Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 11:39 am BST

PDB ID	:	1XCQ
Title	:	Complex HCV core-Fab 19D9D6-Protein L mutant (D55A,L57H,Y64W) in space group P21
Authors	:	Menez, R.; Housden, N.G.; Harrison, S.; Jolivet-Reynaud, C.; Gore, M.G.; Stura, E.A.
Deposited on	:	2004-09-03
Resolution	:	3.50 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

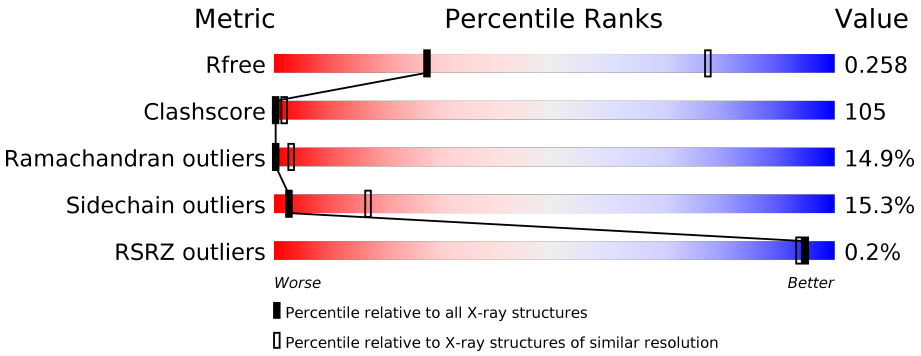
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	P	44	7% 9% 20% 18% 45%
1	Q	44	7% 9% 20% 45% 25%
1	S	44	2% 5% 23% 36% 36%
2	A	220	5% 20% 62% 13%
2	C	220	6% 30% 48% 17%
2	E	220	5% 25% 55% 16%

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Mol	Chain	Length	Quality of chain
2	G	220	5% 32% 46% 17%
3	B	218	6% 22% 54% 17%
3	D	218	25% 54% 17%
3	F	218	5% 28% 50% 17%
3	H	218	30% 52% 13%
4	L	80	5% 28% 39% 11% 18%
4	M	80	20% 36% 19% 23%
4	N	80	21% 41% 15% 20%
4	O	80	5% 18% 48% 8% 23%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 16467 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 Capsid protein C.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	P	24	Total	C	N	O	0	0	0
			167	106	33	28			
1	Q	44	Total	C	N	O	0	0	0
			346	213	75	58			
1	S	44	Total	C	N	O	0	0	0
			346	213	75	58			

- Molecule 2 is a protein called Monoclonal antibody 19D9D6 Light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	220	Total	C	N	O	S	0	0	0
			1708	1063	291	346	8			
2	C	220	Total	C	N	O	S	0	0	0
			1708	1063	291	346	8			
2	E	220	Total	C	N	O	S	0	0	0
			1708	1063	291	346	8			
2	G	219	Total	C	N	O	S	0	0	0
			1701	1060	290	344	7			

- Molecule 3 is a protein called Monoclonal antibody 19D9D6 Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	B	218	Total	C	N	O	S	0	0	0
			1660	1058	270	325	7			
3	D	218	Total	C	N	O	S	0	0	0
			1660	1058	270	325	7			
3	F	218	Total	C	N	O	S	0	0	0
			1660	1058	270	325	7			
3	H	218	Total	C	N	O	S	0	0	0
			1660	1058	270	325	7			

- Molecule 4 is a protein called Protein L.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	L	66	Total	C	N	O	S	0	0	0
			507	322	85	99	1			
4	M	62	Total	C	N	O	S	0	0	0
			480	305	80	94	1			
4	N	64	Total	C	N	O	S	0	0	0
			490	311	82	96	1			
4	O	62	Total	C	N	O	S	0	0	0
			480	305	80	94	1			

- Molecule 5 is water.

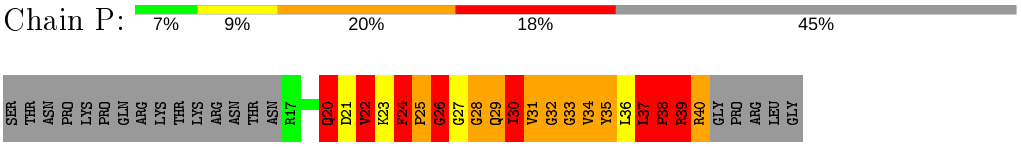
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	P	1	Total	O	0	0
			1	1		
5	A	29	Total	O	0	0
			29	29		
5	B	31	Total	O	0	0
			31	31		
5	L	9	Total	O	0	0
			9	9		
5	C	13	Total	O	0	0
			13	13		
5	D	10	Total	O	0	0
			10	10		
5	Q	6	Total	O	0	0
			6	6		
5	M	3	Total	O	0	0
			3	3		
5	E	17	Total	O	0	0
			17	17		
5	F	34	Total	O	0	0
			34	34		
5	N	7	Total	O	0	0
			7	7		
5	S	3	Total	O	0	0
			3	3		
5	G	11	Total	O	0	0
			11	11		
5	H	9	Total	O	0	0
			9	9		
5	O	3	Total	O	0	0
			3	3		

3 Residue-property plots (i)

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

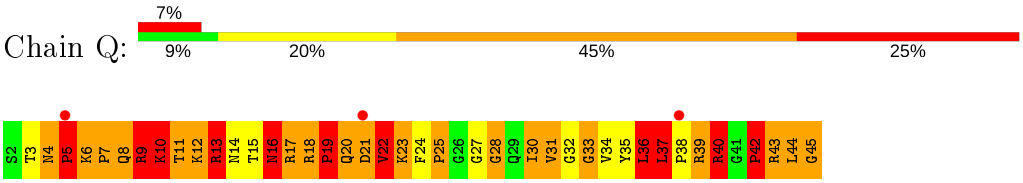
- Molecule 1: Capsid protein C

Chain P:



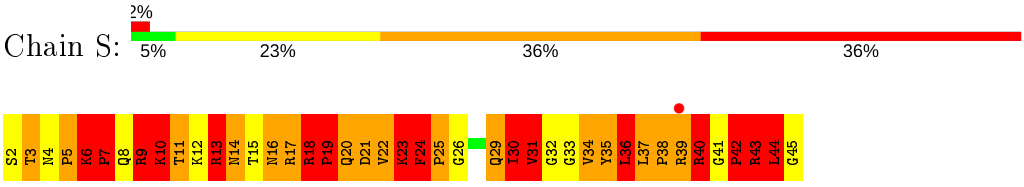
- Molecule 1: Capsid protein C

Chain Q:



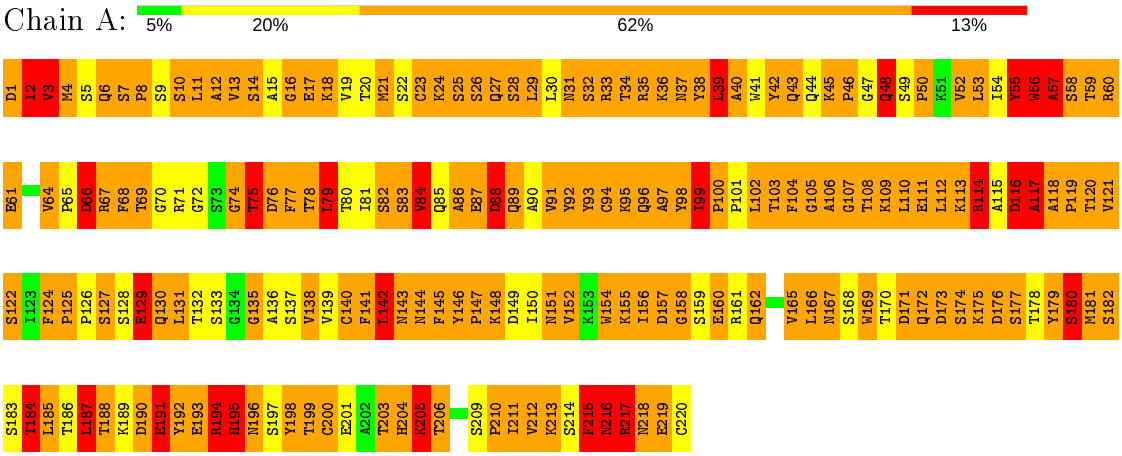
- Molecule 1: Capsid protein C

Chain S:



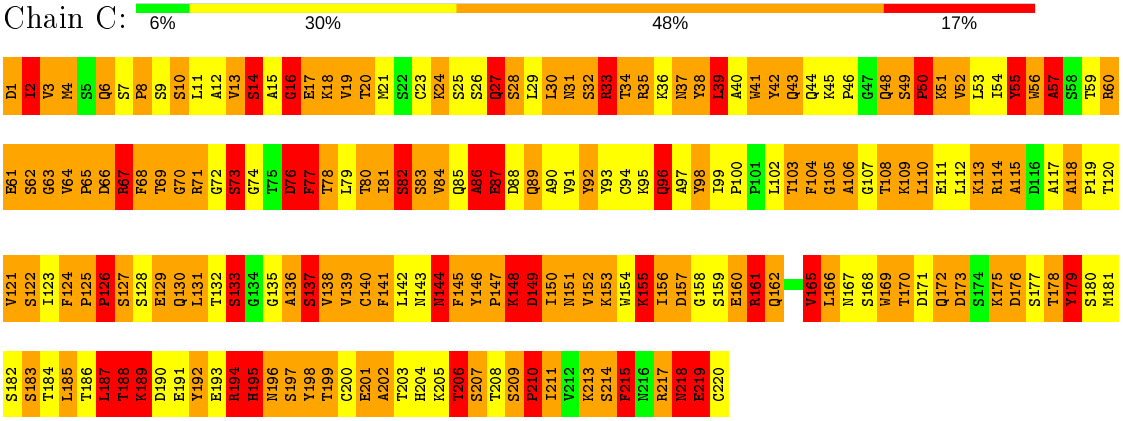
- Molecule 2: Monoclonal antibody 19D9D6 Light chain

Chain A:



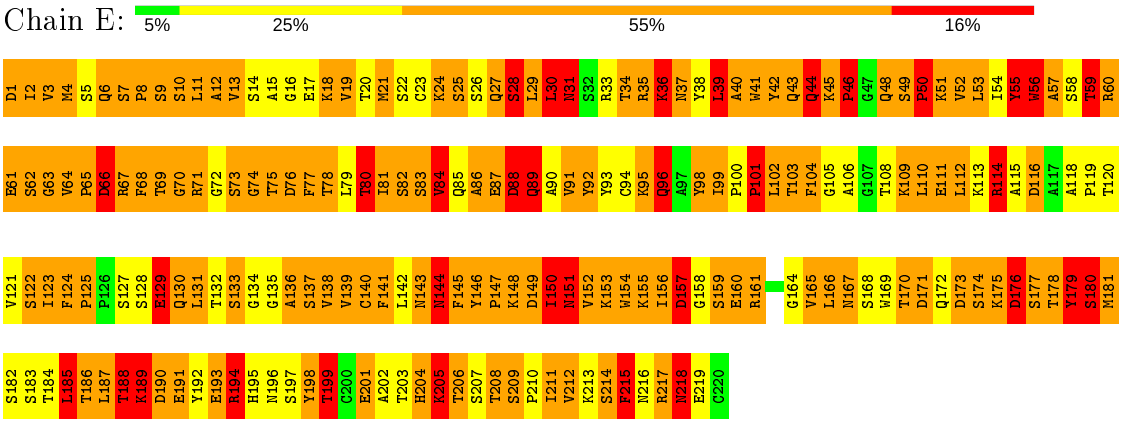
- Molecule 2: Monoclonal antibody 19D9D6 Light chain

Chain C:



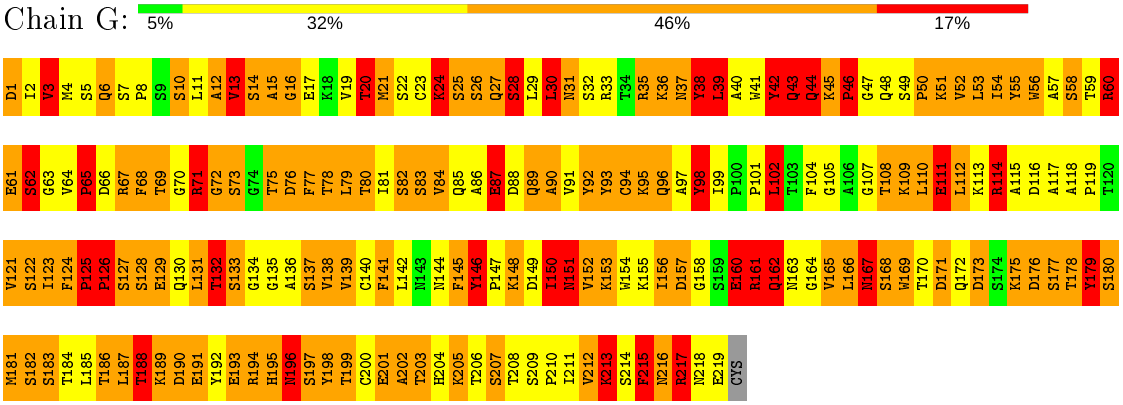
- Molecule 2: Monoclonal antibody 19D9D6 Light chain

Chain E:



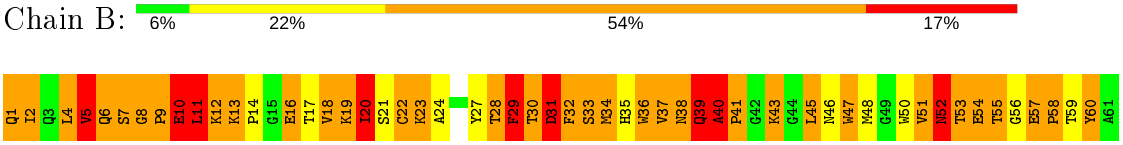
- Molecule 2: Monoclonal antibody 19D9D6 Light chain

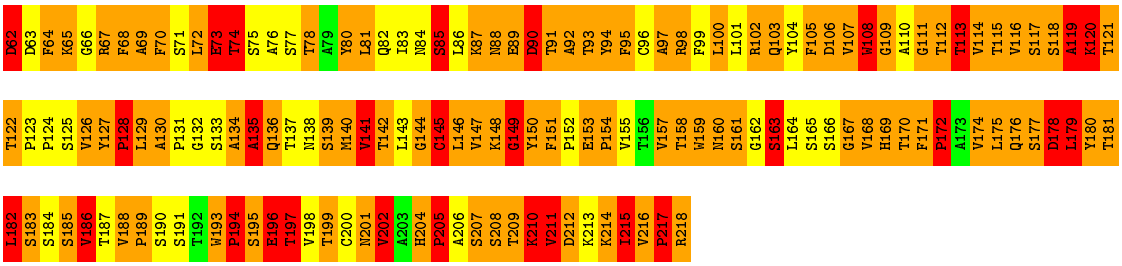
Chain G:



- Molecule 3: Monoclonal antibody 19D9D6 Heavy chain

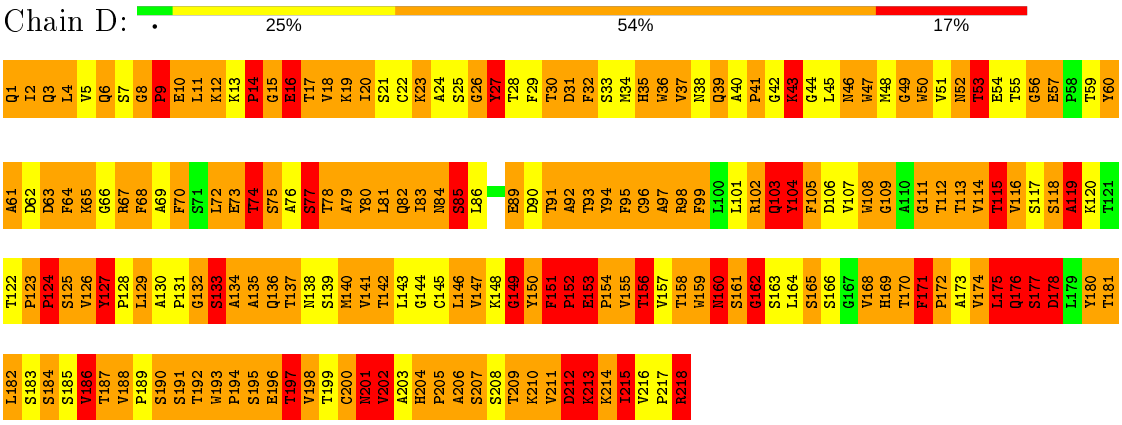
Chain B:





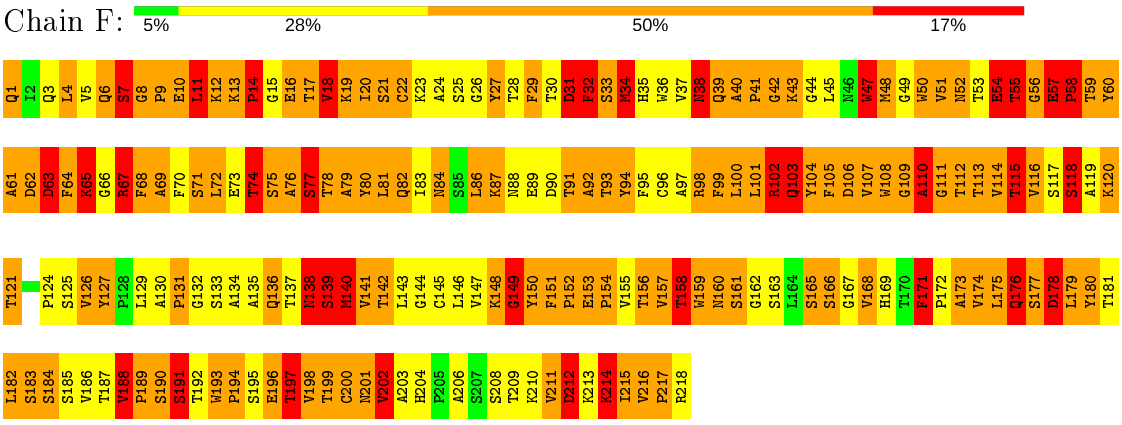
• Molecule 3: Monoclonal antibody 19D9D6 Heavy chain

Chain D:



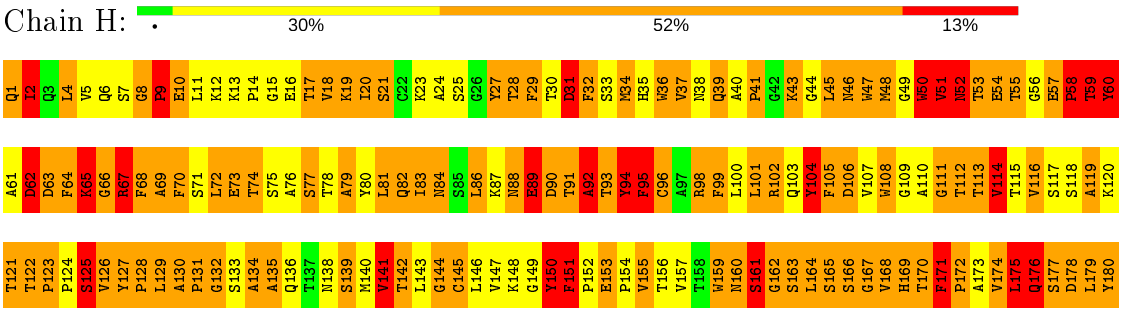
• Molecule 3: Monoclonal antibody 19D9D6 Heavy chain

Chain F:



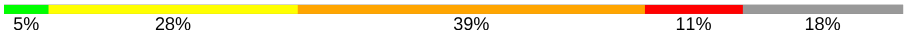
• Molecule 3: Monoclonal antibody 19D9D6 Heavy chain

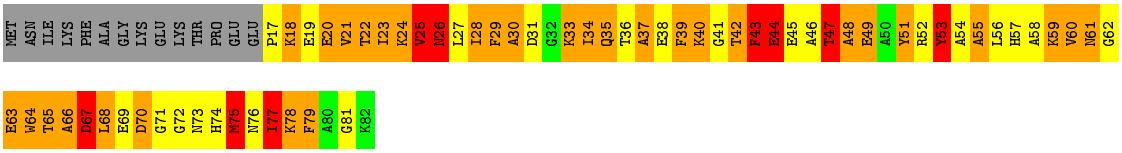
Chain H:



• Molecule 4: Protein L

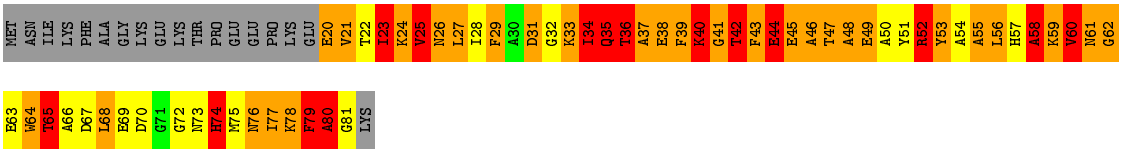
Chain L:





• Molecule 4: Protein L

Chain M:

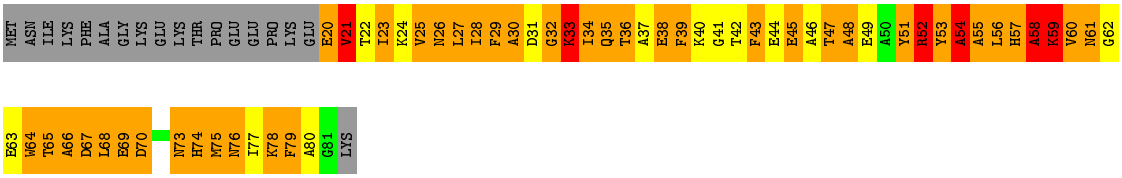


• Molecule 4: Protein L

Chain N:

