SER
1	K	53	SER
1	K	125	LEU
2	L	9	ALA
2	L	14	PRO
2	L	26	GLY
2	L	29	PHE
2	L	51	ILE
2	L	61	GLN
1	M	30	SER
1	M	152	ASN
1	M	156	SER
2	N	25	SER
2	N	53	VAL
2	N	82(B)	SER
2	N	86	ASP
2	N	189	LEU
1	O	138	ASN
2	P	2	VAL
2	P	18	VAL

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Mol	Chain	Res	Type
2	P	29	PHE
2	P	32	TYR
2	P	127	SER
1	A	30	SER
1	A	40	PRO
1	A	138	ASN
1	A	156	SER
2	B	55	GLY
2	B	62	LYS
2	B	82(A)	SER
1	C	28	SER
1	C	67	SER
2	D	30	SER
2	D	116	THR
2	D	202	PRO
1	E	138	ASN
1	E	156	SER
2	F	82(C)	LEU
2	F	144	ASP
2	F	189	LEU
1	G	54	LEU
1	G	168	SER
1	G	186	TYR
2	H	3	GLN
2	H	16	SER
1	I	13	ALA
1	I	152	ASN
2	J	9	ALA
2	J	29	PHE
2	J	82(B)	SER
2	L	187	SER
1	M	78	LEU
2	N	6	GLN
2	N	127	SER
2	N	204	ASN
1	O	51	ALA
2	P	56	SER
2	P	82(B)	SER
2	P	100(L)	MET
2	P	177	SER
2	B	14	PRO
2	B	51	ILE

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Mol	Chain	Res	Type
2	B	52(A)	PRO
1	C	186	TYR
2	D	3	GLN
2	D	52(A)	PRO
2	D	114	ALA
2	D	144	ASP
2	D	192	GLN
1	E	84	ALA
1	E	108	ARG
2	F	101	ASP
1	G	11	LEU
1	G	76	SER
1	G	184	ALA
2	H	88	ALA
2	H	113	SER
2	H	129	LYS
2	H	147	PRO
2	H	201	LYS
1	I	30	SER
1	I	111	ALA
1	I	138	ASN
1	I	142	ARG
2	J	73	GLU
2	J	126	PRO
1	K	166	GLN
2	L	25	SER
2	L	82(B)	SER
2	L	114	ALA
2	L	144	ASP
1	M	59	PRO
1	M	138	ASN
2	N	72	ASP
2	N	158	ALA
2	P	3	GLN
2	P	30	SER
2	P	52(A)	PRO
1	A	93	SER
1	C	156	SER
1	C	166	GLN
1	C	204	PRO
2	D	60	ALA
2	D	123	PRO

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Mol	Chain	Res	Type
2	H	117	LYS
2	H	124	LEU
1	I	188	LYS
2	J	152	VAL
1	K	109	THR
2	L	74	ALA
2	L	201	LYS
1	M	123	GLU
2	N	31	SER
2	P	33	ALA
2	P	62	LYS
2	P	74	ALA
2	P	201	LYS
2	B	155	ASN
1	E	40	PRO
2	F	88	ALA
2	F	123	PRO
1	G	30	SER
2	H	61	GLN
2	J	18	VAL
2	J	202	PRO
1	K	93	SER
2	L	177	SER
1	M	81	GLU
2	N	106	GLY
1	O	43	VAL
2	P	202	PRO
1	K	44	PRO
1	K	204	PRO
1	M	204	PRO
1	O	112	ALA
2	H	150	VAL
2	J	53	VAL
2	J	100(K)	GLY
2	H	152	VAL
2	H	185	PRO
2	H	195	ILE
2	J	52(A)	PRO
2	B	149	PRO
2	N	149	PRO
1	K	141	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	187/188 (100%)	156 (83%)	31 (17%)	2	7
1	C	188/188 (100%)	157 (84%)	31 (16%)	2	8
1	E	187/188 (100%)	158 (84%)	29 (16%)	2	9
1	G	187/188 (100%)	163 (87%)	24 (13%)	4	14
1	I	187/188 (100%)	166 (89%)	21 (11%)	6	19
1	K	187/188 (100%)	166 (89%)	21 (11%)	6	19
1	M	187/188 (100%)	162 (87%)	25 (13%)	4	12
1	O	187/188 (100%)	160 (86%)	27 (14%)	3	11
2	B	176/189 (93%)	150 (85%)	26 (15%)	3	10
2	D	176/189 (93%)	159 (90%)	17 (10%)	8	25
2	F	177/189 (94%)	156 (88%)	21 (12%)	5	16
2	H	176/189 (93%)	158 (90%)	18 (10%)	7	23
2	J	176/189 (93%)	155 (88%)	21 (12%)	5	16
2	L	176/189 (93%)	158 (90%)	18 (10%)	7	23
2	N	176/189 (93%)	157 (89%)	19 (11%)	6	21
2	P	176/189 (93%)	152 (86%)	24 (14%)	3	12
All	All	2906/3016 (96%)	2533 (87%)	373 (13%)	4	14