• Molecule 4: Protein L

Chain O:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	43.60Å 230.52Å 123.64Å 90.00° 91.67° 90.00°	Depositor
Resolution (Å)	21.62 – 3.50 21.60 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.4 (21.62-3.50) 99.4 (21.60-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.17	Depositor
$< I/\sigma(I) >$ [1]	1.30 (at 3.53Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.192 , 0.264 0.196 , 0.258	Depositor DCC
R_{free} test set	1535 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	72.1	Xtriage
Anisotropy	0.156	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 114.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	0.116 for h,-k,-l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	16467	wwPDB-VP
Average B, all atoms (Å^2)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.11% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	P	2.91	16/170 (9.4%)	2.24	7/229 (3.1%)
1	Q	3.71	60/353 (17.0%)	2.35	15/472 (3.2%)
1	S	3.33	39/353 (11.0%)	2.12	14/472 (3.0%)
2	A	3.90	300/1745 (17.2%)	2.20	77/2366 (3.3%)
2	C	3.73	280/1745 (16.0%)	2.19	57/2366 (2.4%)
2	E	4.10	328/1745 (18.8%)	2.40	95/2366 (4.0%)
2	G	3.78	269/1738 (15.5%)	2.22	73/2358 (3.1%)
3	B	4.01	330/1707 (19.3%)	2.24	84/2335 (3.6%)
3	D	3.78	293/1707 (17.2%)	2.12	67/2335 (2.9%)
3	F	3.95	312/1707 (18.3%)	2.22	79/2335 (3.4%)
3	H	3.82	282/1707 (16.5%)	2.18	65/2335 (2.8%)
4	L	4.08	98/517 (19.0%)	2.34	23/695 (3.3%)
4	M	4.13	94/489 (19.2%)	2.35	29/659 (4.4%)
4	N	4.05	96/499 (19.2%)	2.07	15/673 (2.2%)
4	O	3.83	95/489 (19.4%)	2.15	17/659 (2.6%)
All	All	3.88	2892/16671 (17.3%)	2.22	717/22655 (3.2%)

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
2	C	0	1
2	E	0	3
2	G	0	2
3	D	0	1
3	F	0	1
3	H	0	1
4	L	0	1
All	All	0	10

All (2892) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	93	TYR	CG-CD1	-22.17	1.10	1.39
3	H	89	GLU	CG-CD	20.91	1.83	1.51
3	D	127	TYR	CE1-CZ	-20.53	1.11	1.38
1	S	31	VAL	CB-CG1	20.39	1.95	1.52
2	G	193	GLU	CD-OE1	20.15	1.47	1.25
2	E	93	TYR	CE1-CZ	-19.67	1.12	1.38
4	N	53	TYR	CE2-CZ	-19.64	1.13	1.38
2	E	28	SER	CB-OG	19.10	1.67	1.42
2	E	145	PHE	CG-CD1	-18.60	1.10	1.38
3	B	104	TYR	CE1-CZ	-17.96	1.15	1.38
4	L	51	TYR	CE2-CZ	-17.84	1.15	1.38
4	M	64	TRP	CG-CD1	-17.65	1.12	1.36
3	D	202	VAL	CB-CG1	-17.63	1.15	1.52
2	E	38	TYR	CE2-CZ	-17.35	1.16	1.38
2	C	56	TRP	CB-CG	17.32	1.81	1.50
2	E	179	TYR	CG-CD2	-16.28	1.18	1.39
3	H	203	ALA	CA-CB	-16.18	1.18	1.52
2	E	198	TYR	CG-CD2	-16.04	1.18	1.39
2	G	93	TYR	CE1-CZ	-15.98	1.17	1.38
2	A	38	TYR	CD1-CE1	-15.88	1.15	1.39
2	A	121	VAL	CA-CB	-15.82	1.21	1.54
2	E	215	PHE	CG-CD1	-15.81	1.15	1.38
2	G	93	TYR	CD2-CE2	-15.81	1.15	1.39
3	B	151	PHE	CE1-CZ	-15.75	1.07	1.37
3	B	94	TYR	CD2-CE2	-15.71	1.15	1.39
2	G	177	SER	CB-OG	15.71	1.62	1.42
3	D	73	GLU	CD-OE2	15.67	1.42	1.25
3	B	127	TYR	CE1-CZ	-15.65	1.18	1.38
3	F	104	TYR	CE2-CZ	-15.56	1.18	1.38
2	G	36	LYS	CE-NZ	15.45	1.87	1.49
2	C	179	TYR	CE1-CZ	-15.40	1.18	1.38
2	E	68	PHE	CG-CD1	-15.19	1.16	1.38
3	F	150	TYR	CD1-CE1	-15.10	1.16	1.39
3	B	151	PHE	CG-CD2	-15.04	1.16	1.38
2	A	61	GLU	CD-OE2	15.03	1.42	1.25
3	F	94	TYR	CG-CD2	-15.00	1.19	1.39
2	A	179	TYR	CG-CD1	-14.98	1.19	1.39
2	G	5	SER	C-O	14.98	1.51	1.23
2	E	192	TYR	CE1-CZ	-14.93	1.19	1.38
2	E	41	TRP	CB-CG	14.85	1.76	1.50
2	G	35	ARG	NE-CZ	14.84	1.52	1.33
4	L	53	TYR	CE2-CZ	-14.84	1.19	1.38
4	M	51	TYR	CE2-CZ	-14.74	1.19	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	93	TYR	CG-CD2	-14.73	1.20	1.39
3	B	151	PHE	CD2-CE2	-14.63	1.09	1.39
2	G	192	TYR	CE2-CZ	-14.57	1.19	1.38
3	F	102	ARG	CG-CD	14.48	1.88	1.51
2	A	192	TYR	CG-CD2	-14.40	1.20	1.39
3	D	127	TYR	CE2-CZ	-14.35	1.19	1.38
2	E	42	TYR	CG-CD2	-14.34	1.20	1.39
2	A	135	GLY	C-O	14.19	1.46	1.23
2	E	98	TYR	CG-CD1	-14.17	1.20	1.39
3	B	119	ALA	CA-CB	14.13	1.82	1.52
2	C	10	SER	CA-CB	14.10	1.74	1.52
2	G	146	TYR	CG-CD1	-14.08	1.20	1.39
3	F	159	TRP	CB-CG	-14.03	1.25	1.50
3	F	151	PHE	CE1-CZ	-14.02	1.10	1.37
3	B	98	ARG	NE-CZ	-13.99	1.14	1.33
3	H	151	PHE	CB-CG	-13.97	1.27	1.51
2	G	104	PHE	CE2-CZ	-13.96	1.10	1.37
3	H	68	PHE	CE2-CZ	13.90	1.63	1.37
4	N	73	ASN	CB-CG	13.81	1.82	1.51
2	A	120	THR	CB-CG2	-13.79	1.06	1.52
3	B	151	PHE	CD1-CE1	-13.76	1.11	1.39
2	C	198	TYR	CG-CD1	-13.76	1.21	1.39
2	G	198	TYR	CB-CG	-13.70	1.31	1.51
3	F	110	ALA	N-CA	-13.69	1.19	1.46
3	F	150	TYR	CE1-CZ	-13.65	1.20	1.38
4	M	79	PHE	CE2-CZ	-13.58	1.11	1.37
2	C	41	TRP	CD2-CE2	-13.42	1.25	1.41
2	C	129	GLU	CB-CG	13.41	1.77	1.52
3	F	202	VAL	CB-CG2	-13.39	1.24	1.52
3	F	36	TRP	CB-CG	-13.39	1.26	1.50
3	H	9	PRO	CA-C	-13.28	1.26	1.52
3	D	73	GLU	CG-CD	13.18	1.71	1.51
3	H	89	GLU	CD-OE1	13.16	1.40	1.25
2	A	146	TYR	CD1-CE1	-13.14	1.19	1.39
2	C	41	TRP	CG-CD1	-13.12	1.18	1.36
2	C	124	PHE	CD1-CE1	-13.12	1.13	1.39
2	A	76	ASP	CB-CG	13.11	1.79	1.51
4	O	23	ILE	C-O	-13.11	0.98	1.23
3	B	29	PHE	CE1-CZ	-13.10	1.12	1.37
2	C	104	PHE	CB-CG	-13.08	1.29	1.51
2	E	98	TYR	CE2-CZ	-13.06	1.21	1.38
3	B	104	TYR	CG-CD2	-13.06	1.22	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	94	TYR	CD2-CE2	-12.98	1.19	1.39
3	B	92	ALA	CA-CB	-12.97	1.25	1.52
2	G	201	GLU	CB-CG	12.90	1.76	1.52
4	N	43	PHE	CG-CD2	-12.88	1.19	1.38
4	M	51	TYR	CG-CD1	-12.87	1.22	1.39
2	E	8	PRO	CA-C	-12.86	1.27	1.52
3	B	9	PRO	CA-CB	-12.85	1.27	1.53
3	H	150	TYR	CG-CD1	-12.84	1.22	1.39
3	H	198	VAL	CB-CG2	12.84	1.79	1.52
2	C	64	VAL	CB-CG1	-12.80	1.25	1.52
2	G	77	PHE	CD2-CE2	-12.80	1.13	1.39
3	B	161	SER	CA-CB	12.79	1.72	1.52
3	F	167	GLY	C-O	12.78	1.44	1.23
3	D	102	ARG	CG-CD	12.70	1.83	1.51
4	L	38	GLU	CD-OE2	-12.66	1.11	1.25
3	F	104	TYR	CG-CD1	-12.65	1.22	1.39
3	D	99	PHE	CE1-CZ	12.64	1.61	1.37
2	G	152	VAL	CA-CB	-12.63	1.28	1.54
2	A	38	TYR	CD2-CE2	-12.63	1.20	1.39
4	N	53	TYR	CD1-CE1	-12.59	1.20	1.39
3	H	50	TRP	CB-CG	12.59	1.73	1.50
3	B	107	VAL	CB-CG1	-12.58	1.26	1.52
3	D	50	TRP	CE2-CZ2	-12.58	1.18	1.39
2	E	141	PHE	CG-CD1	-12.56	1.20	1.38
3	D	96	CYS	N-CA	-12.54	1.21	1.46
1	Q	40	ARG	NE-CZ	12.52	1.49	1.33
4	O	43	PHE	CG-CD2	12.52	1.57	1.38
4	L	79	PHE	CD1-CE1	-12.49	1.14	1.39
2	A	1	ASP	CB-CG	12.48	1.77	1.51
2	E	161	ARG	CZ-NH1	12.46	1.49	1.33
4	O	58	ALA	CA-CB	12.46	1.78	1.52
4	M	29	PHE	CE1-CZ	12.45	1.61	1.37
3	D	99	PHE	CG-CD2	12.44	1.57	1.38
2	G	193	GLU	CG-CD	12.44	1.70	1.51
3	D	36	TRP	CG-CD1	-12.40	1.19	1.36
2	A	68	PHE	CD1-CE1	-12.39	1.14	1.39
3	D	159	TRP	CD2-CE2	-12.39	1.26	1.41
3	D	57	GLU	CG-CD	12.37	1.70	1.51
2	G	42	TYR	CD2-CE2	-12.37	1.20	1.39
2	E	194	ARG	CG-CD	12.36	1.82	1.51
3	F	196	GLU	CD-OE1	12.33	1.39	1.25
2	G	35	ARG	CZ-NH2	12.31	1.49	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	N	61	ASN	C-O	12.30	1.46	1.23
2	G	67	ARG	CG-CD	12.29	1.82	1.51
2	A	106	ALA	CA-C	-12.28	1.21	1.52
3	H	216	VAL	CA-CB	12.26	1.80	1.54
2	E	160	GLU	CD-OE1	12.26	1.39	1.25
2	E	141	PHE	CG-CD2	-12.22	1.20	1.38
2	E	129	GLU	CG-CD	12.18	1.70	1.51
3	H	36	TRP	CG-CD1	-12.18	1.19	1.36
3	F	177	SER	C-O	-12.14	1.00	1.23
3	H	208	SER	CA-CB	-12.14	1.34	1.52
4	O	79	PHE	CE2-CZ	12.09	1.60	1.37
4	M	65	THR	CB-CG2	12.07	1.92	1.52
2	A	135	GLY	CA-C	12.04	1.71	1.51
3	F	174	VAL	CB-CG1	-12.02	1.27	1.52
2	G	193	GLU	CB-CG	12.00	1.75	1.52
2	E	198	TYR	CD2-CE2	-11.98	1.21	1.39
3	H	47	TRP	CE2-CZ2	-11.98	1.19	1.39
3	B	168	VAL	CA-CB	-11.98	1.29	1.54
3	F	183	SER	CA-CB	-11.96	1.35	1.52
3	F	202	VAL	CA-CB	-11.96	1.29	1.54
4	M	51	TYR	CD1-CE1	-11.90	1.21	1.39
2	E	12	ALA	CA-CB	11.90	1.77	1.52
3	B	150	TYR	CE1-CZ	-11.86	1.23	1.38
2	C	138	VAL	CB-CG2	-11.82	1.28	1.52
3	F	159	TRP	CG-CD1	-11.82	1.20	1.36
2	A	160	GLU	CG-CD	11.78	1.69	1.51
2	A	41	TRP	CD2-CE2	-11.77	1.27	1.41
4	M	39	PHE	CE1-CZ	-11.75	1.15	1.37
3	H	131	PRO	CA-C	-11.75	1.29	1.52
4	M	45	GLU	CD-OE2	11.74	1.38	1.25
3	B	116	VAL	CB-CG2	-11.73	1.28	1.52
1	S	17	ARG	NE-CZ	11.70	1.48	1.33
2	C	165	VAL	CB-CG1	11.70	1.77	1.52
2	C	129	GLU	CD-OE2	11.68	1.38	1.25
2	G	91	VAL	CA-CB	-11.66	1.30	1.54
3	B	104	TYR	CG-CD1	-11.66	1.24	1.39
4	L	52	ARG	CZ-NH2	11.63	1.48	1.33
3	F	33	SER	CA-CB	11.63	1.70	1.52
4	L	39	PHE	CD2-CE2	-11.58	1.16	1.39
2	E	179	TYR	CD1-CE1	-11.57	1.22	1.39
3	H	95	PHE	CE1-CZ	-11.54	1.15	1.37
3	F	188	VAL	CB-CG2	-11.52	1.28	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	103	GLN	CG-CD	11.50	1.77	1.51
4	M	48	ALA	C-O	11.49	1.45	1.23
2	G	93	TYR	CD1-CE1	-11.48	1.22	1.39
2	A	191	GLU	N-CA	11.48	1.69	1.46
3	D	127	TYR	CG-CD1	-11.48	1.24	1.39
2	A	219	GLU	CD-OE2	-11.46	1.13	1.25
2	A	42	TYR	CD2-CE2	-11.45	1.22	1.39
1	Q	35	TYR	CG-CD2	11.44	1.54	1.39
2	E	28	SER	CA-CB	11.44	1.70	1.52
3	H	171	PHE	C-O	-11.43	1.01	1.23
1	S	40	ARG	CZ-NH2	11.40	1.47	1.33
3	H	70	PHE	CD1-CE1	-11.36	1.16	1.39
2	E	111	GLU	CD-OE2	-11.35	1.13	1.25
2	A	118	ALA	CA-CB	11.35	1.76	1.52
3	B	193	TRP	CD2-CE3	-11.35	1.23	1.40
1	Q	13	ARG	CZ-NH2	11.34	1.47	1.33
2	C	71	ARG	NE-CZ	11.34	1.47	1.33
3	F	33	SER	CB-OG	11.32	1.56	1.42
3	H	180	TYR	CG-CD2	11.30	1.53	1.39
2	E	38	TYR	CD1-CE1	-11.30	1.22	1.39
2	C	35	ARG	CD-NE	11.30	1.65	1.46
3	F	88	ASN	CB-CG	-11.30	1.25	1.51
3	F	165	SER	CB-OG	11.29	1.56	1.42
2	C	93	TYR	CD2-CE2	-11.28	1.22	1.39
2	A	12	ALA	C-O	11.27	1.44	1.23
2	C	179	TYR	CG-CD2	-11.24	1.24	1.39
4	O	20	GLU	CG-CD	11.23	1.68	1.51
2	A	38	TYR	CB-CG	11.20	1.68	1.51
2	G	42	TYR	CD1-CE1	-11.20	1.22	1.39
4	L	55	ALA	CA-CB	11.19	1.75	1.52
2	A	160	GLU	CB-CG	11.19	1.73	1.52
2	E	145	PHE	CE2-CZ	-11.18	1.16	1.37
2	C	82	SER	CA-CB	11.15	1.69	1.52
1	Q	31	VAL	CA-CB	11.12	1.78	1.54
4	N	53	TYR	CG-CD1	-11.12	1.24	1.39
3	F	180	TYR	CD2-CE2	-11.10	1.22	1.39
4	L	79	PHE	CE2-CZ	-11.10	1.16	1.37
2	C	148	LYS	CG-CD	11.08	1.90	1.52
2	E	55	TYR	CE2-CZ	-11.05	1.24	1.38
4	M	20	GLU	CG-CD	11.04	1.68	1.51
3	D	37	VAL	CA-CB	-11.02	1.31	1.54
2	G	26	SER	CB-OG	-11.02	1.27	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	16	GLU	CD-OE2	11.01	1.37	1.25
2	E	41	TRP	CE2-CZ2	-11.01	1.21	1.39
3	H	89	GLU	CB-CG	11.00	1.73	1.52
2	E	141	PHE	CD1-CE1	-10.97	1.17	1.39
2	G	1	ASP	CB-CG	10.96	1.74	1.51
2	G	198	TYR	CG-CD1	-10.96	1.24	1.39
4	M	24	LYS	CB-CG	10.93	1.82	1.52
3	B	159	TRP	CE2-CZ2	-10.93	1.21	1.39
2	G	141	PHE	CG-CD2	10.92	1.55	1.38
2	A	89	GLN	CB-CG	10.92	1.82	1.52
2	A	169	TRP	CE3-CZ3	10.92	1.57	1.38
4	L	43	PHE	CE1-CZ	10.87	1.57	1.37
3	H	46	ASN	N-CA	-10.84	1.24	1.46
3	F	108	TRP	CG-CD1	-10.84	1.21	1.36
3	F	26	GLY	C-O	-10.82	1.06	1.23
3	B	105	PHE	CE1-CZ	-10.82	1.16	1.37
2	A	86	ALA	C-O	-10.82	1.02	1.23
4	L	53	TYR	CE1-CZ	-10.81	1.24	1.38
3	B	211	VAL	CA-CB	-10.81	1.32	1.54
2	G	104	PHE	CG-CD1	-10.80	1.22	1.38
3	H	116	VAL	CA-CB	-10.79	1.32	1.54
4	M	31	ASP	CB-CG	-10.77	1.29	1.51
2	G	205	LYS	CD-CE	10.76	1.78	1.51
2	C	138	VAL	CB-CG1	-10.75	1.30	1.52
3	B	126	VAL	CB-CG2	10.73	1.75	1.52
4	N	20	GLU	CG-CD	10.73	1.68	1.51
2	G	146	TYR	CE2-CZ	-10.72	1.24	1.38
3	B	151	PHE	CE2-CZ	-10.72	1.17	1.37
3	B	99	PHE	CG-CD1	-10.69	1.22	1.38
2	C	192	TYR	CG-CD2	10.69	1.53	1.39
2	C	168	SER	CA-CB	10.68	1.69	1.52
3	H	217	PRO	N-CA	-10.68	1.29	1.47
3	B	116	VAL	CB-CG1	-10.64	1.30	1.52
2	G	95	LYS	CD-CE	-10.64	1.24	1.51
2	A	162	GLN	CG-CD	10.63	1.75	1.51
3	F	47	TRP	CB-CG	-10.61	1.31	1.50
3	H	39	GLN	CD-OE1	10.60	1.47	1.24
4	M	39	PHE	CD1-CE1	-10.59	1.18	1.39
3	F	214	LYS	CE-NZ	10.59	1.75	1.49
3	F	98	ARG	CZ-NH2	10.57	1.46	1.33
2	E	38	TYR	CG-CD1	-10.56	1.25	1.39
2	A	67	ARG	CZ-NH2	-10.56	1.19	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	179	TYR	CE2-CZ	-10.56	1.24	1.38
2	E	42	TYR	CG-CD1	-10.54	1.25	1.39
3	B	95	PHE	CG-CD2	-10.53	1.23	1.38
3	F	99	PHE	CD1-CE1	-10.53	1.18	1.39
3	F	151	PHE	CG-CD1	-10.52	1.23	1.38
4	N	20	GLU	CD-OE2	10.52	1.37	1.25
2	E	194	ARG	NE-CZ	10.51	1.46	1.33
4	N	33	LYS	CE-NZ	10.51	1.75	1.49
2	A	33	ARG	CA-CB	10.50	1.77	1.53
2	C	141	PHE	CD2-CE2	-10.48	1.18	1.39
4	N	64	TRP	CE3-CZ3	10.47	1.56	1.38
4	M	20	GLU	N-CA	10.46	1.67	1.46
3	F	120	LYS	CG-CD	10.46	1.88	1.52
4	L	25	VAL	CA-CB	-10.45	1.32	1.54
3	F	159	TRP	CG-CD2	-10.45	1.25	1.43
4	L	77	ILE	CB-CG2	-10.44	1.20	1.52
3	D	47	TRP	CZ3-CH2	-10.43	1.23	1.40
2	C	121	VAL	CB-CG2	-10.43	1.30	1.52
3	B	1	GLN	N-CA	10.42	1.67	1.46
3	D	132	GLY	C-O	10.42	1.40	1.23
4	O	43	PHE	CD1-CE1	-10.41	1.18	1.39
3	B	95	PHE	CD1-CE1	-10.40	1.18	1.39
1	S	36	LEU	CG-CD2	10.39	1.90	1.51
4	N	25	VAL	CB-CG1	-10.38	1.31	1.52
3	B	66	GLY	CA-C	-10.37	1.35	1.51
2	E	118	ALA	CA-CB	-10.36	1.30	1.52
3	H	188	VAL	CB-CG2	10.36	1.74	1.52
2	G	43	GLN	CD-NE2	10.36	1.58	1.32
2	E	145	PHE	CE1-CZ	-10.36	1.17	1.37
4	M	52	ARG	NE-CZ	10.35	1.46	1.33
3	H	95	PHE	CE2-CZ	-10.34	1.17	1.37
3	D	31	ASP	CB-CG	10.33	1.73	1.51
3	F	16	GLU	C-O	-10.33	1.03	1.23
3	D	210	LYS	CD-CE	10.32	1.77	1.51
3	H	95	PHE	CG-CD2	-10.32	1.23	1.38
2	C	113	LYS	CE-NZ	10.32	1.74	1.49
2	A	95	LYS	C-O	-10.32	1.03	1.23
2	A	198	TYR	CG-CD2	-10.31	1.25	1.39
2	C	145	PHE	CD2-CE2	-10.31	1.18	1.39
3	F	149	GLY	CA-C	10.31	1.68	1.51
3	F	151	PHE	CG-CD2	-10.30	1.23	1.38
2	A	125	PRO	C-O	-10.29	1.02	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	129	GLU	CG-CD	10.29	1.67	1.51
2	G	198	TYR	CG-CD2	-10.29	1.25	1.39
2	A	219	GLU	CD-OE1	10.29	1.36	1.25
3	B	64	PHE	CD2-CE2	-10.29	1.18	1.39
3	B	110	ALA	N-CA	-10.28	1.25	1.46
4	O	73	ASN	CA-C	10.27	1.79	1.52
3	D	90	ASP	CB-CG	-10.26	1.30	1.51
3	H	43	LYS	CD-CE	-10.26	1.25	1.51
4	L	39	PHE	CG-CD1	-10.24	1.23	1.38
2	A	101	PRO	N-CA	-10.24	1.29	1.47
2	A	55	TYR	CD1-CE1	10.24	1.54	1.39
2	G	87	GLU	CD-OE2	10.23	1.36	1.25
4	M	25	VAL	CB-CG2	-10.21	1.31	1.52
2	E	179	TYR	CE1-CZ	-10.19	1.25	1.38
3	H	29	PHE	C-O	-10.19	1.03	1.23
3	F	156	THR	CA-CB	10.18	1.79	1.53
2	E	105	GLY	C-O	-10.17	1.07	1.23
2	G	213	LYS	CE-NZ	10.17	1.74	1.49
2	A	77	PHE	CA-CB	-10.16	1.31	1.53
4	L	53	TYR	CZ-OH	-10.16	1.20	1.37
3	F	155	VAL	CB-CG2	-10.16	1.31	1.52
2	C	73	SER	CA-CB	10.15	1.68	1.52
2	C	161	ARG	CG-CD	10.15	1.77	1.51
2	G	146	TYR	C-N	-10.15	1.15	1.34
3	D	125	SER	C-O	-10.14	1.04	1.23
2	E	95	LYS	CD-CE	10.14	1.76	1.51
4	M	50	ALA	CA-CB	-10.14	1.31	1.52
3	D	18	VAL	CB-CG1	10.13	1.74	1.52
2	E	129	GLU	CD-OE1	10.13	1.36	1.25
3	D	166	SER	CB-OG	10.12	1.55	1.42
3	D	143	LEU	C-O	-10.11	1.04	1.23
2	E	74	GLY	N-CA	10.10	1.61	1.46
3	F	102	ARG	NE-CZ	10.10	1.46	1.33
3	B	150	TYR	CE2-CZ	-10.10	1.25	1.38
3	F	94	TYR	CG-CD1	10.10	1.52	1.39
3	F	183	SER	C-O	-10.09	1.04	1.23
3	D	154	PRO	N-CD	-10.09	1.33	1.47
3	F	218	ARG	CZ-NH1	10.09	1.46	1.33
4	N	39	PHE	CE1-CZ	-10.08	1.18	1.37
3	F	108	TRP	CD2-CE2	-10.08	1.29	1.41
3	F	60	TYR	CE1-CZ	10.07	1.51	1.38
2	C	71	ARG	CZ-NH2	10.07	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	99	PHE	CA-CB	10.05	1.76	1.53
4	L	39	PHE	CE2-CZ	-10.04	1.18	1.37
2	C	57	ALA	CA-CB	10.04	1.73	1.52
3	F	120	LYS	CD-CE	10.02	1.76	1.51
4	N	68	LEU	CA-C	10.01	1.78	1.52
3	B	171	PHE	CD2-CE2	-10.01	1.19	1.39
3	B	98	ARG	CG-CD	10.00	1.76	1.51
2	E	55	TYR	CG-CD2	-10.00	1.26	1.39
2	G	21	MET	CB-CG	9.98	1.83	1.51
3	B	36	TRP	CD2-CE3	-9.97	1.25	1.40
2	C	48	GLN	CD-OE1	9.97	1.45	1.24
3	D	60	TYR	CE2-CZ	-9.96	1.25	1.38
3	F	49	GLY	C-O	-9.96	1.07	1.23
3	H	9	PRO	CG-CD	9.96	1.83	1.50
3	B	145	CYS	CA-CB	-9.94	1.32	1.53
4	L	45	GLU	CA-C	-9.94	1.27	1.52
4	O	59	LYS	CB-CG	9.93	1.79	1.52
2	A	36	LYS	CE-NZ	9.92	1.73	1.49
2	A	192	TYR	CA-C	-9.92	1.27	1.52
2	G	52	VAL	CA-CB	-9.92	1.33	1.54
3	H	59	THR	CB-CG2	9.91	1.85	1.52
2	A	86	ALA	CA-CB	9.91	1.73	1.52
2	C	189	LYS	CA-CB	9.91	1.75	1.53
1	Q	22	VAL	CA-CB	9.91	1.75	1.54
3	F	50	TRP	CB-CG	-9.91	1.32	1.50
2	E	204	HIS	CB-CG	-9.89	1.32	1.50
2	G	215	PHE	CD2-CE2	-9.89	1.19	1.39