All (373) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ILE
1	A	3	GLN
1	A	8	PRO
1	A	11	LEU
1	A	18	ARG
1	A	19	VAL
1	A	20	THR
1	A	26	SER

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Mol	Chain	Res	Type
1	A	27	GLN
1	A	33	LEU
1	A	56	SER
1	A	65	SER
1	A	72	THR
1	A	74	THR
1	A	75	ILE
1	A	81	GLU
1	A	90	GLN
1	A	94	THR
1	A	102	THR
1	A	103	LYS
1	A	105	GLU
1	A	106	ILE
1	A	132	VAL
1	A	135	LEU
1	A	154	LEU
1	A	158	ASN
1	A	175	LEU
1	A	180	THR
1	A	181	LEU
1	A	195	GLU
1	A	211	ARG
2	B	5	LEU
2	B	17	SER
2	B	20	VAL
2	B	28	THR
2	B	30	SER
2	B	53	VAL
2	B	54	PHE
2	B	58	ASN
2	B	61	GLN
2	B	66	ARG
2	B	73	GLU
2	B	85	GLU
2	B	100(J)	HIS
2	B	100(L)	MET
2	B	101	ASP
2	B	135	THR
2	B	141	LEU
2	B	149	PRO
2	B	169	VAL

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Mol	Chain	Res	Type
2	B	170	LEU
2	B	175	LEU
2	B	178	LEU
2	B	187	SER
2	B	191	THR
2	B	193	THR
2	B	199	ASN
1	C	3	GLN
1	C	5	THR
1	C	6	GLN
1	C	8	PRO
1	C	10	SER
1	C	11	LEU
1	C	23	CYS
1	C	47	LEU
1	C	49	TYR
1	C	62	PHE
1	C	70	ASP
1	C	72	THR
1	C	75	ILE
1	C	80	PRO
1	C	89	GLN
1	C	90	GLN
1	C	94	THR
1	C	104	LEU
1	C	105	GLU
1	C	117	ILE
1	C	127	SER
1	C	129	THR
1	C	136	LEU
1	C	163	VAL
1	C	164	THR
1	C	176	SER
1	C	180	THR
1	C	195	GLU
1	C	197	THR
1	C	204	PRO
1	C	205	VAL
2	D	6	GLN
2	D	21	SER
2	D	29	PHE
2	D	37	VAL

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Mol	Chain	Res	Type
2	D	39	GLN
2	D	59	TYR
2	D	61	GLN
2	D	62	LYS
2	D	101	ASP
2	D	102	VAL
2	D	138	LEU
2	D	151	THR
2	D	161	SER
2	D	178	LEU
2	D	182	VAL
2	D	193	THR
2	D	205	THR
1	E	15	VAL
1	E	22	THR
1	E	26	SER
1	E	40	PRO
1	E	47	LEU
1	E	49	TYR
1	E	63	SER
1	E	72	THR
1	E	76	SER
1	E	85	THR
1	E	90	GLN
1	E	93	SER
1	E	98	PHE
1	E	105	GLU
1	E	126	LYS
1	E	127	SER
1	E	129	THR
1	E	131	SER
1	E	143	GLU
1	E	152	ASN
1	E	154	LEU
1	E	158	ASN
1	E	161	GLU
1	E	163	VAL
1	E	175	LEU
1	E	179	LEU
1	E	180	THR
1	E	197	THR
1	E	210	ASN

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Mol	Chain	Res	Type
2	F	21	SER
2	F	22	CYS
2	F	34	ILE
2	F	54	PHE
2	F	67	VAL
2	F	78	THR
2	F	84	SER
2	F	94	LYS
2	F	103	TRP
2	F	108	THR
2	F	135	THR
2	F	145	TYR
2	F	147	PRO
2	F	164	HIS
2	F	172	SER
2	F	180	SER
2	F	182	VAL
2	F	184	VAL
2	F	193	THR
2	F	199	ASN
2	F	205	THR
1	G	2	ILE
1	G	11	LEU
1	G	22	THR
1	G	24	ARG
1	G	34	ASN
1	G	48	ILE
1	G	54	LEU
1	G	72	THR
1	G	78	LEU
1	G	79	GLN
1	G	89	GLN
1	G	90	GLN
1	G	94	THR
1	G	102	THR
1	G	106	ILE
1	G	118	PHE
1	G	123	GLU
1	G	137	ASN
1	G	158	ASN
1	G	166	GLN
1	G	175	LEU