2	E	93	TYR	CD1-CE1	9.89	1.54	1.39
2	E	119	PRO	C-O	-9.88	1.03	1.23
2	G	180	SER	CB-OG	9.88	1.55	1.42
3	H	95	PHE	CG-CD1	-9.88	1.24	1.38
2	E	155	LYS	CE-NZ	9.87	1.73	1.49
3	F	150	TYR	CB-CG	9.87	1.66	1.51
2	E	41	TRP	CE3-CZ3	-9.87	1.21	1.38
2	E	82	SER	CA-CB	-9.86	1.38	1.52
2	G	117	ALA	C-O	-9.86	1.04	1.23
3	H	172	PRO	CG-CD	9.86	1.83	1.50
3	D	171	PHE	CD2-CE2	9.85	1.58	1.39
3	H	197	THR	CA-CB	-9.84	1.27	1.53
2	G	124	PHE	CE2-CZ	9.81	1.55	1.37
2	C	119	PRO	CA-C	-9.80	1.33	1.52
3	F	80	TYR	CG-CD1	-9.81	1.26	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	150	TYR	CG-CD2	-9.80	1.26	1.39
2	E	71	ARG	NE-CZ	9.79	1.45	1.33
2	C	207	SER	CA-CB	9.79	1.67	1.52
2	A	205	LYS	CB-CG	9.78	1.78	1.52
2	G	192	TYR	CG-CD1	-9.78	1.26	1.39
2	A	3	VAL	CB-CG2	9.77	1.73	1.52
2	E	59	THR	C-O	-9.76	1.04	1.23
3	D	197	THR	CA-CB	9.76	1.78	1.53
2	E	106	ALA	CA-CB	9.75	1.73	1.52
2	A	154	TRP	CD2-CE2	-9.75	1.29	1.41
3	F	180	TYR	CG-CD2	9.75	1.51	1.39
3	B	218	ARG	CA-C	9.74	1.78	1.52
2	E	179	TYR	CG-CD1	-9.74	1.26	1.39
3	H	27	TYR	CE2-CZ	9.74	1.51	1.38
2	C	19	VAL	CB-CG1	-9.74	1.32	1.52
3	D	39	GLN	CD-OE1	-9.74	1.02	1.24
2	G	6	GLN	C-O	-9.72	1.04	1.23
3	D	36	TRP	CB-CG	-9.71	1.32	1.50
2	G	56	TRP	CD2-CE2	-9.72	1.29	1.41
2	C	38	TYR	CB-CG	9.71	1.66	1.51
3	D	23	LYS	CB-CG	9.70	1.78	1.52
3	F	202	VAL	CB-CG1	-9.68	1.32	1.52
3	H	68	PHE	CB-CG	-9.67	1.34	1.51
2	E	36	LYS	C-O	-9.66	1.04	1.23
1	S	23	LYS	CE-NZ	9.66	1.73	1.49
4	L	39	PHE	CD1-CE1	-9.65	1.20	1.39
2	E	17	GLU	CD-OE2	9.64	1.36	1.25
2	G	146	TYR	C-O	-9.64	1.05	1.23
2	A	56	TRP	C-O	-9.63	1.05	1.23
3	B	149	GLY	C-O	-9.62	1.08	1.23
3	D	197	THR	CB-CG2	9.62	1.84	1.52
2	C	108	THR	CB-CG2	9.61	1.84	1.52
3	F	198	VAL	CA-CB	-9.61	1.34	1.54
1	Q	28	GLY	CA-C	9.60	1.67	1.51
4	O	48	ALA	CA-CB	-9.60	1.32	1.52
2	A	124	PHE	CB-CG	-9.60	1.35	1.51
2	A	218	ASN	CB-CG	-9.59	1.28	1.51
3	B	130	ALA	CA-CB	-9.56	1.32	1.52
2	C	67	ARG	CG-CD	9.56	1.75	1.51
3	D	196	GLU	C-O	-9.56	1.05	1.23
2	E	98	TYR	CD1-CE1	-9.55	1.25	1.39
3	B	176	GLN	CG-CD	9.54	1.73	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	141	PHE	CE1-CZ	9.54	1.55	1.37
4	O	52	ARG	CB-CG	9.53	1.78	1.52
2	G	114	ARG	CZ-NH2	9.53	1.45	1.33
3	B	105	PHE	CD1-CE1	-9.53	1.20	1.39
2	E	25	SER	CA-C	-9.53	1.28	1.52
3	H	89	GLU	N-CA	-9.53	1.27	1.46
3	H	41	PRO	CA-CB	-9.49	1.34	1.53
3	B	21	SER	CB-OG	9.48	1.54	1.42
2	G	199	THR	CA-CB	-9.47	1.28	1.53
2	E	57	ALA	CA-CB	-9.46	1.32	1.52
2	A	13	VAL	CB-CG2	-9.46	1.32	1.52
3	B	9	PRO	CA-C	-9.45	1.33	1.52
2	G	26	SER	CA-CB	-9.45	1.38	1.52
3	H	196	GLU	CD-OE2	9.44	1.36	1.25
2	C	55	TYR	CB-CG	-9.44	1.37	1.51
2	G	179	TYR	CD1-CE1	-9.44	1.25	1.39
2	A	77	PHE	CE2-CZ	9.44	1.55	1.37
4	M	64	TRP	NE1-CE2	-9.44	1.25	1.37
2	E	37	ASN	C-O	-9.43	1.05	1.23
2	C	215	PHE	CG-CD2	9.43	1.52	1.38
2	C	38	TYR	CE1-CZ	9.42	1.50	1.38
3	F	155	VAL	CB-CG1	-9.42	1.33	1.52
4	N	33	LYS	CD-CE	9.42	1.74	1.51
3	H	151	PHE	CG-CD1	-9.41	1.24	1.38
2	E	104	PHE	CE2-CZ	-9.41	1.19	1.37
3	D	99	PHE	C-O	-9.40	1.05	1.23
2	G	101	PRO	CA-C	-9.39	1.34	1.52
3	H	131	PRO	CA-CB	-9.39	1.34	1.53
3	D	159	TRP	CA-C	-9.38	1.28	1.52
1	Q	23	LYS	CD-CE	9.38	1.74	1.51
2	G	201	GLU	CD-OE2	9.38	1.35	1.25
3	H	180	TYR	CD2-CE2	-9.38	1.25	1.39
3	H	215	ILE	CA-CB	-9.38	1.33	1.54
2	C	19	VAL	N-CA	-9.37	1.27	1.46
3	F	150	TYR	CE2-CZ	-9.37	1.26	1.38
3	H	108	TRP	CG-CD1	-9.37	1.23	1.36
3	H	54	GLU	CG-CD	9.37	1.66	1.51
2	A	176	ASP	C-O	-9.36	1.05	1.23
2	E	74	GLY	CA-C	9.36	1.66	1.51
2	G	71	ARG	CG-CD	9.36	1.75	1.51
1	Q	12	LYS	CD-CE	9.35	1.74	1.51
2	E	215	PHE	CE2-CZ	-9.35	1.19	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	89	GLN	C-O	-9.35	1.05	1.23
3	H	109	GLY	CA-C	-9.35	1.36	1.51
4	M	81	GLY	C-O	9.34	1.38	1.23
3	D	111	GLY	C-O	-9.34	1.08	1.23
2	E	104	PHE	CG-CD2	-9.33	1.24	1.38
3	B	150	TYR	CG-CD2	-9.32	1.27	1.39
3	H	68	PHE	CG-CD1	9.32	1.52	1.38
3	B	171	PHE	CG-CD1	-9.32	1.24	1.38
4	O	39	PHE	CD2-CE2	9.31	1.57	1.39
3	D	159	TRP	C-O	-9.30	1.05	1.23
2	C	93	TYR	CE2-CZ	-9.30	1.26	1.38
2	E	24	LYS	CD-CE	9.30	1.74	1.51
3	H	155	VAL	CA-CB	-9.26	1.35	1.54
3	H	157	VAL	CB-CG2	9.25	1.72	1.52
3	D	12	LYS	CD-CE	9.25	1.74	1.51
4	L	21	VAL	CB-CG1	9.24	1.72	1.52
2	E	25	SER	C-O	-9.23	1.05	1.23
4	N	43	PHE	CD1-CE1	-9.23	1.20	1.39
3	B	1	GLN	CA-CB	9.23	1.74	1.53
3	F	180	TYR	CG-CD1	-9.23	1.27	1.39
3	H	180	TYR	CB-CG	9.23	1.65	1.51
3	F	7	SER	N-CA	-9.22	1.27	1.46
2	E	21	MET	CA-CB	-9.22	1.33	1.53
2	E	73	SER	CA-CB	-9.22	1.39	1.52
3	H	126	VAL	CB-CG1	-9.22	1.33	1.52
2	E	121	VAL	CB-CG2	-9.20	1.33	1.52
2	A	82	SER	CB-OG	-9.19	1.30	1.42
3	H	36	TRP	CD2-CE2	-9.19	1.30	1.41
3	D	151	PHE	CB-CG	9.19	1.67	1.51
2	C	3	VAL	CB-CG2	9.19	1.72	1.52
2	G	126	PRO	N-CA	-9.18	1.31	1.47
3	H	168	VAL	CA-CB	-9.17	1.35	1.54
3	B	80	TYR	CD1-CE1	9.16	1.53	1.39
3	F	195	SER	CA-CB	9.15	1.66	1.52
2	C	169	TRP	CZ3-CH2	9.15	1.54	1.40
4	N	39	PHE	CG-CD1	-9.14	1.25	1.38
3	B	70	PHE	CE2-CZ	-9.13	1.20	1.37
3	D	178	ASP	CB-CG	-9.12	1.32	1.51
3	B	126	VAL	CB-CG1	-9.12	1.33	1.52
2	C	37	ASN	CB-CG	9.12	1.72	1.51
3	F	150	TYR	CD2-CE2	-9.11	1.25	1.39
2	E	93	TYR	CG-CD1	-9.11	1.27	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	91	THR	N-CA	9.10	1.64	1.46
3	H	98	ARG	CZ-NH1	9.10	1.44	1.33
3	D	166	SER	C-O	-9.09	1.06	1.23
3	F	51	VAL	N-CA	-9.09	1.28	1.46
3	B	134	ALA	CA-CB	9.08	1.71	1.52
3	B	154	PRO	N-CA	-9.07	1.31	1.47
3	H	10	GLU	CD-OE1	9.07	1.35	1.25
3	H	47	TRP	CB-CG	9.07	1.66	1.50
3	H	55	THR	CA-CB	9.06	1.76	1.53
4	L	29	PHE	CD1-CE1	9.05	1.57	1.39
2	E	20	THR	CB-OG1	-9.04	1.25	1.43
3	F	156	THR	N-CA	-9.04	1.28	1.46
4	N	38	GLU	CG-CD	9.03	1.65	1.51
3	B	202	VAL	CB-CG1	-9.03	1.33	1.52
3	D	170	THR	CB-CG2	9.02	1.82	1.52
3	B	211	VAL	CB-CG1	-9.01	1.33	1.52
3	D	159	TRP	CZ3-CH2	-9.01	1.25	1.40
2	E	56	TRP	CD2-CE2	9.01	1.52	1.41
2	E	98	TYR	CG-CD2	-9.00	1.27	1.39
2	G	77	PHE	CD1-CE1	-9.00	1.21	1.39
2	C	41	TRP	CZ3-CH2	-8.99	1.25	1.40
4	N	49	GLU	CD-OE2	8.99	1.35	1.25
2	A	77	PHE	CG-CD1	8.98	1.52	1.38
4	O	79	PHE	CD1-CE1	8.98	1.57	1.39
3	B	32	PHE	CD2-CE2	-8.97	1.21	1.39
2	E	42	TYR	CB-CG	-8.97	1.38	1.51
3	D	159	TRP	CE2-CZ2	-8.97	1.24	1.39
3	B	41	PRO	N-CD	-8.95	1.35	1.47
2	A	199	THR	CB-CG2	8.95	1.81	1.52
4	L	79	PHE	CD2-CE2	-8.94	1.21	1.39
4	M	64	TRP	CG-CD2	-8.94	1.28	1.43
3	D	130	ALA	C-O	8.93	1.40	1.23
2	C	165	VAL	CA-CB	8.92	1.73	1.54
3	F	91	THR	CB-CG2	-8.92	1.23	1.52
2	A	92	TYR	CE2-CZ	-8.91	1.26	1.38
1	Q	9	ARG	CZ-NH1	8.91	1.44	1.33
3	B	105	PHE	CE2-CZ	-8.91	1.20	1.37
3	D	47	TRP	CD2-CE2	-8.91	1.30	1.41
3	B	90	ASP	CB-CG	-8.90	1.33	1.51
3	B	159	TRP	CG-CD2	-8.90	1.28	1.43
2	E	78	THR	CA-C	-8.90	1.29	1.52
2	C	4	MET	CA-C	-8.90	1.29	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	79	PHE	CG-CD2	8.90	1.52	1.38
2	A	110	LEU	N-CA	-8.89	1.28	1.46
2	E	52	VAL	CB-CG2	8.88	1.71	1.52
3	H	65	LYS	CD-CE	8.88	1.73	1.51
2	A	38	TYR	CZ-OH	8.88	1.52	1.37
4	N	43	PHE	CE1-CZ	-8.88	1.20	1.37
3	H	70	PHE	CG-CD2	-8.88	1.25	1.38
2	A	206	THR	C-O	8.87	1.40	1.23
3	D	115	THR	CB-CG2	-8.87	1.23	1.52
3	B	45	LEU	CA-CB	-8.86	1.33	1.53
3	B	210	LYS	CG-CD	8.86	1.82	1.52
3	D	50	TRP	CB-CG	8.86	1.66	1.50
2	E	60	ARG	CG-CD	8.86	1.74	1.51
3	D	159	TRP	CG-CD1	-8.86	1.24	1.36
1	Q	9	ARG	CZ-NH2	8.86	1.44	1.33
3	H	195	SER	C-O	8.86	1.40	1.23
2	G	129	GLU	CD-OE1	8.84	1.35	1.25
4	L	37	ALA	CA-CB	-8.84	1.33	1.52
2	E	55	TYR	CD2-CE2	8.84	1.52	1.39
3	D	170	THR	N-CA	-8.84	1.28	1.46
4	M	38	GLU	C-O	-8.83	1.06	1.23
4	N	67	ASP	CB-CG	-8.83	1.33	1.51
4	L	28	ILE	C-O	-8.82	1.06	1.23
4	O	78	LYS	CD-CE	8.82	1.73	1.51
4	L	49	GLU	CD-OE1	-8.82	1.16	1.25
3	H	19	LYS	CB-CG	8.81	1.76	1.52
2	E	96	GLN	C-O	-8.81	1.06	1.23
4	O	79	PHE	CB-CG	-8.81	1.36	1.51
2	C	55	TYR	CD1-CE1	-8.80	1.26	1.39
2	A	125	PRO	CA-C	-8.79	1.35	1.52
2	A	177	SER	CA-CB	-8.79	1.39	1.52
4	N	39	PHE	CE2-CZ	-8.77	1.20	1.37
2	A	146	TYR	CZ-OH	8.77	1.52	1.37
2	C	38	TYR	CG-CD2	8.76	1.50	1.39
2	C	92	TYR	CE1-CZ	-8.75	1.27	1.38
3	F	68	PHE	CG-CD2	-8.75	1.25	1.38
3	F	78	THR	C-O	-8.74	1.06	1.23
4	L	51	TYR	CG-CD1	-8.74	1.27	1.39
3	F	1	GLN	CB-CG	8.74	1.76	1.52
4	L	48	ALA	C-O	8.73	1.40	1.23
2	A	55	TYR	CD2-CE2	8.72	1.52	1.39
4	M	29	PHE	CB-CG	-8.72	1.36	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	93	TYR	CB-CG	-8.72	1.38	1.51
2	E	179	TYR	CA-CB	8.72	1.73	1.53
2	G	80	THR	CA-CB	-8.72	1.30	1.53
3	H	18	VAL	CA-CB	-8.72	1.36	1.54
2	G	207	SER	CA-CB	8.71	1.66	1.52
3	B	127	TYR	CG-CD2	-8.71	1.27	1.39
2	C	42	TYR	CG-CD1	-8.71	1.27	1.39
2	A	188	THR	C-O	-8.70	1.06	1.23
1	S	37	LEU	CG-CD2	8.69	1.83	1.51
4	N	34	ILE	CA-CB	-8.68	1.34	1.54
3	B	71	SER	CB-OG	-8.68	1.30	1.42
3	B	194	PRO	C-O	8.67	1.40	1.23
4	N	72	GLY	CA-C	-8.67	1.38	1.51
2	A	198	TYR	CE1-CZ	-8.66	1.27	1.38
3	B	90	ASP	C-O	8.66	1.39	1.23
2	C	33	ARG	CG-CD	8.64	1.73	1.51
2	A	187	LEU	C-O	-8.63	1.06	1.23
2	A	40	ALA	N-CA	-8.62	1.29	1.46
4	N	51	TYR	CE2-CZ	8.62	1.49	1.38
3	F	163	SER	CA-CB	8.62	1.65	1.52
3	F	218	ARG	CG-CD	8.62	1.73	1.51
3	D	180	TYR	CD1-CE1	-8.61	1.26	1.39
1	Q	11	THR	CA-CB	8.61	1.75	1.53
3	B	41	PRO	CA-CB	-8.60	1.36	1.53
2	E	153	LYS	CB-CG	8.59	1.75	1.52
3	B	201	ASN	CB-CG	-8.59	1.31	1.51
4	O	27	LEU	C-O	8.58	1.39	1.23
3	B	108	TRP	CB-CG	-8.58	1.34	1.50
2	E	161	ARG	NE-CZ	8.57	1.44	1.33
4	N	51	TYR	CD1-CE1	8.56	1.52	1.39
3	F	209	THR	N-CA	-8.56	1.29	1.46
2	C	14	SER	CB-OG	8.55	1.53	1.42
2	E	77	PHE	C-O	8.55	1.39	1.23
3	F	114	VAL	CA-CB	8.55	1.72	1.54
2	G	166	LEU	CG-CD1	8.55	1.83	1.51
2	A	111	GLU	C-O	-8.53	1.07	1.23
2	E	81	ILE	C-O	8.52	1.39	1.23
2	C	160	GLU	CB-CG	8.52	1.68	1.52
2	E	89	GLN	CB-CG	8.52	1.75	1.52
3	D	94	TYR	CE1-CZ	8.52	1.49	1.38
2	E	92	TYR	CE2-CZ	-8.52	1.27	1.38
3	D	47	TRP	CD2-CE3	-8.51	1.27	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	199	THR	CA-CB	-8.51	1.31	1.53
2	G	55	TYR	CG-CD1	-8.51	1.28	1.39
3	F	94	TYR	CA-CB	-8.50	1.35	1.53
3	F	99	PHE	C-O	-8.49	1.07	1.23
2	G	93	TYR	CG-CD2	-8.49	1.28	1.39
1	Q	35	TYR	CD2-CE2	8.49	1.52	1.39
2	C	113	LYS	CD-CE	8.48	1.72	1.51
2	E	31	ASN	C-O	-8.48	1.07	1.23
3	F	111	GLY	CA-C	8.48	1.65	1.51
2	C	125	PRO	CA-C	-8.48	1.35	1.52
3	F	60	TYR	CZ-OH	8.48	1.52	1.37
2	E	17	GLU	CG-CD	8.48	1.64	1.51
3	F	96	CYS	CB-SG	-8.47	1.67	1.82
4	M	51	TYR	CD2-CE2	-8.46	1.26	1.39
3	F	32	PHE	CG-CD2	-8.46	1.26	1.38
3	F	168	VAL	CA-CB	-8.46	1.36	1.54
3	F	188	VAL	CB-CG1	8.46	1.70	1.52
4	O	49	GLU	CD-OE2	8.45	1.34	1.25
2	A	82	SER	CA-CB	-8.45	1.40	1.52
3	H	65	LYS	CA-CB	8.45	1.72	1.53
3	H	208	SER	N-CA	-8.44	1.29	1.46
3	F	74	THR	CB-CG2	8.44	1.80	1.52
4	N	65	THR	CB-CG2	8.44	1.80	1.52
2	E	124	PHE	C-O	-8.44	1.07	1.23
2	A	68	PHE	CG-CD2	-8.43	1.26	1.38
1	Q	10	LYS	CE-NZ	8.43	1.70	1.49
3	H	14	PRO	C-O	8.43	1.40	1.23
3	H	175	LEU	CG-CD2	8.43	1.83	1.51
4	L	20	GLU	CD-OE1	8.42	1.34	1.25
1	S	7	PRO	CG-CD	8.42	1.78	1.50
2	C	92	TYR	N-CA	8.41	1.63	1.46
2	C	179	TYR	CE2-CZ	-8.41	1.27	1.38
3	H	114	VAL	CA-CB	-8.41	1.37	1.54
3	H	205	PRO	N-CD	-8.41	1.36	1.47
3	B	97	ALA	CA-CB	-8.40	1.34	1.52
3	D	47	TRP	CZ2-CH2	-8.40	1.21	1.37
3	H	73	GLU	CD-OE1	8.40	1.34	1.25
2	C	92	TYR	CG-CD2	-8.40	1.28	1.39
3	B	181	THR	C-O	8.39	1.39	1.23
3	D	185	SER	C-O	-8.39	1.07	1.23
2	E	40	ALA	CA-CB	-8.39	1.34	1.52
3	F	57	GLU	CG-CD	8.39	1.64	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	158	GLY	N-CA	8.39	1.58	1.46
3	F	48	MET	CG-SD	8.37	2.02	1.81
2	E	165	VAL	CB-CG1	8.37	1.70	1.52
3	D	153	GLU	N-CA	-8.37	1.29	1.46
4	L	29	PHE	CE1-CZ	8.36	1.53	1.37
2	C	124	PHE	CD2-CE2	-8.36	1.22	1.39
3	H	187	THR	CA-CB	-8.36	1.31	1.53
4	L	40	LYS	CD-CE	8.35	1.72	1.51
2	G	198	TYR	CE2-CZ	8.35	1.49	1.38
3	H	64	PHE	CE1-CZ	8.35	1.53	1.37
3	B	172	PRO	CA-CB	-8.34	1.36	1.53
3	D	210	LYS	CE-NZ	8.34	1.69	1.49
2	E	165	VAL	CB-CG2	8.33	1.70	1.52
4	M	80	ALA	CA-CB	-8.33	1.34	1.52
4	L	51	TYR	CE1-CZ	8.33	1.49	1.38
4	O	76	ASN	CB-CG	8.33	1.70	1.51
3	F	104	TYR	CG-CD2	-8.33	1.28	1.39
2	A	77	PHE	CG-CD2	8.32	1.51	1.38
3	F	29	PHE	CG-CD1	-8.31	1.26	1.38
3	H	218	ARG	N-CA	8.31	1.62	1.46
3	B	94	TYR	CG-CD1	8.30	1.50	1.39
3	D	202	VAL	CA-CB	-8.30	1.37	1.54
4	O	43	PHE	CD2-CE2	-8.29	1.22	1.39
1	S	2	SER	CB-OG	8.29	1.53	1.42
2	G	184	THR	CA-CB	-8.29	1.31	1.53
3	B	155	VAL	CB-CG2	-8.28	1.35	1.52
4	M	44	GLU	CD-OE2	8.28	1.34	1.25
2	G	138	VAL	CB-CG1	8.28	1.70	1.52
3	D	188	VAL	C-O	-8.28	1.07	1.23
2	C	196	ASN	CB-CG	-8.27	1.32	1.51
3	D	157	VAL	CA-CB	-8.27	1.37	1.54
3	B	34	MET	CG-SD	-8.26	1.59	1.81
3	D	152	PRO	N-CD	-8.26	1.36	1.47
2	A	100	PRO	CA-C	-8.26	1.36	1.52
2	A	211	ILE	CA-CB	-8.26	1.35	1.54
4	O	43	PHE	CE1-CZ	8.25	1.53	1.37
2	A	75	THR	N-CA	8.25	1.62	1.46
2	A	55	TYR	CG-CD2	-8.24	1.28	1.39
2	A	96	GLN	CB-CG	8.24	1.74	1.52
4	L	44	GLU	CA-C	8.24	1.74	1.52
2	G	87	GLU	CG-CD	8.24	1.64	1.51
3	D	176	GLN	CG-CD	8.24	1.70	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	41	PRO	CG-CD	8.23	1.77	1.50
2	G	41	TRP	CG-CD1	-8.23	1.25	1.36
2	G	42	TYR	CE1-CZ	-8.23	1.27	1.38
2	C	43	GLN	CG-CD	8.23	1.70	1.51
1	P	31	VAL	CB-CG2	8.22	1.70	1.52
2	C	145	PHE	CD1-CE1	-8.22	1.22	1.39
2	C	183	SER	CA-CB	8.22	1.65	1.52
3	B	24	ALA	CA-C	-8.21	1.31	1.52
3	B	151	PHE	CG-CD1	-8.21	1.26	1.38
2	E	214	SER	CA-CB	-8.21	1.40	1.52
2	E	71	ARG	CB-CG	8.21	1.74	1.52
2	A	89	GLN	CA-C	-8.20	1.31	1.52
3	B	167	GLY	C-O	8.20	1.36	1.23
2	A	181	MET	N-CA	8.20	1.62	1.46
3	H	205	PRO	CA-CB	-8.19	1.37	1.53
2	G	189	LYS	CD-CE	8.19	1.71	1.51
2	A	146	TYR	CG-CD2	-8.18	1.28	1.39
3	F	43	LYS	CA-CB	-8.18	1.35	1.53
2	A	1	ASP	CA-CB	8.18	1.72	1.53
4	M	61	ASN	CB-CG	8.17	1.69	1.51
2	A	16	GLY	CA-C	8.16	1.65	1.51
3	B	80	TYR	CD2-CE2	8.16	1.51	1.39
3	B	165	SER	CA-CB	8.15	1.65	1.52
2	G	119	PRO	CA-C	-8.15	1.36	1.52
3	H	166	SER	CB-OG	8.15	1.52	1.42
2	A	124	PHE	N-CA	-8.15	1.30	1.46
2	G	56	TRP	CZ3-CH2	-8.14	1.27	1.40
1	Q	24	PHE	CG-CD1	8.14	1.50	1.38
3	B	55	THR	N-CA	-8.13	1.30	1.46
2	G	56	TRP	CG-CD2	-8.13	1.29	1.43
4	L	79	PHE	CG-CD1	-8.13	1.26	1.38
3	F	184	SER	CA-C	-8.13	1.31	1.52
2	E	84	VAL	CA-C	-8.12	1.31	1.52
1	Q	23	LYS	CG-CD	8.10	1.79	1.52
2	C	93	TYR	N-CA	-8.10	1.30	1.46
3	F	99	PHE	CD2-CE2	-8.10	1.23	1.39
2	A	77	PHE	CD2-CE2	8.09	1.55	1.39
3	H	171	PHE	CE2-CZ	8.09	1.52	1.37
3	D	3	GLN	CB-CG	8.09	1.74	1.52
1	S	34	VAL	CB-CG1	8.08	1.69	1.52
2	E	71	ARG	CZ-NH2	8.08	1.43	1.33
2	E	168	SER	CA-CB	8.08	1.65	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	161	SER	C-O	8.08	1.38	1.23
3	D	153	GLU	CB-CG	8.07	1.67	1.52
3	F	31	ASP	CB-CG	8.07	1.68	1.51
3	H	46	ASN	CB-CG	8.07	1.69	1.51
2	G	139	VAL	CB-CG1	-8.07	1.35	1.52
3	H	126	VAL	N-CA	8.07	1.62	1.46
3	D	39	GLN	C-O	8.07	1.38	1.23
2	A	12	ALA	N-CA	-8.06	1.30	1.46
2	A	195	HIS	N-CA	-8.06	1.30	1.46
2	G	92	TYR	CB-CG	-8.06	1.39	1.51
3	H	139	SER	CB-OG	8.06	1.52	1.42
3	B	195	SER	CB-OG	8.06	1.52	1.42
2	E	150	ILE	CA-CB	8.05	1.73	1.54
4	N	21	VAL	CB-CG2	8.05	1.69	1.52
2	A	192	TYR	CB-CG	-8.05	1.39	1.51
2	C	122	SER	CA-CB	-8.04	1.40	1.52
3	H	118	SER	N-CA	8.04	1.62	1.46
2	G	141	PHE	CE2-CZ	8.04	1.52	1.37
3	F	37	VAL	CB-CG1	8.04	1.69	1.52
3	B	1	GLN	CB-CG	8.04	1.74	1.52
2	C	192	TYR	CB-CG	8.04	1.63	1.51
3	H	36	TRP	CE3-CZ3	8.04	1.52	1.38
4	O	52	ARG	CA-CB	8.03	1.71	1.53
3	B	159	TRP	N-CA	8.03	1.62	1.46
4	M	69	GLU	CD-OE2	8.03	1.34	1.25
3	F	99	PHE	CG-CD1	-8.03	1.26	1.38
2	G	161	ARG	NE-CZ	8.03	1.43	1.33
4	O	34	ILE	CA-CB	8.03	1.73	1.54
2	C	201	GLU	CB-CG	8.02	1.67	1.52
3	D	211	VAL	CA-CB	-8.02	1.38	1.54
2	E	35	ARG	CG-CD	8.02	1.72	1.51
2	A	60	ARG	CG-CD	8.02	1.72	1.51
3	H	63	ASP	C-O	8.02	1.38	1.23
3	F	131	PRO	CG-CD	8.01	1.77	1.50
3	B	202	VAL	N-CA	-8.01	1.30	1.46
3	F	64	PHE	CE1-CZ	-8.01	1.22	1.37
3	B	60	TYR	CG-CD1	8.00	1.49	1.39
3	F	159	TRP	CE3-CZ3	8.00	1.52	1.38
2	A	120	THR	C-O	8.00	1.38	1.23
2	C	51	LYS	CE-NZ	8.00	1.69	1.49
3	B	147	VAL	CB-CG1	-7.99	1.36	1.52
3	H	27	TYR	CZ-OH	7.99	1.51	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	194	ARG	CD-NE	7.99	1.60	1.46
3	F	61	ALA	CA-CB	-7.99	1.35	1.52
4	O	20	GLU	CD-OE2	7.98	1.34	1.25
2	C	78	THR	N-CA	-7.98	1.30	1.46
2	C	109	LYS	C-O	7.98	1.38	1.23
4	N	43	PHE	CD2-CE2	-7.97	1.23	1.39
3	H	131	PRO	N-CD	-7.97	1.36	1.47
3	D	169	HIS	C-N	-7.97	1.15	1.34
3	H	151	PHE	CA-CB	-7.96	1.36	1.53
2	C	39	LEU	N-CA	7.96	1.62	1.46
2	E	154	TRP	CD2-CE2	-7.96	1.31	1.41
3	F	10	GLU	N-CA	-7.96	1.30	1.46
2	G	36	LYS	CG-CD	7.96	1.79	1.52
4	N	39	PHE	CD2-CE2	-7.95	1.23	1.39
2	E	213	LYS	CD-CE	7.94	1.71	1.51
3	B	144	GLY	C-O	-7.94	1.10	1.23
3	F	65	LYS	C-O	7.94	1.38	1.23
4	O	53	TYR	CD1-CE1	-7.94	1.27	1.39
4	L	52	ARG	CA-C	7.94	1.73	1.52
3	H	73	GLU	CG-CD	7.94	1.63	1.51
2	G	161	ARG	CG-CD	7.94	1.71	1.51
2	A	52	VAL	CA-CB	-7.93	1.38	1.54
4	N	80	ALA	C-O	-7.93	1.08	1.23
2	C	16	GLY	CA-C	7.93	1.64	1.51
3	H	18	VAL	CB-CG2	7.93	1.69	1.52
1	S	43	ARG	NE-CZ	7.92	1.43	1.33
2	A	93	TYR	CD2-CE2	7.91	1.51	1.39
3	F	120	LYS	CA-CB	-7.91	1.36	1.53
3	D	105	PHE	CD1-CE1	-7.91	1.23	1.39
4	M	58	ALA	C-O	-7.90	1.08	1.23
3	F	64	PHE	C-O	7.90	1.38	1.23
2	C	19	VAL	C-O	-7.90	1.08	1.23
4	M	35	GLN	CG-CD	7.90	1.69	1.51
3	B	113	THR	CB-CG2	7.90	1.78	1.52
3	D	97	ALA	C-O	7.89	1.38	1.23
2	C	70	GLY	C-O	7.89	1.36	1.23
2	G	112	LEU	C-O	7.89	1.38	1.23
1	Q	13	ARG	CB-CG	7.88	1.73	1.52
3	F	27	TYR	CD1-CE1	-7.88	1.27	1.39
3	B	144	GLY	CA-C	7.88	1.64	1.51
2	C	137	SER	C-O	-7.88	1.08	1.23
2	G	179	TYR	CE1-CZ	7.88	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	114	ARG	CB-CG	7.88	1.73	1.52
2	A	113	LYS	C-O	-7.87	1.08	1.23
2	G	169	TRP	CD2-CE3	-7.87	1.28	1.40
3	B	70	PHE	CD2-CE2	7.87	1.54	1.39
1	Q	35	TYR	CG-CD1	7.87	1.49	1.39
3	B	64	PHE	N-CA	7.86	1.62	1.46
2	C	187	LEU	CG-CD1	7.86	1.80	1.51
2	C	179	TYR	CB-CG	7.86	1.63	1.51
2	A	169	TRP	CB-CG	7.86	1.64	1.50
2	E	70	GLY	C-O	7.86	1.36	1.23
2	E	211	ILE	CA-CB	-7.86	1.36	1.54
4	O	33	LYS	CD-CE	7.86	1.70	1.51
2	A	34	THR	CB-CG2	-7.86	1.26	1.52
2	A	38	TYR	CG-CD2	-7.85	1.28	1.39
3	F	12	LYS	CD-CE	7.85	1.70	1.51
3	F	183	SER	CB-OG	-7.84	1.32	1.42
2	E	168	SER	CA-C	-7.84	1.32	1.52
3	B	174	VAL	CB-CG2	-7.84	1.36	1.52
2	C	18	LYS	CG-CD	7.84	1.79	1.52
3	F	87	LYS	C-O	-7.84	1.08	1.23
1	Q	12	LYS	CB-CG	-7.83	1.31	1.52
3	B	127	TYR	CG-CD1	-7.83	1.28	1.39
3	D	83	ILE	CB-CG2	-7.82	1.28	1.52
3	B	31	ASP	C-O	7.82	1.38	1.23
4	L	61	ASN	CB-CG	-7.82	1.33	1.51
2	A	24	LYS	C-O	-7.81	1.08	1.23
2	A	161	ARG	NE-CZ	7.81	1.43	1.33
2	G	156	ILE	CB-CG2	7.81	1.77	1.52
3	D	124	PRO	CG-CD	7.80	1.76	1.50
2	A	154	TRP	CG-CD1	-7.80	1.25	1.36
3	B	51	VAL	CB-CG2	7.80	1.69	1.52
3	B	88	ASN	CB-CG	7.80	1.69	1.51
4	O	39	PHE	CG-CD2	-7.79	1.27	1.38
4	L	23	ILE	CA-CB	-7.79	1.36	1.54
3	D	127	TYR	CD1-CE1	7.79	1.51	1.39
3	H	57	GLU	CD-OE2	-7.79	1.17	1.25
3	F	54	GLU	CB-CG	-7.79	1.37	1.52
3	H	175	LEU	CA-CB	7.79	1.71	1.53
3	D	56	GLY	C-O	-7.78	1.11	1.23
3	D	194	PRO	CA-C	-7.77	1.37	1.52
2	E	198	TYR	CE2-CZ	7.77	1.48	1.38
2	E	137	SER	CB-OG	-7.77	1.32	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	162	GLY	CA-C	-7.77	1.39	1.51
2	G	138	VAL	N-CA	-7.76	1.30	1.46
3	H	94	TYR	CG-CD1	-7.76	1.29	1.39
2	C	18	LYS	CB-CG	7.76	1.73	1.52
2	G	193	GLU	CD-OE2	7.76	1.34	1.25
2	A	60	ARG	C-O	-7.76	1.08	1.23
3	F	193	TRP	C-N	-7.76	1.19	1.34
2	A	216	ASN	CG-OD1	7.75	1.41	1.24
2	G	1	ASP	CA-CB	7.75	1.71	1.53
3	B	205	PRO	N-CA	-7.74	1.34	1.47
3	D	175	LEU	CG-CD2	7.74	1.80	1.51
4	N	36	THR	CA-CB	-7.74	1.33	1.53
3	D	77	SER	CB-OG	7.74	1.52	1.42
2	A	190	ASP	CA-CB	7.73	1.71	1.53
3	F	133	SER	CB-OG	7.73	1.52	1.42
1	S	23	LYS	CA-CB	-7.73	1.36	1.53
3	D	77	SER	CA-CB	7.73	1.64	1.52
3	B	155	VAL	CA-CB	7.73	1.71	1.54
4	M	79	PHE	CA-C	7.72	1.73	1.52
2	G	177	SER	CA-CB	7.72	1.64	1.52
2	A	180	SER	C-O	7.72	1.38	1.23
4	O	67	ASP	C-O	7.72	1.38	1.23
3	H	208	SER	CA-C	-7.71	1.32	1.52
2	G	5	SER	CB-OG	-7.71	1.32	1.42
4	O	51	TYR	C-O	-7.71	1.08	1.23
2	A	130	GLN	CB-CG	7.71	1.73	1.52
1	Q	34	VAL	CB-CG1	7.70	1.69	1.52
2	C	14	SER	CA-CB	7.70	1.64	1.52
2	C	43	GLN	CA-C	-7.70	1.32	1.52
4	O	35	GLN	CA-CB	-7.70	1.37	1.53
3	B	171	PHE	CE1-CZ	-7.70	1.22	1.37
2	A	145	PHE	CD1-CE1	-7.70	1.23	1.39
4	L	39	PHE	CG-CD2	-7.70	1.27	1.38
3	H	162	GLY	C-O	7.69	1.35	1.23
2	G	55	TYR	CZ-OH	-7.69	1.24	1.37
2	C	82	SER	CB-OG	7.69	1.52	1.42
3	D	114	VAL	CB-CG1	7.69	1.69	1.52
3	B	12	LYS	CB-CG	7.69	1.73	1.52
2	C	73	SER	N-CA	7.68	1.61	1.46
3	H	32	PHE	CE2-CZ	7.68	1.51	1.37
2	G	181	MET	N-CA	7.68	1.61	1.46
3	H	27	TYR	CE1-CZ	-7.68	1.28	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	56	TRP	CG-CD1	7.68	1.47	1.36
3	F	139	SER	CB-OG	7.67	1.52	1.42
1	Q	43	ARG	CB-CG	7.67	1.73	1.52
3	F	8	GLY	C-O	7.67	1.35	1.23
3	D	103	GLN	CB-CG	7.66	1.73	1.52
2	E	1	ASP	N-CA	7.66	1.61	1.46
3	B	50	TRP	C-O	7.66	1.37	1.23
3	H	145	CYS	CB-SG	7.65	1.95	1.82
4	O	58	ALA	N-CA	7.65	1.61	1.46
3	H	143	LEU	CA-CB	-7.65	1.36	1.53
3	F	6	GLN	CA-C	7.64	1.72	1.52
3	F	191	SER	N-CA	-7.64	1.31	1.46
3	H	51	VAL	CA-C	7.64	1.72	1.52
3	B	140	MET	SD-CE	7.64	2.20	1.77
3	F	67	ARG	CD-NE	-7.64	1.33	1.46
4	N	60	VAL	CA-CB	7.63	1.70	1.54
3	H	28	THR	CA-CB	7.63	1.73	1.53
2	A	141	PHE	CG-CD1	-7.63	1.27	1.38
3	D	127	TYR	N-CA	-7.63	1.31	1.46
3	D	198	VAL	CB-CG1	-7.63	1.36	1.52
2	A	152	VAL	CB-CG2	-7.62	1.36	1.52
3	F	88	ASN	CA-C	7.62	1.72	1.52
4	O	57	HIS	CA-C	-7.62	1.33	1.52
4	O	55	ALA	N-CA	-7.62	1.31	1.46
3	B	171	PHE	CD1-CE1	-7.62	1.24	1.39
3	F	109	GLY	C-O	-7.61	1.11	1.23
3	F	153	GLU	CD-OE2	7.61	1.34	1.25
3	B	90	ASP	CA-CB	-7.61	1.37	1.53
3	F	214	LYS	CD-CE	7.61	1.70	1.51
2	G	45	LYS	CB-CG	7.61	1.73	1.52
3	H	213	LYS	CA-CB	-7.61	1.37	1.53
3	F	171	PHE	CA-CB	-7.60	1.37	1.53
3	H	184	SER	CB-OG	-7.59	1.32	1.42
3	D	152	PRO	CA-C	7.59	1.68	1.52
2	A	217	ARG	NE-CZ	7.58	1.42	1.33
2	A	188	THR	CA-C	-7.57	1.33	1.52
3	H	105	PHE	CG-CD2	-7.57	1.27	1.38
4	O	20	GLU	CD-OE1	7.57	1.33	1.25
3	B	94	TYR	CD1-CE1	-7.57	1.27	1.39
2	C	33	ARG	NE-CZ	7.57	1.42	1.33
2	A	124	PHE	CE2-CZ	7.57	1.51	1.37
4	L	52	ARG	CB-CG	7.57	1.73	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	192	TYR	CB-CG	7.56	1.62	1.51
2	C	150	ILE	C-O	7.56	1.37	1.23
3	B	104	TYR	CD2-CE2	-7.56	1.28	1.39
2	E	99	ILE	CB-CG2	-7.55	1.29	1.52
3	B	125	SER	CA-C	-7.55	1.33	1.52
2	E	180	SER	CB-OG	7.55	1.52	1.42
4	N	49	GLU	CG-CD	-7.54	1.40	1.51
4	M	44	GLU	CD-OE1	-7.54	1.17	1.25
2	A	17	GLU	CD-OE2	-7.54	1.17	1.25
2	G	169	TRP	CB-CG	-7.53	1.36	1.50
3	H	68	PHE	CE1-CZ	7.53	1.51	1.37
3	D	21	SER	CB-OG	-7.53	1.32	1.42
3	F	97	ALA	C-O	-7.53	1.09	1.23
2	G	192	TYR	CA-C	-7.52	1.33	1.52
2	C	24	LYS	C-O	7.52	1.37	1.23
2	E	36	LYS	CB-CG	7.52	1.72	1.52
4	L	45	GLU	CB-CG	7.51	1.66	1.52
2	E	68	PHE	CE1-CZ	-7.51	1.23	1.37
4	L	17	PRO	C-O	7.51	1.38	1.23
2	E	66	ASP	C-O	-7.51	1.09	1.23
4	N	32	GLY	CA-C	-7.51	1.39	1.51
3	H	171	PHE	N-CA	-7.50	1.31	1.46
4	O	29	PHE	CD2-CE2	-7.50	1.24	1.39
1	Q	20	GLN	CG-CD	7.50	1.68	1.51
3	H	168	VAL	CB-CG2	7.50	1.68	1.52
3	H	171	PHE	CG-CD1	7.49	1.50	1.38
3	B	212	ASP	CB-CG	7.49	1.67	1.51
2	E	19	VAL	CB-CG1	7.49	1.68	1.52
4	N	35	GLN	C-O	-7.49	1.09	1.23
2	E	177	SER	CB-OG	-7.48	1.32	1.42
2	G	110	LEU	C-O	-7.48	1.09	1.23
3	H	64	PHE	CE2-CZ	-7.48	1.23	1.37
3	B	157	VAL	CA-CB	7.48	1.70	1.54
2	E	42	TYR	CE2-CZ	-7.48	1.28	1.38
4	L	28	ILE	CB-CG2	7.48	1.76	1.52
3	D	67	ARG	CA-C	7.48	1.72	1.52
3	D	159	TRP	CB-CG	7.48	1.63	1.50
3	D	68	PHE	CD1-CE1	-7.48	1.24	1.39
2	G	28	SER	CB-OG	7.47	1.51	1.42
3	H	9	PRO	C-O	-7.47	1.08	1.23
2	E	123	ILE	CA-C	7.47	1.72	1.52
3	D	193	TRP	CE3-CZ3	7.47	1.51	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1	GLN	CA-C	7.46	1.72	1.52
3	H	37	VAL	CA-CB	-7.46	1.39	1.54
3	B	159	TRP	CZ2-CH2	7.46	1.51	1.37
2	C	127	SER	CA-CB	-7.46	1.41	1.52
3	B	171	PHE	CG-CD2	-7.46	1.27	1.38
2	C	92	TYR	CG-CD1	7.45	1.48	1.39
4	M	33	LYS	C-O	-7.45	1.09	1.23
1	S	24	PHE	CG-CD2	7.45	1.50	1.38
3	H	32	PHE	CB-CG	7.45	1.64	1.51
3	H	67	ARG	NE-CZ	-7.44	1.23	1.33
2	E	95	LYS	CB-CG	7.44	1.72	1.52
2	E	192	TYR	CD2-CE2	7.44	1.50	1.39
3	B	176	GLN	CD-NE2	7.43	1.51	1.32
4	O	34	ILE	C-O	-7.43	1.09	1.23
2	E	102	LEU	N-CA	-7.43	1.31	1.46
2	A	172	GLN	CA-C	-7.42	1.33	1.52
2	G	13	VAL	CA-CB	7.42	1.70	1.54
2	G	109	LYS	CG-CD	7.41	1.77	1.52
3	H	1	GLN	CB-CG	7.41	1.72	1.52
3	B	4	LEU	C-O	-7.41	1.09	1.23
2	C	160	GLU	CD-OE2	7.41	1.33	1.25
2	G	43	GLN	CG-CD	7.41	1.68	1.51
3	B	12	LYS	CA-C	-7.40	1.33	1.52
3	B	180	TYR	CD2-CE2	-7.40	1.28	1.39
4	O	33	LYS	CG-CD	7.40	1.77	1.52
2	G	52	VAL	CB-CG2	7.40	1.68	1.52
3	B	216	VAL	CB-CG1	7.40	1.68	1.52
2	A	92	TYR	CB-CG	7.39	1.62	1.51
3	D	140	MET	SD-CE	7.39	2.19	1.77
4	N	34	ILE	C-O	7.39	1.37	1.23
2	A	149	ASP	CA-CB	7.39	1.70	1.53
2	E	143	ASN	CA-C	7.38	1.72	1.52
2	E	198	TYR	CZ-OH	7.38	1.50	1.37
2	A	33	ARG	CB-CG	7.38	1.72	1.52
2	G	110	LEU	C-N	-7.37	1.17	1.34
3	B	193	TRP	CG-CD2	-7.37	1.31	1.43
4	O	45	GLU	N-CA	7.37	1.61	1.46
3	D	81	LEU	CG-CD1	7.37	1.79	1.51
2	A	98	TYR	CE2-CZ	-7.37	1.28	1.38
2	A	209	SER	CA-CB	7.36	1.64	1.52
3	F	212	ASP	N-CA	-7.36	1.31	1.46
2	C	206	THR	CB-CG2	7.36	1.76	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	213	LYS	CE-NZ	7.36	1.67	1.49
2	A	41	TRP	CE3-CZ3	-7.36	1.25	1.38
2	C	145	PHE	CG-CD1	-7.36	1.27	1.38
4	N	73	ASN	CA-CB	7.36	1.72	1.53
3	B	33	SER	CB-OG	7.35	1.51	1.42
2	C	126	PRO	C-O	7.35	1.38	1.23
2	E	194	ARG	CZ-NH1	7.35	1.42	1.33
3	H	5	VAL	CB-CG1	7.35	1.68	1.52
2	E	119	PRO	CG-CD	-7.35	1.26	1.50
3	D	188	VAL	CA-CB	7.35	1.70	1.54
2	A	195	HIS	CB-CG	-7.34	1.36	1.50
3	H	150	TYR	CD2-CE2	-7.34	1.28	1.39
4	N	38	GLU	CD-OE1	7.34	1.33	1.25
3	H	50	TRP	CA-CB	7.34	1.70	1.53
4	N	21	VAL	CA-CB	7.34	1.70	1.54
2	A	33	ARG	CZ-NH2	7.34	1.42	1.33
3	B	64	PHE	CD1-CE1	-7.33	1.24	1.39
2	E	133	SER	C-O	7.33	1.37	1.23
3	D	2	ILE	N-CA	7.33	1.61	1.46
2	C	91	VAL	CB-CG2	7.32	1.68	1.52
2	C	138	VAL	N-CA	-7.32	1.31	1.46
3	D	99	PHE	CD1-CE1	7.32	1.53	1.39
3	F	131	PRO	C-N	-7.32	1.19	1.33
2	C	93	TYR	CD1-CE1	-7.32	1.28	1.39
4	O	54	ALA	CA-CB	7.32	1.67	1.52
2	C	207	SER	CA-C	-7.32	1.33	1.52
2	E	38	TYR	CG-CD2	-7.31	1.29	1.39
2	C	104	PHE	CA-CB	-7.31	1.37	1.53
2	G	124	PHE	CD2-CE2	7.31	1.53	1.39
3	D	27	TYR	CG-CD2	-7.30	1.29	1.39
3	B	121	THR	C-O	-7.30	1.09	1.23
3	F	27	TYR	CB-CG	7.30	1.62	1.51
2	G	197	SER	CB-OG	7.30	1.51	1.42
2	E	215	PHE	C-O	-7.30	1.09	1.23
2	A	103	THR	CA-CB	-7.29	1.34	1.53
4	O	38	GLU	CD-OE1	7.29	1.33	1.25
2	E	149	ASP	CA-C	7.28	1.71	1.52
2	A	93	TYR	CZ-OH	-7.28	1.25	1.37
3	B	47	TRP	CZ3-CH2	-7.28	1.28	1.40
2	C	169	TRP	N-CA	-7.28	1.31	1.46
2	G	132	THR	CA-CB	-7.28	1.34	1.53
2	C	15	ALA	CA-C	-7.28	1.34	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	47	THR	C-O	-7.28	1.09	1.23
3	F	21	SER	C-O	-7.28	1.09	1.23
2	A	161	ARG	CZ-NH1	7.27	1.42	1.33
1	Q	40	ARG	CA-C	7.27	1.71	1.52
2	C	27	GLN	CD-NE2	7.27	1.51	1.32
3	D	217	PRO	CA-CB	7.27	1.68	1.53
2	G	116	ASP	CB-CG	7.27	1.67	1.51
4	M	61	ASN	C-O	-7.27	1.09	1.23
2	A	77	PHE	CD1-CE1	7.27	1.53	1.39
3	D	174	VAL	CB-CG2	7.26	1.68	1.52
2	G	14	SER	CA-CB	-7.26	1.42	1.52
3	H	59	THR	N-CA	7.26	1.60	1.46
3	D	102	ARG	CA-CB	-7.26	1.38	1.53
3	F	84	ASN	CA-CB	7.26	1.72	1.53
2	C	124	PHE	N-CA	-7.25	1.31	1.46
2	C	210	PRO	N-CA	-7.25	1.34	1.47
3	F	142	THR	N-CA	7.25	1.60	1.46
3	F	77	SER	CA-CB	7.25	1.63	1.52
2	A	114	ARG	CZ-NH2	7.25	1.42	1.33
3	D	79	ALA	C-O	-7.24	1.09	1.23
3	D	102	ARG	CZ-NH1	7.24	1.42	1.33
3	B	218	ARG	C-O	7.24	1.37	1.23
4	M	46	ALA	CA-C	7.24	1.71	1.52
2	G	102	LEU	CG-CD1	7.24	1.78	1.51
3	B	159	TRP	NE1-CE2	-7.24	1.28	1.37
2	G	60	ARG	CB-CG	7.24	1.72	1.52
3	H	79	ALA	N-CA	7.23	1.60	1.46
2	C	124	PHE	CG-CD1	-7.23	1.27	1.38
3	H	164	LEU	CG-CD2	7.23	1.78	1.51
2	A	215	PHE	CD2-CE2	-7.22	1.24	1.39
3	F	118	SER	CA-C	-7.22	1.34	1.52
3	F	16	GLU	N-CA	-7.22	1.31	1.46
3	B	87	LYS	C-O	7.21	1.37	1.23
2	E	110	LEU	CG-CD1	-7.21	1.25	1.51