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Mol	Chain	Res	Type
1	G	180	THR
1	G	209	PHE
1	G	210	ASN
2	H	3	GLN
2	H	18	VAL
2	H	38	ARG
2	H	54	PHE
2	H	64	GLN
2	H	69	ILE
2	H	70	THR
2	H	73	GLU
2	H	76	SER
2	H	101	ASP
2	H	110	THR
2	H	131	THR
2	H	176	TYR
2	H	178	LEU
2	H	183	THR
2	H	191	THR
2	H	199	ASN
2	H	206	LYS
1	I	11	LEU
1	I	22	THR
1	I	33	LEU
1	I	34	ASN
1	I	43	VAL
1	I	54	LEU
1	I	72	THR
1	I	73	LEU
1	I	77	SER
1	I	78	LEU
1	I	90	GLN
1	I	109	THR
1	I	127	SER
1	I	154	LEU
1	I	164	THR
1	I	174	SER
1	I	175	LEU
1	I	177	SER
1	I	181	LEU
1	I	207	LYS
1	I	210	ASN

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Mol	Chain	Res	Type
2	J	17	SER
2	J	29	PHE
2	J	43	GLN
2	J	45	LEU
2	J	61	GLN
2	J	66	ARG
2	J	81	GLU
2	J	83	ARG
2	J	85	GLU
2	J	89	VAL
2	J	90	TYR
2	J	91	PHE
2	J	111	VAL
2	J	132	SER
2	J	135	THR
2	J	141	LEU
2	J	149	PRO
2	J	150	VAL
2	J	164	HIS
2	J	191	THR
2	J	208	ASP
1	K	18	ARG
1	K	32	TYR
1	K	44	PRO
1	K	70	ASP
1	K	77	SER
1	K	89	GLN
1	K	94	THR
1	K	100	GLN
1	K	105	GLU
1	K	106	ILE
1	K	110	VAL
1	K	123	GLU
1	K	126	LYS
1	K	152	ASN
1	K	161	GLU
1	K	163	VAL
1	K	179	LEU
1	K	195	GLU
1	K	204	PRO
1	K	206	THR
1	K	210	ASN

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Mol	Chain	Res	Type
2	L	7	SER
2	L	17	SER
2	L	51	ILE
2	L	89	VAL
2	L	102	VAL
2	L	110	THR
2	L	119	PRO
2	L	121	VAL
2	L	140	CYS
2	L	141	LEU
2	L	149	PRO
2	L	159	LEU
2	L	165	THR
2	L	172	SER
2	L	175	LEU
2	L	182	VAL
2	L	197	ASN
2	L	207	VAL
1	M	18	ARG
1	M	22	THR
1	M	33	LEU
1	M	36	TYR
1	M	37	GLN
1	M	44	PRO
1	M	59	PRO
1	M	72	THR
1	M	77	SER
1	M	78	LEU
1	M	80	PRO
1	M	104	LEU
1	M	105	GLU
1	M	110	VAL
1	M	117	ILE
1	M	123	GLU
1	M	136	LEU
1	M	158	ASN
1	M	160	GLN
1	M	163	VAL
1	M	164	THR
1	M	179	LEU
1	M	180	THR
1	M	181	LEU

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Mol	Chain	Res	Type
1	M	210	ASN
2	N	4	LEU
2	N	6	GLN
2	N	7	SER
2	N	11	VAL
2	N	67	VAL
2	N	89	VAL
2	N	109	VAL
2	N	124	LEU
2	N	131	THR
2	N	140	CYS
2	N	147	PRO
2	N	149	PRO
2	N	178	LEU
2	N	181	VAL
2	N	182	VAL
2	N	184	VAL
2	N	186	SER
2	N	196	CYS
2	N	212	GLU
1	O	5	THR
1	O	11	LEU
1	O	20	THR
1	O	21	ILE
1	O	22	THR
1	O	34	ASN
1	O	59	PRO
1	O	69	THR
1	O	77	SER
1	O	78	LEU
1	O	89	GLN
1	O	106	ILE
1	O	108	ARG
1	O	113	PRO
1	O	126	LYS
1	O	129	THR
1	O	131	SER
1	O	135	LEU
1	O	138	ASN
1	O	151	ASP
1	O	154	LEU
1	O	158	ASN