2	E	64	VAL	CA-CB	-7.20	1.39	1.54
2	G	55	TYR	CE2-CZ	-7.20	1.29	1.38
3	D	184	SER	CB-OG	7.20	1.51	1.42
3	B	180	TYR	C-O	-7.20	1.09	1.23
2	E	188	THR	CA-CB	-7.20	1.34	1.53
4	N	81	GLY	CA-C	7.20	1.63	1.51
2	G	158	GLY	CA-C	7.20	1.63	1.51
3	F	157	VAL	C-O	-7.20	1.09	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	N	39	PHE	CG-CD2	-7.19	1.27	1.38
3	D	102	ARG	NE-CZ	7.19	1.42	1.33
4	O	45	GLU	CD-OE2	7.19	1.33	1.25
2	A	91	VAL	N-CA	-7.19	1.31	1.46
3	D	159	TRP	CE3-CZ3	-7.19	1.26	1.38
3	H	94	TYR	CE1-CZ	-7.19	1.29	1.38
2	C	161	ARG	CZ-NH1	7.18	1.42	1.33
2	E	7	SER	C-N	-7.18	1.20	1.34
2	G	63	GLY	N-CA	-7.18	1.35	1.46
2	G	61	GLU	CD-OE2	7.18	1.33	1.25
2	G	71	ARG	CB-CG	7.17	1.72	1.52
2	A	88	ASP	CA-C	7.17	1.71	1.52
4	N	68	LEU	N-CA	7.17	1.60	1.46
2	A	77	PHE	CE1-CZ	7.17	1.50	1.37
3	D	89	GLU	CG-CD	7.17	1.62	1.51
3	D	159	TRP	NE1-CE2	-7.16	1.28	1.37
2	G	66	ASP	CA-C	-7.16	1.34	1.52
2	C	73	SER	CB-OG	7.16	1.51	1.42
4	L	64	TRP	CA-C	-7.16	1.34	1.52
3	B	127	TYR	CE2-CZ	-7.15	1.29	1.38
3	B	135	ALA	CA-CB	7.15	1.67	1.52
2	E	215	PHE	CE1-CZ	-7.15	1.23	1.37
3	B	95	PHE	CE1-CZ	-7.15	1.23	1.37
4	L	34	ILE	N-CA	-7.15	1.32	1.46
3	F	95	PHE	CE1-CZ	-7.15	1.23	1.37
3	D	37	VAL	N-CA	-7.14	1.32	1.46
3	D	161	SER	CA-C	-7.14	1.34	1.52
3	B	88	ASN	CG-OD1	7.14	1.39	1.24
2	A	113	LYS	N-CA	-7.14	1.32	1.46
2	C	138	VAL	CA-CB	-7.13	1.39	1.54
3	D	80	TYR	CD1-CE1	7.13	1.50	1.39
2	C	201	GLU	CD-OE1	-7.13	1.17	1.25
2	A	142	LEU	C-O	-7.13	1.09	1.23
2	A	171	ASP	C-N	-7.13	1.17	1.34
2	E	44	GLN	CA-CB	-7.13	1.38	1.53
1	Q	25	PRO	N-CD	7.12	1.57	1.47
4	M	60	VAL	CA-CB	7.12	1.69	1.54
4	L	65	THR	CA-CB	7.12	1.71	1.53
4	O	24	LYS	N-CA	-7.12	1.32	1.46
4	L	33	LYS	CG-CD	7.12	1.76	1.52
3	B	160	ASN	CA-C	-7.11	1.34	1.52
3	B	204	HIS	C-N	-7.11	1.20	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	89	GLU	CD-OE1	7.11	1.33	1.25
3	F	87	LYS	CB-CG	7.11	1.71	1.52
1	Q	24	PHE	CD1-CE1	7.11	1.53	1.39
2	A	109	LYS	CA-CB	-7.11	1.38	1.53
2	E	4	MET	CA-CB	-7.11	1.38	1.53
3	F	189	PRO	CB-CG	7.11	1.85	1.50
2	G	190	ASP	CB-CG	7.11	1.66	1.51
2	A	169	TRP	CE2-CZ2	7.11	1.51	1.39
2	A	141	PHE	CD1-CE1	-7.10	1.25	1.39
2	C	146	TYR	CB-CG	7.10	1.62	1.51
4	L	29	PHE	CB-CG	-7.10	1.39	1.51
3	D	180	TYR	CB-CG	7.10	1.62	1.51
3	D	201	ASN	CG-OD1	7.10	1.39	1.24
3	D	165	SER	CA-CB	7.10	1.63	1.52
2	G	192	TYR	CE1-CZ	-7.10	1.29	1.38
3	D	186	VAL	CB-CG2	7.09	1.67	1.52
3	F	176	GLN	CG-CD	7.09	1.67	1.51
3	H	71	SER	CA-CB	-7.08	1.42	1.52
3	B	121	THR	CA-C	-7.08	1.34	1.52
4	L	51	TYR	CA-CB	-7.08	1.38	1.53
3	H	214	LYS	CA-C	-7.08	1.34	1.52
3	B	194	PRO	N-CD	-7.08	1.38	1.47
3	F	95	PHE	CG-CD1	-7.08	1.28	1.38
3	H	79	ALA	CA-CB	7.08	1.67	1.52
3	H	192	THR	CA-C	7.08	1.71	1.52
4	N	61	ASN	C-N	7.08	1.45	1.33
3	F	94	TYR	C-O	-7.07	1.09	1.23
4	N	39	PHE	CD1-CE1	-7.07	1.25	1.39
2	G	46	PRO	N-CD	-7.07	1.38	1.47
3	D	46	ASN	CA-C	-7.06	1.34	1.52
1	Q	8	GLN	C-O	7.06	1.36	1.23
4	N	37	ALA	CA-CB	7.06	1.67	1.52
4	L	21	VAL	C-O	-7.06	1.09	1.23
2	E	110	LEU	C-N	7.06	1.50	1.34
2	E	64	VAL	N-CA	-7.06	1.32	1.46
2	E	104	PHE	CE1-CZ	-7.06	1.24	1.37
2	G	31	ASN	CB-CG	7.06	1.67	1.51
4	O	24	LYS	C-O	7.05	1.36	1.23
3	B	155	VAL	N-CA	7.05	1.60	1.46
3	H	67	ARG	C-O	-7.05	1.09	1.23
4	L	39	PHE	CE1-CZ	-7.05	1.24	1.37
2	C	55	TYR	CD2-CE2	-7.05	1.28	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	192	TYR	CB-CG	7.04	1.62	1.51
2	C	118	ALA	N-CA	7.04	1.60	1.46
3	B	73	GLU	C-O	7.04	1.36	1.23
1	S	9	ARG	NE-CZ	7.04	1.42	1.33
3	F	160	ASN	N-CA	-7.04	1.32	1.46
2	C	61	GLU	N-CA	-7.03	1.32	1.46
2	E	139	VAL	CB-CG1	7.03	1.67	1.52
2	G	62	SER	C-O	-7.03	1.09	1.23
2	A	38	TYR	CG-CD1	7.03	1.48	1.39
4	N	58	ALA	C-O	7.03	1.36	1.23
2	C	76	ASP	CA-CB	7.02	1.69	1.53
2	G	124	PHE	CG-CD2	-7.02	1.28	1.38
2	G	146	TYR	CE1-CZ	7.02	1.47	1.38
3	B	106	ASP	CA-CB	7.02	1.69	1.53
2	C	192	TYR	CE1-CZ	7.01	1.47	1.38
3	D	50	TRP	CE3-CZ3	-7.01	1.26	1.38
4	L	43	PHE	C-O	7.01	1.36	1.23
2	C	2	ILE	CA-CB	7.01	1.71	1.54
1	Q	10	LYS	CD-CE	7.00	1.68	1.51
3	D	148	LYS	CE-NZ	-7.00	1.31	1.49
2	A	67	ARG	CZ-NH1	-7.00	1.24	1.33
4	M	79	PHE	CD1-CE1	-7.00	1.25	1.39
2	A	16	GLY	C-O	6.99	1.34	1.23
2	A	147	PRO	N-CD	-6.99	1.38	1.47
4	L	21	VAL	CA-CB	6.99	1.69	1.54
2	G	118	ALA	C-O	6.99	1.36	1.23
2	G	39	LEU	CA-CB	-6.99	1.37	1.53
2	E	170	THR	CB-CG2	-6.99	1.29	1.52
3	D	80	TYR	CE2-CZ	6.98	1.47	1.38
3	B	157	VAL	C-O	6.98	1.36	1.23
3	H	57	GLU	CA-CB	6.98	1.69	1.53
4	O	20	GLU	CB-CG	6.98	1.65	1.52
4	L	21	VAL	CB-CG2	6.98	1.67	1.52
2	C	149	ASP	CG-OD1	6.98	1.41	1.25
2	E	92	TYR	CG-CD1	-6.97	1.30	1.39
2	E	5	SER	CB-OG	6.97	1.51	1.42
2	E	147	PRO	N-CA	-6.97	1.35	1.47
4	N	28	ILE	CB-CG2	6.97	1.74	1.52
2	E	169	TRP	CE2-CZ2	6.97	1.51	1.39
1	S	29	GLN	CB-CG	6.97	1.71	1.52
3	H	118	SER	CB-OG	6.97	1.51	1.42
2	E	56	TRP	CZ3-CH2	6.96	1.51	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	79	ALA	CA-CB	6.96	1.67	1.52
2	A	87	GLU	CA-C	-6.96	1.34	1.52
3	D	53	THR	CA-CB	-6.96	1.35	1.53
2	C	159	SER	CB-OG	6.95	1.51	1.42
2	C	207	SER	CB-OG	6.94	1.51	1.42
2	G	38	TYR	CE1-CZ	6.94	1.47	1.38
3	F	150	TYR	CZ-OH	-6.94	1.26	1.37
4	O	21	VAL	CB-CG2	6.94	1.67	1.52
4	O	33	LYS	CB-CG	6.94	1.71	1.52
4	L	26	ASN	C-O	6.94	1.36	1.23
4	M	45	GLU	CA-C	-6.93	1.34	1.52
4	L	35	GLN	CG-CD	6.93	1.67	1.51
3	D	19	LYS	CA-C	-6.93	1.34	1.52
2	G	175	LYS	N-CA	-6.93	1.32	1.46
4	O	53	TYR	CG-CD2	-6.93	1.30	1.39
2	C	148	LYS	CD-CE	6.93	1.68	1.51
3	F	80	TYR	CG-CD2	-6.93	1.30	1.39
3	H	86	LEU	CG-CD1	6.92	1.77	1.51
3	F	200	CYS	C-O	-6.92	1.10	1.23
3	B	185	SER	CA-CB	6.92	1.63	1.52
2	C	79	LEU	C-O	-6.92	1.10	1.23
3	D	49	GLY	C-O	6.92	1.34	1.23
1	Q	13	ARG	CG-CD	6.92	1.69	1.51
2	E	91	VAL	C-O	6.92	1.36	1.23
2	A	93	TYR	CD1-CE1	6.92	1.49	1.39
3	H	41	PRO	CA-C	-6.92	1.39	1.52
1	P	24	PHE	CE1-CZ	6.92	1.50	1.37
3	D	38	ASN	CA-C	-6.91	1.34	1.52
1	Q	17	ARG	CG-CD	6.91	1.69	1.51
3	F	209	THR	CA-C	-6.91	1.34	1.52
4	N	23	ILE	CB-CG2	-6.91	1.31	1.52
3	D	123	PRO	CA-C	-6.91	1.39	1.52
2	A	219	GLU	N-CA	6.91	1.60	1.46
1	Q	33	GLY	C-O	6.91	1.34	1.23
2	E	37	ASN	CA-C	-6.90	1.35	1.52
2	E	99	ILE	N-CA	6.90	1.60	1.46
2	G	121	VAL	CA-CB	-6.90	1.40	1.54
3	B	40	ALA	N-CA	6.90	1.60	1.46
2	C	192	TYR	CA-C	6.90	1.70	1.52
3	F	127	TYR	CB-CG	-6.90	1.41	1.51
2	G	175	LYS	CG-CD	6.90	1.75	1.52
4	L	33	LYS	CA-C	6.89	1.70	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Q	6	LYS	CD-CE	6.89	1.68	1.51
3	D	151	PHE	N-CA	-6.89	1.32	1.46
4	M	64	TRP	CD2-CE2	-6.89	1.33	1.41
2	E	144	ASN	CA-C	-6.89	1.35	1.52
4	N	23	ILE	C-O	-6.89	1.10	1.23
4	N	81	GLY	C-O	6.89	1.34	1.23
3	F	47	TRP	CG-CD1	-6.89	1.27	1.36
2	A	167	ASN	N-CA	-6.89	1.32	1.46
3	B	126	VAL	CA-C	-6.89	1.35	1.52
4	N	54	ALA	CA-C	6.89	1.70	1.52
3	F	4	LEU	CG-CD1	-6.88	1.26	1.51
2	C	213	LYS	N-CA	6.88	1.60	1.46
3	B	78	THR	CA-C	-6.88	1.35	1.52
2	E	61	GLU	CD-OE2	6.87	1.33	1.25
3	F	204	HIS	C-O	-6.87	1.10	1.23
2	G	109	LYS	CA-CB	-6.87	1.38	1.53
4	L	18	LYS	CA-CB	6.87	1.69	1.53
4	O	23	ILE	CB-CG2	-6.87	1.31	1.52
3	D	171	PHE	CE1-CZ	6.87	1.50	1.37
4	M	52	ARG	CD-NE	6.87	1.58	1.46
3	B	11	LEU	C-O	6.87	1.36	1.23
3	B	90	ASP	N-CA	-6.87	1.32	1.46
3	D	95	PHE	CD1-CE1	-6.87	1.25	1.39
3	F	21	SER	CA-CB	6.87	1.63	1.52
3	B	186	VAL	C-O	-6.86	1.10	1.23
2	E	169	TRP	C-O	-6.86	1.10	1.23
3	B	197	THR	CB-CG2	6.86	1.75	1.52
2	C	175	LYS	C-O	-6.86	1.10	1.23
2	G	93	TYR	CB-CG	6.85	1.61	1.51
3	B	195	SER	N-CA	6.85	1.60	1.46
3	B	20	ILE	CA-CB	6.85	1.70	1.54
2	E	11	LEU	CG-CD1	6.85	1.77	1.51
2	G	176	ASP	N-CA	6.85	1.60	1.46
3	H	145	CYS	C-O	-6.85	1.10	1.23
4	O	64	TRP	CA-C	-6.85	1.35	1.52
2	A	145	PHE	CD2-CE2	-6.85	1.25	1.39
3	H	111	GLY	CA-C	-6.84	1.41	1.51
2	E	44	GLN	CG-CD	6.83	1.66	1.51
2	E	81	ILE	CB-CG2	6.83	1.74	1.52
2	C	62	SER	CB-OG	6.83	1.51	1.42
4	N	53	TYR	CG-CD2	-6.83	1.30	1.39
2	G	164	GLY	CA-C	6.83	1.62	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	149	ASP	CG-OD2	6.82	1.41	1.25
3	D	184	SER	CA-CB	-6.82	1.42	1.52
2	E	76	ASP	CG-OD1	6.82	1.41	1.25
2	G	112	LEU	CG-CD2	6.82	1.77	1.51
3	D	32	PHE	CB-CG	-6.82	1.39	1.51
4	L	29	PHE	CD2-CE2	6.82	1.52	1.39
2	C	155	LYS	CA-C	-6.82	1.35	1.52
2	C	156	ILE	CB-CG2	-6.82	1.31	1.52
3	D	6	GLN	CD-OE1	-6.82	1.08	1.24
4	N	41	GLY	C-O	-6.82	1.12	1.23
1	Q	20	GLN	CD-NE2	6.81	1.49	1.32
2	E	98	TYR	CD2-CE2	-6.81	1.29	1.39
3	B	68	PHE	C-O	6.81	1.36	1.23
3	D	152	PRO	CG-CD	6.81	1.73	1.50
3	D	127	TYR	CZ-OH	-6.81	1.26	1.37
2	G	76	ASP	CB-CG	6.81	1.66	1.51
2	A	130	GLN	CA-CB	6.81	1.69	1.53
2	C	170	THR	C-O	-6.81	1.10	1.23
3	D	65	LYS	CD-CE	6.81	1.68	1.51
3	H	36	TRP	CZ3-CH2	-6.80	1.29	1.40
4	L	28	ILE	CA-C	-6.80	1.35	1.52
3	D	183	SER	N-CA	6.80	1.59	1.46
2	E	56	TRP	C-O	-6.80	1.10	1.23
2	G	181	MET	CB-CG	-6.80	1.29	1.51
2	C	113	LYS	CA-CB	-6.80	1.39	1.53
3	D	115	THR	CA-C	-6.80	1.35	1.52
2	C	141	PHE	CD1-CE1	-6.80	1.25	1.39
3	B	60	TYR	C-O	-6.79	1.10	1.23
2	C	77	PHE	CG-CD1	-6.79	1.28	1.38
1	S	3	THR	CB-CG2	6.79	1.74	1.52
2	E	12	ALA	CA-C	-6.79	1.35	1.52
2	A	210	PRO	CG-CD	6.79	1.73	1.50
2	C	55	TYR	CA-C	6.79	1.70	1.52
2	C	121	VAL	CA-CB	-6.78	1.40	1.54
2	E	84	VAL	CB-CG1	-6.78	1.38	1.52
3	F	173	ALA	CA-CB	6.78	1.66	1.52
2	E	109	LYS	C-O	-6.78	1.10	1.23
3	H	82	GLN	CD-OE1	6.78	1.38	1.24
4	M	81	GLY	CA-C	6.77	1.62	1.51
3	F	109	GLY	CA-C	6.77	1.62	1.51
2	A	43	GLN	CD-NE2	6.77	1.49	1.32
2	C	189	LYS	CD-CE	6.77	1.68	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	68	PHE	N-CA	-6.77	1.32	1.46
2	C	15	ALA	CA-CB	6.76	1.66	1.52
2	C	28	SER	N-CA	6.76	1.59	1.46
2	E	192	TYR	CE2-CZ	-6.76	1.29	1.38
3	F	216	VAL	CB-CG1	6.76	1.67	1.52
2	E	129	GLU	N-CA	-6.75	1.32	1.46
3	H	139	SER	CA-CB	6.75	1.63	1.52
2	A	14	SER	C-O	-6.75	1.10	1.23
2	E	216	ASN	C-O	6.75	1.36	1.23
3	B	168	VAL	CB-CG2	-6.75	1.38	1.52
3	D	145	CYS	CA-CB	-6.75	1.39	1.53
3	H	127	TYR	CD2-CE2	-6.74	1.29	1.39
3	D	161	SER	CB-OG	6.74	1.51	1.42
3	F	18	VAL	CB-CG2	-6.74	1.38	1.52
4	O	23	ILE	CA-CB	-6.74	1.39	1.54
3	F	159	TRP	CD2-CE2	-6.74	1.33	1.41
2	A	98	TYR	CA-C	-6.74	1.35	1.52
2	A	117	ALA	CA-CB	6.74	1.66	1.52
3	H	127	TYR	CA-CB	-6.74	1.39	1.53
3	D	147	VAL	CA-CB	-6.73	1.40	1.54
3	F	84	ASN	CB-CG	6.73	1.66	1.51
3	D	125	SER	CA-CB	6.73	1.63	1.52
3	B	105	PHE	CG-CD1	-6.73	1.28	1.38
3	D	90	ASP	C-O	6.73	1.36	1.23
2	G	110	LEU	CA-C	-6.73	1.35	1.52
2	A	154	TRP	CZ3-CH2	-6.73	1.29	1.40
3	D	126	VAL	CB-CG2	-6.73	1.38	1.52
3	H	138	ASN	CB-CG	6.73	1.66	1.51
2	A	50	PRO	N-CA	-6.72	1.35	1.47
3	B	166	SER	C-N	-6.72	1.21	1.33
3	D	120	LYS	N-CA	6.72	1.59	1.46
3	D	140	MET	CG-SD	6.72	1.98	1.81
3	H	130	ALA	CA-CB	-6.71	1.38	1.52
3	B	179	LEU	CG-CD1	6.71	1.76	1.51
3	B	63	ASP	C-O	6.71	1.36	1.23
2	E	103	THR	CA-CB	-6.71	1.35	1.53
2	A	94	CYS	CB-SG	6.71	1.93	1.82
4	L	42	THR	CA-CB	6.71	1.70	1.53
3	D	204	HIS	CA-C	6.71	1.70	1.52
2	E	110	LEU	C-O	6.71	1.36	1.23
2	E	125	PRO	N-CD	-6.71	1.38	1.47
2	A	169	TRP	CA-C	-6.70	1.35	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	104	TYR	CD1-CE1	-6.70	1.29	1.39
3	F	55	THR	CA-CB	-6.70	1.35	1.53
4	N	68	LEU	C-O	6.70	1.36	1.23
2	A	11	LEU	CB-CG	-6.70	1.33	1.52
3	D	5	VAL	CA-C	-6.70	1.35	1.52
4	N	64	TRP	CZ3-CH2	-6.69	1.29	1.40
2	E	143	ASN	CG-OD1	-6.69	1.09	1.24
3	F	150	TYR	CG-CD1	6.69	1.47	1.39
2	A	85	GLN	C-O	-6.68	1.10	1.23
3	D	176	GLN	CA-CB	6.68	1.68	1.53
3	D	151	PHE	CG-CD2	6.67	1.48	1.38
2	E	154	TRP	CE3-CZ3	-6.67	1.27	1.38
2	A	86	ALA	N-CA	6.67	1.59	1.46
1	S	6	LYS	CB-CG	6.67	1.70	1.52
4	M	43	PHE	CB-CG	6.67	1.62	1.51
3	B	158	THR	CA-CB	-6.66	1.36	1.53
3	F	136	GLN	CG-CD	6.66	1.66	1.51
4	O	34	ILE	CB-CG1	6.66	1.72	1.54
2	A	217	ARG	C-O	6.66	1.36	1.23
2	A	193	GLU	CD-OE1	-6.66	1.18	1.25
3	D	82	GLN	CG-CD	6.66	1.66	1.51
2	A	8	PRO	N-CA	-6.66	1.35	1.47
3	B	111	GLY	CA-C	6.66	1.62	1.51
3	D	36	TRP	CE2-CZ2	6.65	1.51	1.39
3	F	29	PHE	CB-CG	-6.65	1.40	1.51
2	E	7	SER	C-O	-6.65	1.10	1.23
2	E	124	PHE	CG-CD2	-6.65	1.28	1.38
2	A	107	GLY	CA-C	6.65	1.62	1.51
2	G	153	LYS	CA-C	-6.65	1.35	1.52
3	B	171	PHE	CE2-CZ	-6.65	1.24	1.37
2	G	102	LEU	C-O	6.65	1.35	1.23
3	B	208	SER	CB-OG	-6.64	1.33	1.42
3	B	31	ASP	CA-C	6.64	1.70	1.52
4	L	71	GLY	C-O	6.64	1.34	1.23
3	B	89	GLU	CD-OE2	6.64	1.32	1.25
1	Q	42	PRO	CA-CB	6.64	1.66	1.53
2	E	207	SER	CA-CB	6.64	1.62	1.52
2	G	21	MET	CA-C	-6.63	1.35	1.52
2	A	195	HIS	CA-CB	-6.63	1.39	1.53
2	E	71	ARG	CA-C	-6.63	1.35	1.52
3	F	65	LYS	CB-CG	6.62	1.70	1.52
1	Q	42	PRO	CG-CD	6.62	1.72	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	191	GLU	CA-C	-6.62	1.35	1.52
3	F	101	LEU	CG-CD2	6.62	1.76	1.51
3	B	172	PRO	N-CD	-6.62	1.38	1.47
2	A	143	ASN	CB-CG	6.62	1.66	1.51
3	D	16	GLU	CB-CG	6.61	1.64	1.52
3	H	142	THR	CB-CG2	-6.61	1.30	1.52
2	A	138	VAL	CA-CB	6.61	1.68	1.54
2	C	6	GLN	CD-NE2	6.61	1.49	1.32
3	B	51	VAL	CA-C	-6.61	1.35	1.52
2	E	72	GLY	CA-C	6.61	1.62	1.51
1	S	2	SER	CA-CB	6.61	1.62	1.52
2	E	43	GLN	CA-C	6.61	1.70	1.52
3	F	180	TYR	C-O	-6.61	1.10	1.23
4	N	51	TYR	CB-CG	-6.61	1.41	1.51
3	B	31	ASP	CG-OD1	-6.60	1.10	1.25
3	H	159	TRP	CZ3-CH2	6.60	1.50	1.40
4	N	54	ALA	C-O	6.60	1.35	1.23
2	G	41	TRP	CB-CG	6.59	1.62	1.50
3	B	178	ASP	C-O	6.59	1.35	1.23
2	E	136	ALA	CA-C	-6.59	1.35	1.52
4	M	40	LYS	CB-CG	6.59	1.70	1.52
3	F	62	ASP	CG-OD2	6.59	1.40	1.25
2	A	8	PRO	CA-C	6.58	1.66	1.52
4	O	45	GLU	CD-OE1	6.58	1.32	1.25
2	C	33	ARG	C-O	6.58	1.35	1.23
3	F	19	LYS	CG-CD	6.58	1.74	1.52
2	E	51	LYS	CA-C	-6.58	1.35	1.52
3	F	29	PHE	CE2-CZ	6.58	1.49	1.37
2	A	122	SER	N-CA	-6.58	1.33	1.46
4	N	69	GLU	CG-CD	6.58	1.61	1.51
2	A	115	ALA	CA-C	-6.57	1.35	1.52
2	C	129	GLU	CA-C	-6.57	1.35	1.52
3	F	108	TRP	CD2-CE3	-6.57	1.30	1.40
3	D	84	ASN	CB-CG	6.57	1.66	1.51
3	H	110	ALA	CA-C	6.57	1.70	1.52
3	B	102	ARG	NE-CZ	6.57	1.41	1.33
4	L	25	VAL	CB-CG1	6.57	1.66	1.52
2	C	51	LYS	N-CA	6.57	1.59	1.46
2	E	159	SER	CA-C	6.56	1.70	1.52
4	M	55	ALA	C-O	-6.56	1.10	1.23
2	G	109	LYS	CD-CE	6.56	1.67	1.51
3	H	196	GLU	CG-CD	6.56	1.61	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	153	LYS	CA-C	-6.56	1.35	1.52
4	M	43	PHE	C-O	-6.56	1.10	1.23
3	B	20	ILE	N-CA	6.56	1.59	1.46
3	B	81	LEU	N-CA	-6.56	1.33	1.46
3	F	166	SER	C-N	-6.56	1.21	1.33
3	H	51	VAL	CA-CB	6.55	1.68	1.54
3	B	209	THR	C-O	6.55	1.35	1.23
3	F	48	MET	CA-C	6.55	1.70	1.52
2	G	42	TYR	CG-CD2	-6.55	1.30	1.39
2	A	10	SER	CB-OG	-6.55	1.33	1.42
2	C	16	GLY	C-O	6.55	1.34	1.23
2	E	87	GLU	C-O	6.55	1.35	1.23
2	G	179	TYR	CD2-CE2	-6.54	1.29	1.39
2	E	93	TYR	CE2-CZ	-6.54	1.30	1.38
3	H	77	SER	CB-OG	6.54	1.50	1.42
2	G	33	ARG	CG-CD	6.54	1.68	1.51
3	F	95	PHE	N-CA	-6.54	1.33	1.46
4	M	70	ASP	C-N	6.54	1.44	1.33
2	C	146	TYR	CA-C	-6.53	1.35	1.52
3	D	17	THR	C-O	-6.53	1.10	1.23
4	M	62	GLY	CA-C	-6.53	1.41	1.51
3	B	210	LYS	CD-CE	6.53	1.67	1.51
4	L	59	LYS	CB-CG	6.53	1.70	1.52
2	E	8	PRO	N-CD	-6.53	1.38	1.47
4	L	59	LYS	CE-NZ	6.53	1.65	1.49
3	F	67	ARG	NE-CZ	-6.53	1.24	1.33
3	H	52	ASN	CA-C	6.53	1.70	1.52
4	M	73	ASN	CB-CG	6.52	1.66	1.51
2	E	133	SER	CB-OG	-6.52	1.33	1.42
2	A	108	THR	CA-CB	6.52	1.70	1.53
3	H	110	ALA	CA-CB	6.52	1.66	1.52
3	D	157	VAL	N-CA	-6.51	1.33	1.46
2	A	23	CYS	CA-CB	-6.51	1.39	1.53
3	F	92	ALA	CA-CB	-6.51	1.38	1.52
2	A	160	GLU	CD-OE2	6.50	1.32	1.25
3	F	210	LYS	CB-CG	6.50	1.70	1.52
2	A	4	MET	C-O	6.50	1.35	1.23
2	A	97	ALA	CA-CB	-6.50	1.38	1.52
2	C	192	TYR	CE2-CZ	-6.50	1.30	1.38
3	H	29	PHE	CE1-CZ	6.50	1.49	1.37
2	E	174	SER	CA-CB	6.50	1.62	1.52
2	E	193	GLU	CG-CD	6.50	1.61	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	24	LYS	CD-CE	6.50	1.67	1.51
3	F	102	ARG	CZ-NH2	6.50	1.41	1.33
1	P	24	PHE	CG-CD2	6.49	1.48	1.38
3	B	188	VAL	C-O	-6.49	1.11	1.23
2	C	152	VAL	CB-CG1	6.49	1.66	1.52
3	H	89	GLU	CD-OE2	6.49	1.32	1.25
2	C	192	TYR	CD1-CE1	6.49	1.49	1.39
3	F	1	GLN	CA-CB	6.49	1.68	1.53
3	H	120	LYS	N-CA	-6.49	1.33	1.46
4	N	53	TYR	CZ-OH	-6.49	1.26	1.37
3	H	216	VAL	CB-CG2	6.49	1.66	1.52
3	B	73	GLU	N-CA	6.48	1.59	1.46
2	C	72	GLY	CA-C	-6.48	1.41	1.51
3	F	103	GLN	N-CA	6.48	1.59	1.46
2	G	153	LYS	CG-CD	6.48	1.74	1.52
4	O	68	LEU	CA-C	-6.47	1.36	1.52
3	B	99	PHE	CE2-CZ	-6.47	1.25	1.37
2	E	102	LEU	CA-CB	-6.47	1.38	1.53
1	S	9	ARG	CZ-NH1	6.47	1.41	1.33
2	C	114	ARG	CB-CG	-6.46	1.35	1.52
3	F	12	LYS	CE-NZ	6.46	1.65	1.49
2	A	32	SER	CB-OG	6.46	1.50	1.42
3	D	67	ARG	CB-CG	6.46	1.70	1.52
2	E	142	LEU	CG-CD1	-6.46	1.27	1.51
4	O	35	GLN	CA-C	6.46	1.69	1.52
3	F	115	THR	N-CA	-6.45	1.33	1.46
2	A	92	TYR	CG-CD1	-6.45	1.30	1.39
4	M	33	LYS	CG-CD	6.45	1.74	1.52
3	F	100	LEU	CG-CD2	6.45	1.75	1.51
2	A	179	TYR	CE1-CZ	-6.44	1.30	1.38
2	A	41	TRP	CG-CD1	-6.44	1.27	1.36
3	F	5	VAL	CA-CB	6.44	1.68	1.54
3	F	209	THR	C-O	-6.44	1.11	1.23
1	S	35	TYR	CG-CD1	-6.44	1.30	1.39
3	H	214	LYS	CE-NZ	6.44	1.65	1.49
2	C	87	GLU	CD-OE1	-6.43	1.18	1.25
2	G	146	TYR	CA-C	-6.43	1.36	1.52
3	H	112	THR	CB-CG2	6.43	1.73	1.52
3	H	21	SER	CA-CB	6.43	1.62	1.52
3	F	10	GLU	CD-OE1	6.43	1.32	1.25
3	D	85	SER	C-O	6.43	1.35	1.23
2	E	136	ALA	CA-CB	-6.42	1.39	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	108	TRP	CZ2-CH2	-6.42	1.25	1.37
3	B	68	PHE	CE2-CZ	-6.42	1.25	1.37
3	B	105	PHE	N-CA	-6.42	1.33	1.46
3	B	155	VAL	CB-CG1	-6.42	1.39	1.52
2	C	172	GLN	CD-OE1	6.42	1.38	1.24
3	F	68	PHE	CE2-CZ	-6.42	1.25	1.37
3	F	218	ARG	CZ-NH2	6.42	1.41	1.33
3	H	208	SER	CB-OG	-6.41	1.33	1.42
4	L	43	PHE	CA-C	6.40	1.69	1.52
1	Q	18	ARG	NE-CZ	6.40	1.41	1.33
3	D	57	GLU	CB-CG	6.40	1.64	1.52
4	O	35	GLN	C-O	-6.40	1.11	1.23
3	F	214	LYS	CB-CG	6.40	1.69	1.52
3	H	112	THR	CA-CB	-6.40	1.36	1.53
3	B	16	GLU	CD-OE2	-6.40	1.18	1.25
3	B	120	LYS	CA-CB	-6.39	1.39	1.53
4	O	69	GLU	CB-CG	-6.39	1.40	1.52
2	A	37	ASN	CG-ND2	-6.39	1.16	1.32
2	A	175	LYS	CD-CE	6.39	1.67	1.51
3	D	82	GLN	N-CA	6.39	1.59	1.46
2	G	76	ASP	C-O	6.39	1.35	1.23
3	D	12	LYS	CG-CD	6.39	1.74	1.52
2	G	92	TYR	CZ-OH	6.39	1.48	1.37
3	B	36	TRP	CB-CG	-6.38	1.38	1.50
3	H	32	PHE	CG-CD1	6.38	1.48	1.38
2	C	30	LEU	CG-CD1	6.38	1.75	1.51
3	B	180	TYR	CB-CG	6.38	1.61	1.51
4	M	34	ILE	CA-CB	-6.38	1.40	1.54
2	C	48	GLN	CG-CD	6.37	1.65	1.51
2	C	179	TYR	CD1-CE1	-6.37	1.29	1.39
2	E	41	TRP	CG-CD2	6.37	1.54	1.43
2	A	71	ARG	CD-NE	6.37	1.57	1.46
3	F	174	VAL	CB-CG2	-6.37	1.39	1.52
3	F	113	THR	C-N	-6.37	1.19	1.34
2	A	116	ASP	C-O	6.36	1.35	1.23
2	A	165	VAL	CB-CG1	6.36	1.66	1.52
3	B	30	THR	CA-C	-6.36	1.36	1.52
2	E	101	PRO	CA-C	6.36	1.65	1.52
3	D	136	GLN	CB-CG	6.36	1.69	1.52
3	B	37	VAL	CB-CG2	-6.36	1.39	1.52
3	D	128	PRO	CA-C	-6.36	1.40	1.52
2	E	144	ASN	C-O	-6.36	1.11	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	176	GLN	CA-CB	6.36	1.68	1.53
3	B	212	ASP	C-N	-6.36	1.19	1.34
2	C	215	PHE	CB-CG	6.36	1.62	1.51
2	G	104	PHE	CG-CD2	-6.36	1.29	1.38
3	F	67	ARG	CB-CG	6.35	1.69	1.52
2	G	87	GLU	CA-CB	6.35	1.68	1.53
2	C	77	PHE	CE1-CZ	-6.35	1.25	1.37
3	D	126	VAL	CB-CG1	-6.35	1.39	1.52
3	D	149	GLY	CA-C	-6.35	1.41	1.51
2	E	212	VAL	CA-C	-6.35	1.36	1.52
2	E	219	GLU	CG-CD	6.35	1.61	1.51
3	F	21	SER	CA-C	-6.35	1.36	1.52
3	D	31	ASP	CA-CB	6.35	1.68	1.53
4	O	74	HIS	CB-CG	6.35	1.61	1.50
4	O	47	THR	C-O	6.34	1.35	1.23
4	M	64	TRP	CB-CG	-6.34	1.38	1.50
3	B	43	LYS	CD-CE	6.34	1.67	1.51
2	A	42	TYR	CE1-CZ	-6.34	1.30	1.38
2	A	213	LYS	CD-CE	6.34	1.67	1.51
3	B	167	GLY	CA-C	6.34	1.61	1.51
4	M	21	VAL	CA-CB	6.34	1.68	1.54
4	M	45	GLU	CB-CG	6.34	1.64	1.52
3	F	127	TYR	CG-CD1	-6.34	1.30	1.39
4	M	38	GLU	CG-CD	-6.33	1.42	1.51
2	E	96	GLN	CG-CD	6.33	1.65	1.51
2	C	138	VAL	C-O	6.33	1.35	1.23
2	C	162	GLN	CB-CG	6.33	1.69	1.52
4	O	32	GLY	C-O	6.33	1.33	1.23
3	D	142	THR	N-CA	-6.33	1.33	1.46
4	M	77	ILE	CB-CG2	-6.33	1.33	1.52
3	H	10	GLU	CB-CG	-6.33	1.40	1.52
3	H	108	TRP	N-CA	-6.33	1.33	1.46
4	O	64	TRP	CE3-CZ3	-6.33	1.27	1.38
3	H	64	PHE	CG-CD1	-6.32	1.29	1.38
3	F	203	ALA	C-O	-6.31	1.11	1.23
3	D	160	ASN	N-CA	6.31	1.58	1.46
3	D	216	VAL	CB-CG2	6.31	1.66	1.52
3	H	31	ASP	C-O	6.31	1.35	1.23
2	E	9	SER	CA-CB	-6.30	1.43	1.52
3	H	150	TYR	CE2-CZ	-6.30	1.30	1.38
4	M	43	PHE	CA-CB	-6.30	1.40	1.53
3	F	127	TYR	CA-CB	-6.30	1.40	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	O	59	LYS	CD-CE	6.30	1.67	1.51
1	Q	24	PHE	CG-CD2	6.29	1.48	1.38
3	F	163	SER	CB-OG	6.29	1.50	1.42
2	C	189	LYS	CG-CD	-6.29	1.31	1.52
4	N	62	GLY	N-CA	6.29	1.55	1.46
2	C	198	TYR	CE2-CZ	-6.29	1.30	1.38
4	M	38	GLU	CB-CG	6.29	1.64	1.52
4	N	40	LYS	C-O	6.29	1.35	1.23
2	A	11	LEU	CG-CD2	-6.29	1.28	1.51
3	F	18	VAL	N-CA	6.29	1.58	1.46
2	E	75	THR	C-O	-6.28	1.11	1.23
4	L	22	THR	CB-CG2	6.28	1.73	1.52
2	G	68	PHE	CG-CD1	-6.28	1.29	1.38
2	E	20	THR	CA-C	6.28	1.69	1.52
3	B	153	GLU	CD-OE1	6.28	1.32	1.25
3	H	175	LEU	CG-CD1	6.28	1.75	1.51
2	C	178	THR	CA-CB	6.27	1.69	1.53
4	O	35	GLN	CD-NE2	6.27	1.48	1.32
1	Q	7	PRO	CG-CD	6.27	1.71	1.50
2	A	45	LYS	CE-NZ	6.27	1.64	1.49
3	F	107	VAL	N-CA	-6.27	1.33	1.46
2	A	148	LYS	CA-C	6.27	1.69	1.52
3	D	84	ASN	C-O	-6.26	1.11	1.23
2	E	198	TYR	CB-CG	-6.26	1.42	1.51
3	B	82	GLN	CG-CD	6.26	1.65	1.51
3	D	184	SER	C-O	6.25	1.35	1.23
3	B	145	CYS	N-CA	-6.25	1.33	1.46
4	M	59	LYS	CB-CG	6.25	1.69	1.52
2	A	50	PRO	C-O	6.25	1.35	1.23
3	B	27	TYR	CD1-CE1	-6.25	1.29	1.39
2	C	145	PHE	CG-CD2	-6.25	1.29	1.38
2	E	5	SER	CA-C	-6.25	1.36	1.52
2	E	217	ARG	NE-CZ	6.25	1.41	1.33
2	G	98	TYR	N-CA	6.25	1.58	1.46
2	C	139	VAL	CB-CG2	6.24	1.66	1.52
2	E	104	PHE	C-O	-6.24	1.11	1.23
2	G	69	THR	CA-CB	6.24	1.69	1.53
3	B	140	MET	CB-CG	-6.23	1.31	1.51
2	A	69	THR	CA-CB	6.23	1.69	1.53
2	E	99	ILE	CA-C	-6.23	1.36	1.52
3	F	218	ARG	C-OXT	6.23	1.35	1.23
2	A	50	PRO	CB-CG	-6.23	1.18	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S	26	GLY	C-O	-6.23	1.13	1.23
3	H	102	ARG	CA-C	-6.23	1.36	1.52
3	B	47	TRP	CE3-CZ3	-6.23	1.27	1.38
3	F	39	GLN	CD-NE2	-6.23	1.17	1.32
3	B	108	TRP	CA-C	6.22	1.69	1.52
3	B	188	VAL	CB-CG2	-6.22	1.39	1.52
3	D	99	PHE	CD2-CE2	6.22	1.51	1.39
4	M	45	GLU	CG-CD	6.21	1.61	1.51
4	L	64	TRP	CG-CD1	-6.21	1.28	1.36
4	L	73	ASN	N-CA	6.21	1.58	1.46
2	C	208	THR	N-CA	6.21	1.58	1.46
4	M	78	LYS	CD-CE	6.21	1.66	1.51
3	D	165	SER	CB-OG	6.21	1.50	1.42
2	G	15	ALA	CA-CB	-6.21	1.39	1.52
3	F	77	SER	CB-OG	6.21	1.50	1.42
3	D	195	SER	N-CA	6.20	1.58	1.46
2	C	27	GLN	CD-OE1	6.20	1.37	1.24
2	E	121	VAL	C-O	-6.20	1.11	1.23
4	N	80	ALA	CA-C	-6.20	1.36	1.52
2	A	106	ALA	C-N	-6.20	1.21	1.33
4	L	45	GLU	CG-CD	6.20	1.61	1.51
2	C	161	ARG	NE-CZ	6.20	1.41	1.33
2	E	175	LYS	CA-C	-6.20	1.36	1.52
2	A	119	PRO	CA-C	-6.19	1.40	1.52
2	E	216	ASN	N-CA	6.19	1.58	1.46
2	C	61	GLU	CB-CG	6.19	1.64	1.52
3	F	157	VAL	CA-CB	-6.19	1.41	1.54
4	N	25	VAL	N-CA	6.19	1.58	1.46
4	L	30	ALA	N-CA	-6.19	1.33	1.46
2	C	20	THR	CA-C	-6.18	1.36	1.52
2	E	116	ASP	CB-CG	6.18	1.64	1.51
4	L	78	LYS	N-CA	6.18	1.58	1.46
2	G	27	GLN	CG-CD	-6.18	1.36	1.51
3	D	90	ASP	CA-C	6.17	1.69	1.52
2	G	38	TYR	CB-CG	-6.17	1.42	1.51
2	G	179	TYR	CZ-OH	6.17	1.48	1.37
3	B	60	TYR	CD2-CE2	6.17	1.48	1.39
2	C	203	THR	C-O	6.17	1.35	1.23
3	D	97	ALA	CA-C	6.16	1.69	1.52
4	M	24	LYS	CG-CD	6.16	1.73	1.52
2	G	3	VAL	CA-CB	6.16	1.67	1.54
3	H	58	PRO	C-O	6.16	1.35	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	157	ASP	N-CA	-6.16	1.34	1.46
3	B	94	TYR	CB-CG	6.16	1.60	1.51
4	L	55	ALA	N-CA	6.16	1.58	1.46
2	A	179	TYR	CD1-CE1	-6.16	1.30	1.39
3	D	156	THR	CA-CB	6.16	1.69	1.53
3	H	157	VAL	CA-C	-6.16	1.36	1.52
3	D	42	GLY	CA-C	-6.16	1.42	1.51
2	E	62	SER	C-O	-6.16	1.11	1.23
2	E	179	TYR	CZ-OH	6.16	1.48	1.37
1	Q	3	THR	CB-CG2	6.15	1.72	1.52
2	E	28	SER	C-O	-6.15	1.11	1.23
3	D	127	TYR	CG-CD2	-6.15	1.31	1.39
4	L	53	TYR	CD1-CE1	6.15	1.48	1.39
2	G	98	TYR	CE1-CZ	6.15	1.46	1.38
2	C	68	PHE	C-O	-6.14	1.11	1.23
3	H	116	VAL	CB-CG1	6.14	1.65	1.52
3	F	45	LEU	CB-CG	-6.14	1.34	1.52
2	A	83	SER	C-O	-6.14	1.11	1.23
2	G	209	SER	C-O	-6.14	1.11	1.23
3	H	132	GLY	N-CA	6.14	1.55	1.46
3	D	92	ALA	CA-C	-6.14	1.36	1.52
3	F	72	LEU	CB-CG	-6.14	1.34	1.52
1	P	29	GLN	N-CA	6.14	1.58	1.46
4	L	75	MET	CG-SD	6.14	1.97	1.81
3	H	141	VAL	CB-CG1	6.14	1.65	1.52
2	G	129	GLU	N-CA	-6.13	1.34	1.46
4	M	38	GLU	CD-OE2	-6.13	1.19	1.25
2	G	125	PRO	CG-CD	6.13	1.70	1.50
2	A	117	ALA	N-CA	6.13	1.58	1.46
4	M	60	VAL	CB-CG1	6.13	1.65	1.52
3	F	162	GLY	C-O	-6.13	1.13	1.23
4	O	59	LYS	CG-CD	6.13	1.73	1.52
1	S	22	VAL	CB-CG1	6.13	1.65	1.52
3	D	73	GLU	CB-CG	6.12	1.63	1.52
1	Q	8	GLN	CA-C	6.12	1.68	1.52
2	A	27	GLN	CB-CG	-6.12	1.36	1.52
3	B	62	ASP	CA-CB	6.12	1.67	1.53
2	E	154	TRP	CA-C	-6.12	1.37	1.52
2	G	35	ARG	CG-CD	6.12	1.67	1.51
2	C	215	PHE	CE1-CZ	6.12	1.49	1.37
3	B	47	TRP	CD2-CE2	-6.11	1.34	1.41
2	G	160	GLU	CG-CD	6.11	1.61	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	180	TYR	CD2-CE2	-6.11	1.30	1.39
3	F	90	ASP	CG-OD1	6.11	1.39	1.25
3	B	112	THR	CA-CB	-6.11	1.37	1.53
2	G	60	ARG	CA-CB	6.11	1.67	1.53
2	G	192	TYR	CD1-CE1	-6.11	1.30	1.39
3	D	102	ARG	CD-NE	6.11	1.56	1.46
3	H	125	SER	CA-CB	6.11	1.62	1.52
4	L	64	TRP	C-O	-6.10	1.11	1.23
3	F	27	TYR	CE1-CZ	-6.10	1.30	1.38
3	B	94	TYR	CA-CB	-6.10	1.40	1.53
4	L	59	LYS	CG-CD	6.10	1.73	1.52
3	F	38	ASN	C-O	-6.10	1.11	1.23
3	D	80	TYR	CD2-CE2	6.10	1.48	1.39
3	B	39	GLN	CA-C	-6.10	1.37	1.52
1	Q	28	GLY	C-O	6.09	1.33	1.23
3	H	181	THR	CA-CB	-6.09	1.37	1.53
1	Q	35	TYR	CB-CG	6.09	1.60	1.51
3	F	11	LEU	C-O	6.09	1.34	1.23
3	H	125	SER	CB-OG	6.09	1.50	1.42
4	L	49	GLU	CB-CG	-6.09	1.40	1.52
3	B	169	HIS	CA-CB	6.09	1.67	1.53
3	F	64	PHE	CG-CD1	-6.09	1.29	1.38
3	D	34	MET	C-O	6.08	1.34	1.23
3	D	108	TRP	CB-CG	-6.08	1.39	1.50
2	C	33	ARG	CD-NE	6.08	1.56	1.46
3	B	93	THR	CB-CG2	-6.07	1.32	1.52
4	M	62	GLY	C-O	-6.07	1.14	1.23
4	O	53	TYR	N-CA	6.07	1.58	1.46
4	L	20	GLU	CG-CD	6.07	1.61	1.51
2	C	21	MET	C-O	-6.07	1.11	1.23
2	E	188	THR	CB-CG2	6.07	1.72	1.52
2	G	167	ASN	CG-OD1	6.07	1.37	1.24
2	E	191	GLU	CD-OE1	6.07	1.32	1.25
2	G	93	TYR	CG-CD1	-6.07	1.31	1.39
2	G	212	VAL	CB-CG1	-6.07	1.40	1.52
3	B	183	SER	CA-C	-6.06	1.37	1.52
2	C	60	ARG	CZ-NH1	6.06	1.41	1.33
3	D	178	ASP	C-O	-6.06	1.11	1.23
3	B	105	PHE	CB-CG	6.06	1.61	1.51
3	B	186	VAL	N-CA	-6.06	1.34	1.46
2	C	24	LYS	CD-CE	6.06	1.66	1.51
3	H	145	CYS	N-CA	-6.06	1.34	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	22	VAL	CA-CB	6.05	1.67	1.54
2	G	1	ASP	C-O	-6.05	1.11	1.23
2	E	120	THR	N-CA	-6.05	1.34	1.46
1	P	31	VAL	CB-CG1	6.05	1.65	1.52
3	B	97	ALA	C-O	-6.05	1.11	1.23
3	H	106	ASP	C-O	6.05	1.34	1.23
3	B	54	GLU	CD-OE1	-6.05	1.19	1.25
3	D	11	LEU	CG-CD1	-6.05	1.29	1.51
1	S	9	ARG	CB-CG	6.05	1.68	1.52
2	A	135	GLY	N-CA	6.04	1.55	1.46
3	H	135	ALA	CA-CB	-6.04	1.39	1.52
2	A	216	ASN	CB-CG	6.04	1.65	1.51
2	E	154	TRP	CD2-CE3	-6.04	1.31	1.40
2	G	203	THR	CA-CB	6.04	1.69	1.53
3	H	95	PHE	CD2-CE2	-6.04	1.27	1.39
3	F	40	ALA	C-O	-6.04	1.11	1.23
3	F	13	LYS	CB-CG	6.04	1.68	1.52
2	C	115	ALA	CA-CB	-6.04	1.39	1.52
2	E	10	SER	CB-OG	-6.04	1.34	1.42
2	A	46	PRO	CA-C	-6.04	1.40	1.52
2	C	160	GLU	C-O	6.04	1.34	1.23
3	D	47	TRP	CG-CD1	-6.04	1.28	1.36
3	D	217	PRO	CA-C	6.03	1.65	1.52
2	G	139	VAL	C-O	-6.03	1.11	1.23
4	O	39	PHE	CE2-CZ	-6.03	1.25	1.37
2	G	201	GLU	CG-CD	6.03	1.60	1.51
2	C	146	TYR	CD2-CE2	-6.03	1.30	1.39
2	G	123	ILE	CB-CG2	-6.03	1.34	1.52
3	F	54	GLU	CD-OE1	6.02	1.32	1.25
2	A	162	GLN	CB-CG	6.02	1.68	1.52
4	L	22	THR	N-CA	-6.02	1.34	1.46
2	E	151	ASN	C-O	-6.02	1.11	1.23
3	B	189	PRO	CA-C	-6.02	1.40	1.52
3	F	107	VAL	C-O	-6.02	1.11	1.23
2	G	28	SER	CA-CB	6.02	1.61	1.52
4	O	25	VAL	CB-CG1	6.02	1.65	1.52
2	E	94	CYS	CA-CB	-6.02	1.40	1.53
2	E	148	LYS	CA-CB	6.02	1.67	1.53
3	H	65	LYS	CE-NZ	6.02	1.64	1.49
2	C	81	ILE	CA-CB	6.01	1.68	1.54
2	A	105	GLY	CA-C	6.01	1.61	1.51
2	E	44	GLN	N-CA	-6.01	1.34	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	60	ARG	N-CA	6.01	1.58	1.46
3	B	32	PHE	CG-CD2	-6.00	1.29	1.38
1	Q	21	ASP	CB-CG	6.00	1.64	1.51
1	Q	28	GLY	N-CA	6.00	1.55	1.46