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Mol	Chain	Res	Type
1	O	164	THR
1	O	181	LEU
1	O	199	GLN
1	O	202	SER
1	O	209	PHE
2	P	7	SER
2	P	22	CYS
2	P	32	TYR
2	P	69	ILE
2	P	101	ASP
2	P	116	THR
2	P	135	THR
2	P	138	LEU
2	P	140	CYS
2	P	146	PHE
2	P	148	GLU
2	P	150	VAL
2	P	159	LEU
2	P	160	THR
2	P	161	SER
2	P	170	LEU
2	P	172	SER
2	P	182	VAL
2	P	183	THR
2	P	189	LEU
2	P	193	THR
2	P	196	CYS
2	P	202	PRO
2	P	212	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (98) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	27	GLN
1	A	38	GLN
1	A	89	GLN
1	A	124	GLN
1	A	137	ASN
1	A	138	ASN
1	A	158	ASN
1	A	210	ASN

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Mol	Chain	Res	Type
2	B	43	GLN
2	B	64	GLN
2	B	164	HIS
2	B	192	GLN
2	B	199	ASN
1	C	3	GLN
1	C	27	GLN
1	C	38	GLN
1	C	79	GLN
1	C	89	GLN
1	C	90	GLN
1	C	147	GLN
1	C	160	GLN
1	C	189	HIS
1	C	198	HIS
1	C	199	GLN
1	C	210	ASN
2	D	61	GLN
2	D	64	GLN
2	D	171	GLN
1	E	27	GLN
1	E	37	GLN
1	E	96	HIS
1	E	137	ASN
1	E	138	ASN
1	E	147	GLN
1	E	189	HIS
1	E	210	ASN
2	F	100(J)	HIS
2	F	199	ASN
1	G	79	GLN
1	G	137	ASN
1	G	155	GLN
1	G	210	ASN
2	H	1	GLN
2	H	43	GLN
2	H	155	ASN
2	H	164	HIS
2	H	171	GLN
2	H	192	GLN
2	H	199	ASN
1	I	34	ASN

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Mol	Chain	Res	Type
1	I	55	GLN
1	I	96	HIS
1	I	100	GLN
1	I	124	GLN
1	I	138	ASN
1	I	158	ASN
1	I	199	GLN
1	I	210	ASN
2	J	39	GLN
2	J	61	GLN
2	J	105	GLN
2	J	164	HIS
2	J	171	GLN
2	J	199	ASN
1	K	89	GLN
1	K	100	GLN
1	K	147	GLN
1	K	152	ASN
1	K	210	ASN
2	L	1	GLN
2	L	39	GLN
2	L	64	GLN
2	L	164	HIS
1	M	3	GLN
1	M	37	GLN
1	M	38	GLN
1	M	55	GLN
1	M	96	HIS
1	M	137	ASN
1	M	138	ASN
1	M	147	GLN
1	M	189	HIS
1	M	198	HIS
1	M	210	ASN
2	N	39	GLN
2	N	199	ASN
1	O	79	GLN
1	O	89	GLN
1	O	96	HIS
1	O	124	GLN
1	O	138	ASN
1	O	199	GLN

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Mol	Chain	Res	Type
2	P	39	GLN
2	P	155	ASN
2	P	192	GLN
2	P	199	ASN
2	P	200	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	211/212 (99%)	-1.61	0 100 100	27, 49, 72, 79	0
1	C	212/212 (100%)	-1.66	0 100 100	24, 45, 68, 75	0
1	E	211/212 (99%)	-1.66	0 100 100	30, 49, 65, 76	0
1	G	211/212 (99%)	-1.62	0 100 100	33, 53, 86, 100	0
1	I	211/212 (99%)	-1.63	0 100 100	31, 50, 71, 82	0
1	K	211/212 (99%)	-1.66	0 100 100	36, 52, 66, 76	0
1	M	211/212 (99%)	-1.65	0 100 100	24, 45, 59, 75	0
1	O	211/212 (99%)	-1.65	0 100 100	25, 44, 61, 67	0
2	B	216/230 (93%)	-1.57	0 100 100	32, 58, 81, 89	0
2	D	216/230 (93%)	-1.60	0 100 100	27, 58, 87, 99	0
2	F	217/230 (94%)	-1.54	0 100 100	28, 64, 93, 105	0
2	H	216/230 (93%)	-1.49	0 100 100	39, 71, 96, 99	0
2	J	216/230 (93%)	-1.53	0 100 100	39, 65, 91, 96	0
2	L	215/230 (93%)	-1.52	0 100 100	37, 63, 82, 100	0
2	N	216/230 (93%)	-1.63	0 100 100	29, 54, 75, 87	0
2	P	216/230 (93%)	-1.58	0 100 100	28, 52, 86, 92	0
All	All	3417/3536 (96%)	-1.60	0 100 100	24, 53, 84, 105	0

There are no RSRZ outliers to report.

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.