2	E	83	SER	CA-CB	6.00	1.61	1.52
2	E	101	PRO	C-O	6.00	1.35	1.23
3	H	188	VAL	CA-CB	6.00	1.67	1.54
2	A	18	LYS	CG-CD	5.99	1.72	1.52
3	F	27	TYR	C-O	-5.99	1.11	1.23
4	N	67	ASP	CA-C	-5.99	1.37	1.52
4	O	36	THR	N-CA	-5.99	1.34	1.46
2	E	215	PHE	CD2-CE2	-5.99	1.27	1.39
2	C	202	ALA	N-CA	5.99	1.58	1.46
3	H	43	LYS	CB-CG	5.99	1.68	1.52
4	N	68	LEU	CG-CD2	5.99	1.74	1.51
2	G	20	THR	CA-CB	5.99	1.69	1.53
2	G	145	PHE	CE1-CZ	-5.99	1.25	1.37
3	H	184	SER	CA-CB	-5.98	1.44	1.52
3	H	143	LEU	C-N	-5.98	1.22	1.33
2	A	91	VAL	CA-CB	-5.98	1.42	1.54
2	C	18	LYS	CA-CB	5.98	1.67	1.53
4	M	78	LYS	CG-CD	5.97	1.72	1.52
4	M	79	PHE	CE1-CZ	5.97	1.48	1.37
2	G	50	PRO	N-CD	-5.97	1.39	1.47
2	E	161	ARG	CZ-NH2	5.97	1.40	1.33
4	L	17	PRO	C-N	5.97	1.47	1.34
3	F	99	PHE	CA-CB	-5.97	1.40	1.53
4	O	28	ILE	CA-CB	-5.97	1.41	1.54
3	B	137	THR	C-O	5.97	1.34	1.23
2	G	68	PHE	N-CA	-5.97	1.34	1.46
2	C	160	GLU	CG-CD	5.97	1.60	1.51
3	D	17	THR	CA-C	-5.96	1.37	1.52
3	D	74	THR	CA-C	5.96	1.68	1.52
2	A	91	VAL	CB-CG1	5.96	1.65	1.52
3	F	138	ASN	CA-CB	5.96	1.68	1.53
2	G	35	ARG	CZ-NH1	5.96	1.40	1.33
2	G	79	LEU	C-O	5.95	1.34	1.23
3	H	127	TYR	CE2-CZ	-5.95	1.30	1.38
2	A	117	ALA	C-O	-5.95	1.12	1.23
3	F	34	MET	C-O	-5.95	1.12	1.23
1	P	33	GLY	CA-C	5.95	1.61	1.51
2	G	73	SER	CA-C	-5.95	1.37	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	84	VAL	CA-CB	5.95	1.67	1.54
3	H	8	GLY	C-O	-5.95	1.14	1.23
2	G	39	LEU	CA-C	-5.94	1.37	1.52
3	D	16	GLU	CG-CD	5.94	1.60	1.51
3	D	124	PRO	CB-CG	-5.94	1.20	1.50
3	H	121	THR	CA-CB	5.94	1.68	1.53
2	E	46	PRO	C-O	-5.94	1.11	1.23
4	N	66	ALA	C-O	5.94	1.34	1.23
3	F	98	ARG	CZ-NH1	5.94	1.40	1.33
4	N	44	GLU	CD-OE2	5.94	1.32	1.25
2	G	42	TYR	CZ-OH	5.93	1.48	1.37
3	B	212	ASP	C-O	-5.93	1.12	1.23
2	C	180	SER	CA-C	-5.93	1.37	1.52
3	D	190	SER	CA-C	5.93	1.68	1.52
2	A	152	VAL	N-CA	-5.93	1.34	1.46
4	L	17	PRO	CA-CB	5.93	1.65	1.53
3	F	101	LEU	C-O	-5.93	1.12	1.23
3	D	153	GLU	CD-OE1	-5.93	1.19	1.25
3	H	141	VAL	CA-CB	-5.93	1.42	1.54
3	D	45	LEU	CG-CD2	-5.93	1.29	1.51
3	F	197	THR	C-O	5.93	1.34	1.23
2	G	96	GLN	CD-NE2	-5.93	1.18	1.32
4	L	26	ASN	N-CA	5.92	1.58	1.46
1	S	37	LEU	CG-CD1	5.92	1.73	1.51
2	A	56	TRP	CE2-CZ2	-5.92	1.29	1.39
3	B	62	ASP	CB-CG	5.92	1.64	1.51
3	H	70	PHE	CG-CD1	5.92	1.47	1.38
4	O	39	PHE	CB-CG	-5.92	1.41	1.51
2	A	41	TRP	CG-CD2	-5.92	1.33	1.43
3	B	117	SER	C-O	-5.92	1.12	1.23
2	A	147	PRO	C-O	5.91	1.35	1.23
2	E	187	LEU	N-CA	5.91	1.58	1.46
3	B	39	GLN	N-CA	5.91	1.58	1.46
2	C	81	ILE	CA-C	-5.91	1.37	1.52
2	G	112	LEU	CB-CG	-5.91	1.35	1.52
2	G	69	THR	CB-CG2	5.91	1.71	1.52
3	H	102	ARG	CG-CD	5.91	1.66	1.51
2	C	209	SER	CA-C	5.90	1.68	1.52
2	E	146	TYR	CG-CD2	-5.90	1.31	1.39
2	A	179	TYR	CD2-CE2	-5.90	1.30	1.39
3	F	127	TYR	CD1-CE1	5.90	1.48	1.39
3	B	45	LEU	CG-CD2	-5.90	1.30	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Q	21	ASP	C-O	5.90	1.34	1.23
2	A	203	THR	C-O	-5.90	1.12	1.23
2	A	185	LEU	CG-CD2	5.90	1.73	1.51
3	B	105	PHE	CG-CD2	-5.90	1.29	1.38
3	F	51	VAL	CB-CG1	5.90	1.65	1.52
3	F	97	ALA	CA-CB	-5.90	1.40	1.52
4	N	35	GLN	C-N	-5.90	1.20	1.34
2	G	82	SER	CA-CB	5.90	1.61	1.52
3	B	50	TRP	CZ3-CH2	5.90	1.49	1.40
3	B	99	PHE	N-CA	5.89	1.58	1.46
3	D	158	THR	N-CA	5.89	1.58	1.46
2	E	154	TRP	CA-CB	-5.89	1.41	1.53
4	N	49	GLU	CB-CG	-5.89	1.41	1.52
2	C	152	VAL	CB-CG2	5.89	1.65	1.52
2	E	143	ASN	C-O	-5.89	1.12	1.23
4	N	44	GLU	CD-OE1	5.89	1.32	1.25
4	N	64	TRP	CB-CG	-5.89	1.39	1.50
1	P	26	GLY	C-N	5.88	1.43	1.33
2	E	74	GLY	C-O	-5.88	1.14	1.23
2	A	41	TRP	CZ2-CH2	-5.88	1.26	1.37
3	D	182	LEU	N-CA	-5.88	1.34	1.46
3	H	48	MET	CG-SD	-5.88	1.65	1.81
3	B	141	VAL	CB-CG1	-5.88	1.40	1.52
3	D	143	LEU	CA-C	-5.88	1.37	1.52
3	F	112	THR	C-O	-5.88	1.12	1.23
2	E	7	SER	CA-CB	-5.87	1.44	1.52
2	C	32	SER	CA-C	5.87	1.68	1.52
4	N	40	LYS	N-CA	5.87	1.58	1.46
2	G	49	SER	C-N	-5.87	1.23	1.34
2	A	171	ASP	C-O	-5.87	1.12	1.23
4	M	74	HIS	C-O	-5.87	1.12	1.23
2	E	48	GLN	CB-CG	5.87	1.68	1.52
3	F	43	LYS	CE-NZ	5.87	1.63	1.49
2	G	76	ASP	CA-CB	5.87	1.66	1.53
3	D	36	TRP	CA-C	5.87	1.68	1.52
3	B	214	LYS	CD-CE	5.87	1.66	1.51
2	E	186	THR	N-CA	-5.86	1.34	1.46
3	F	30	THR	CA-C	-5.86	1.37	1.52
2	G	124	PHE	CB-CG	-5.86	1.41	1.51
3	B	139	SER	CA-CB	5.86	1.61	1.52
2	G	24	LYS	CG-CD	5.86	1.72	1.52
2	E	98	TYR	CE1-CZ	-5.85	1.30	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	83	ILE	CA-C	5.85	1.68	1.52
2	C	66	ASP	CA-C	-5.85	1.37	1.52
3	F	157	VAL	C-N	-5.85	1.20	1.34
3	F	184	SER	C-O	-5.85	1.12	1.23
3	H	210	LYS	CB-CG	-5.85	1.36	1.52
3	D	81	LEU	CA-CB	-5.84	1.40	1.53
2	C	104	PHE	CE2-CZ	5.84	1.48	1.37
2	C	187	LEU	CA-C	-5.84	1.37	1.52
2	C	146	TYR	CZ-OH	-5.84	1.27	1.37
2	C	150	ILE	CA-C	5.84	1.68	1.52
2	E	198	TYR	CE1-CZ	-5.84	1.30	1.38
3	B	193	TRP	CZ2-CH2	-5.84	1.26	1.37
3	D	30	THR	CA-CB	5.84	1.68	1.53
2	A	41	TRP	CD2-CE3	-5.83	1.31	1.40
2	A	74	GLY	CA-C	-5.83	1.42	1.51
3	B	68	PHE	CE1-CZ	5.83	1.48	1.37
4	M	42	THR	C-O	5.83	1.34	1.23
2	G	119	PRO	CA-CB	-5.83	1.41	1.53
3	D	15	GLY	C-O	-5.83	1.14	1.23
4	M	23	ILE	C-O	-5.83	1.12	1.23
2	E	178	THR	CA-CB	-5.83	1.38	1.53
3	B	201	ASN	CA-C	5.82	1.68	1.52
4	L	33	LYS	CD-CE	5.82	1.65	1.51
3	B	69	ALA	CA-C	-5.82	1.37	1.52
3	D	131	PRO	C-O	5.82	1.34	1.23
3	F	211	VAL	CA-CB	-5.82	1.42	1.54
2	A	99	ILE	N-CA	5.82	1.57	1.46
3	D	51	VAL	CB-CG1	-5.82	1.40	1.52
3	D	14	PRO	CA-C	-5.82	1.41	1.52
2	E	124	PHE	CG-CD1	-5.82	1.30	1.38
1	Q	10	LYS	CB-CG	5.82	1.68	1.52
2	E	204	HIS	CA-CB	-5.82	1.41	1.53
2	C	156	ILE	CA-CB	-5.81	1.41	1.54
3	D	98	ARG	CB-CG	5.81	1.68	1.52
3	B	39	GLN	CG-CD	-5.81	1.37	1.51
3	F	68	PHE	CG-CD1	-5.81	1.30	1.38
3	H	207	SER	C-N	-5.80	1.20	1.34
2	A	64	VAL	CB-CG1	5.80	1.65	1.52
3	B	30	THR	C-O	-5.80	1.12	1.23
3	D	173	ALA	N-CA	5.80	1.57	1.46
3	H	140	MET	CG-SD	5.80	1.96	1.81
2	A	71	ARG	CG-CD	5.80	1.66	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	49	GLU	CA-C	5.80	1.68	1.52
3	D	70	PHE	CE1-CZ	5.79	1.48	1.37
2	G	178	THR	CA-CB	-5.79	1.38	1.53
3	B	50	TRP	CG-CD1	-5.79	1.28	1.36
3	D	1	GLN	CG-CD	5.79	1.64	1.51
3	H	23	LYS	CB-CG	5.79	1.68	1.52
2	C	193	GLU	CD-OE1	5.79	1.32	1.25
3	D	11	LEU	CA-CB	5.79	1.67	1.53
3	D	190	SER	C-O	5.79	1.34	1.23
2	E	56	TRP	CD2-CE3	-5.79	1.31	1.40
2	G	41	TRP	CD2-CE2	-5.79	1.34	1.41
1	S	29	GLN	CD-OE1	5.79	1.36	1.24
3	H	128	PRO	CB-CG	-5.79	1.21	1.50
2	C	146	TYR	N-CA	-5.79	1.34	1.46
3	D	93	THR	C-O	5.79	1.34	1.23
2	C	98	TYR	N-CA	5.79	1.57	1.46
2	A	78	THR	CA-C	-5.79	1.38	1.52
2	A	181	MET	CG-SD	-5.79	1.66	1.81
3	H	167	GLY	C-O	-5.79	1.14	1.23
2	C	98	TYR	CA-C	5.78	1.68	1.52
3	F	100	LEU	N-CA	-5.78	1.34	1.46
3	H	90	ASP	C-O	-5.78	1.12	1.23
3	B	89	GLU	CB-CG	5.78	1.63	1.52
2	A	28	SER	CA-CB	-5.78	1.44	1.52
2	C	129	GLU	CA-CB	5.78	1.66	1.53
2	A	196	ASN	CA-CB	-5.78	1.38	1.53
3	F	67	ARG	CZ-NH1	-5.78	1.25	1.33
3	H	159	TRP	CA-CB	-5.78	1.41	1.53
2	C	180	SER	CB-OG	5.77	1.49	1.42
2	A	8	PRO	N-CD	-5.77	1.39	1.47
2	C	137	SER	C-N	-5.77	1.20	1.34
3	H	112	THR	C-O	-5.77	1.12	1.23
3	H	144	GLY	C-O	5.77	1.32	1.23
3	B	73	GLU	CG-CD	-5.77	1.43	1.51
4	M	76	ASN	CA-CB	-5.77	1.38	1.53
3	F	194	PRO	CA-CB	5.77	1.65	1.53
2	A	210	PRO	CB-CG	-5.77	1.21	1.50
3	B	182	LEU	N-CA	5.77	1.57	1.46
3	D	10	GLU	N-CA	5.77	1.57	1.46
2	G	160	GLU	CA-C	-5.77	1.38	1.52
3	B	70	PHE	CG-CD1	-5.76	1.30	1.38
3	B	104	TYR	CE2-CZ	-5.76	1.31	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	119	ALA	N-CA	-5.76	1.34	1.46
2	C	77	PHE	CD1-CE1	-5.76	1.27	1.39
3	F	174	VAL	CA-CB	-5.76	1.42	1.54
2	C	143	ASN	CG-ND2	5.76	1.47	1.32
2	G	75	THR	CB-CG2	5.75	1.71	1.52
2	A	98	TYR	CG-CD1	-5.75	1.31	1.39
2	A	79	LEU	N-CA	5.75	1.57	1.46
3	D	188	VAL	CA-C	-5.75	1.38	1.52
3	D	32	PHE	CG-CD1	-5.75	1.30	1.38
3	F	105	PHE	CD1-CE1	-5.75	1.27	1.39
2	G	95	LYS	CE-NZ	-5.75	1.34	1.49
1	P	27	GLY	N-CA	5.75	1.54	1.46
2	A	30	LEU	C-O	-5.75	1.12	1.23
3	D	99	PHE	CA-C	-5.75	1.38	1.52
4	N	28	ILE	CB-CG1	5.75	1.70	1.54
2	G	104	PHE	CA-CB	5.74	1.66	1.53
3	D	120	LYS	CA-CB	5.74	1.66	1.53
3	H	212	ASP	CA-CB	5.74	1.66	1.53
2	A	6	GLN	CA-C	-5.74	1.38	1.52
2	A	200	CYS	CB-SG	-5.74	1.72	1.81
2	E	19	VAL	CB-CG2	5.74	1.64	1.52
1	S	10	LYS	CB-CG	5.74	1.68	1.52
3	H	212	ASP	CB-CG	5.74	1.63	1.51
2	A	58	SER	CB-OG	5.74	1.49	1.42
3	B	209	THR	CA-CB	-5.74	1.38	1.53
2	G	126	PRO	CA-C	-5.74	1.41	1.52
3	H	53	THR	CA-CB	-5.74	1.38	1.53
1	S	42	PRO	N-CD	5.73	1.55	1.47
3	H	10	GLU	C-O	5.73	1.34	1.23
3	B	67	ARG	CB-CG	-5.73	1.37	1.52
3	H	60	TYR	CD1-CE1	5.73	1.48	1.39
3	F	206	ALA	CA-CB	-5.73	1.40	1.52
3	H	2	ILE	C-O	-5.73	1.12	1.23
2	C	170	THR	CA-C	-5.73	1.38	1.52
2	A	182	SER	CB-OG	5.72	1.49	1.42
2	C	108	THR	N-CA	-5.72	1.34	1.46
1	S	29	GLN	CG-CD	5.72	1.64	1.51
1	S	7	PRO	CA-CB	5.72	1.65	1.53
2	E	145	PHE	CD2-CE2	-5.72	1.27	1.39
3	B	127	TYR	C-N	-5.72	1.23	1.34
2	C	27	GLN	CB-CG	-5.72	1.37	1.52
3	D	14	PRO	CB-CG	-5.72	1.21	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	93	TYR	CE2-CZ	-5.72	1.31	1.38
2	E	38	TYR	CE1-CZ	-5.71	1.31	1.38
3	F	82	GLN	CD-OE1	5.71	1.36	1.24
2	G	111	GLU	CA-CB	5.71	1.66	1.53
4	M	77	ILE	CA-CB	-5.71	1.41	1.54
3	F	172	PRO	CA-CB	5.71	1.65	1.53
2	G	67	ARG	CB-CG	5.71	1.68	1.52
4	O	43	PHE	CB-CG	5.71	1.61	1.51
1	Q	24	PHE	CD2-CE2	5.71	1.50	1.39
3	F	66	GLY	N-CA	-5.71	1.37	1.46
3	H	196	GLU	N-CA	5.71	1.57	1.46
2	A	121	VAL	CB-CG2	-5.71	1.40	1.52
3	D	129	LEU	C-O	-5.71	1.12	1.23
2	E	202	ALA	N-CA	5.71	1.57	1.46
2	G	47	GLY	CA-C	-5.71	1.42	1.51
3	D	162	GLY	N-CA	5.70	1.54	1.46
1	S	5	PRO	CG-CD	5.70	1.69	1.50
3	B	142	THR	CB-OG1	5.70	1.54	1.43
3	D	46	ASN	C-O	-5.70	1.12	1.23
3	F	9	PRO	N-CD	-5.70	1.39	1.47
3	H	147	VAL	CB-CG1	-5.70	1.40	1.52
3	B	91	THR	C-N	-5.70	1.21	1.34
1	P	24	PHE	CB-CG	5.70	1.61	1.51
2	E	53	LEU	C-O	5.70	1.34	1.23
3	F	171	PHE	CA-C	-5.70	1.38	1.52
2	G	205	LYS	CB-CG	5.70	1.68	1.52
3	B	100	LEU	C-N	5.69	1.47	1.34
2	G	197	SER	CA-CB	5.69	1.61	1.52
2	A	48	GLN	CA-C	5.69	1.67	1.52
3	B	91	THR	CA-CB	5.69	1.68	1.53
3	H	206	ALA	CA-CB	-5.69	1.40	1.52
2	G	150	ILE	C-O	5.69	1.34	1.23
3	B	57	GLU	CD-OE2	5.69	1.31	1.25
3	F	127	TYR	CG-CD2	-5.69	1.31	1.39
3	H	4	LEU	N-CA	5.69	1.57	1.46
3	D	168	VAL	CB-CG2	5.68	1.64	1.52
4	M	29	PHE	CG-CD2	5.68	1.47	1.38
2	G	72	GLY	N-CA	5.68	1.54	1.46
3	F	67	ARG	CA-CB	5.68	1.66	1.53
2	A	172	GLN	N-CA	-5.68	1.34	1.46
4	M	41	GLY	N-CA	5.68	1.54	1.46
4	M	52	ARG	C-O	5.68	1.34	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	193	GLU	CA-CB	5.68	1.66	1.53
3	B	194	PRO	CA-CB	-5.68	1.42	1.53
3	F	214	LYS	CG-CD	5.68	1.71	1.52
2	E	11	LEU	C-O	5.67	1.34	1.23
2	E	138	VAL	C-O	-5.67	1.12	1.23
3	B	130	ALA	C-O	-5.67	1.12	1.23
2	G	1	ASP	N-CA	5.67	1.57	1.46
2	G	148	LYS	CD-CE	-5.67	1.37	1.51
2	A	192	TYR	CD1-CE1	5.67	1.47	1.39
2	C	198	TYR	CD1-CE1	-5.67	1.30	1.39
3	D	155	VAL	CB-CG1	-5.67	1.41	1.52
3	H	5	VAL	CB-CG2	5.67	1.64	1.52
2	A	24	LYS	CA-CB	5.67	1.66	1.53
2	A	130	GLN	CA-C	5.67	1.67	1.52
4	N	71	GLY	CA-C	5.67	1.60	1.51
3	B	10	GLU	CG-CD	5.67	1.60	1.51
2	A	172	GLN	C-O	-5.66	1.12	1.23
3	B	41	PRO	CG-CD	-5.66	1.31	1.50
3	F	54	GLU	CG-CD	-5.66	1.43	1.51
2	C	2	ILE	N-CA	5.66	1.57	1.46
3	B	47	TRP	CE2-CZ2	-5.66	1.30	1.39
3	B	199	THR	N-CA	-5.66	1.35	1.46
3	D	116	VAL	N-CA	5.66	1.57	1.46
2	E	111	GLU	CA-C	-5.66	1.38	1.52
2	G	170	THR	CA-C	-5.66	1.38	1.52
3	D	90	ASP	CG-OD1	-5.66	1.12	1.25
3	B	196	GLU	C-O	5.66	1.34	1.23
3	D	12	LYS	C-O	5.66	1.34	1.23
3	F	107	VAL	CA-CB	-5.66	1.42	1.54
3	D	188	VAL	CB-CG1	5.65	1.64	1.52
4	O	47	THR	N-CA	-5.65	1.35	1.46
2	C	41	TRP	NE1-CE2	-5.65	1.30	1.37
2	A	177	SER	C-O	-5.65	1.12	1.23
2	G	89	GLN	CB-CG	-5.65	1.37	1.52
3	D	192	THR	C-O	5.64	1.34	1.23
1	P	35	TYR	C-O	5.64	1.34	1.23
3	B	69	ALA	N-CA	-5.64	1.35	1.46
3	F	22	CYS	CA-CB	-5.64	1.41	1.53
2	G	105	GLY	CA-C	-5.64	1.42	1.51
4	O	26	ASN	CG-OD1	5.64	1.36	1.24
4	O	40	LYS	CB-CG	5.64	1.67	1.52
2	A	75	THR	C-O	-5.64	1.12	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	1	GLN	C-N	5.63	1.47	1.34
3	H	82	GLN	CG-CD	5.63	1.64	1.51
4	O	76	ASN	C-O	-5.63	1.12	1.23
3	B	52	ASN	CA-C	5.63	1.67	1.52
3	B	38	ASN	C-O	5.63	1.34	1.23
3	B	58	PRO	N-CD	-5.63	1.40	1.47
2	E	206	THR	C-N	5.63	1.47	1.34
4	O	52	ARG	CA-C	-5.63	1.38	1.52
3	B	99	PHE	CB-CG	-5.63	1.41	1.51
2	C	86	ALA	CA-CB	5.63	1.64	1.52
2	E	87	GLU	CB-CG	5.63	1.62	1.52
4	M	61	ASN	C-N	-5.63	1.23	1.33
2	E	96	GLN	N-CA	-5.63	1.35	1.46
3	F	60	TYR	CD2-CE2	-5.63	1.30	1.39
3	F	105	PHE	CG-CD1	5.63	1.47	1.38
2	E	4	MET	CA-C	-5.62	1.38	1.52
2	G	55	TYR	CE1-CZ	-5.62	1.31	1.38
3	B	207	SER	C-O	-5.62	1.12	1.23
2	G	87	GLU	CB-CG	5.62	1.62	1.52
2	C	146	TYR	CE1-CZ	-5.62	1.31	1.38
2	G	58	SER	CB-OG	5.62	1.49	1.42
1	P	39	ARG	CA-CB	5.62	1.66	1.53
2	C	51	LYS	CD-CE	5.62	1.65	1.51
2	C	104	PHE	CG-CD2	-5.62	1.30	1.38
3	F	172	PRO	CA-C	5.62	1.64	1.52
2	A	161	ARG	CG-CD	5.61	1.66	1.51
4	L	64	TRP	CE2-CZ2	5.61	1.49	1.39
3	D	120	LYS	CB-CG	5.61	1.67	1.52
2	E	55	TYR	CD1-CE1	5.61	1.47	1.39
3	F	78	THR	CA-C	-5.61	1.38	1.52
3	F	36	TRP	CE3-CZ3	-5.61	1.28	1.38
3	F	37	VAL	CA-CB	-5.61	1.43	1.54
2	E	205	LYS	C-O	-5.61	1.12	1.23
2	C	160	GLU	CA-CB	5.60	1.66	1.53
3	H	104	TYR	CE1-CZ	-5.60	1.31	1.38
3	H	104	TYR	C-O	-5.60	1.12	1.23
2	A	32	SER	CA-CB	5.60	1.61	1.52
2	E	104	PHE	CA-C	-5.60	1.38	1.52
3	F	180	TYR	CD1-CE1	-5.60	1.30	1.39
3	D	116	VAL	CB-CG1	-5.60	1.41	1.52
2	A	66	ASP	CA-CB	5.59	1.66	1.53
2	E	189	LYS	CA-CB	5.59	1.66	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	35	ARG	NE-CZ	5.59	1.40	1.33
1	Q	16	ASN	C-O	5.59	1.33	1.23
2	G	151	ASN	CG-ND2	5.59	1.46	1.32
2	C	27	GLN	CG-CD	5.59	1.64	1.51
4	N	51	TYR	N-CA	-5.59	1.35	1.46
3	H	69	ALA	N-CA	-5.59	1.35	1.46
3	D	108	TRP	CG-CD1	5.59	1.44	1.36
3	H	67	ARG	N-CA	5.59	1.57	1.46
4	L	53	TYR	C-O	-5.59	1.12	1.23
2	E	152	VAL	CB-CG2	5.59	1.64	1.52
3	F	98	ARG	NE-CZ	5.58	1.40	1.33
3	H	92	ALA	CA-C	5.58	1.67	1.52
2	A	36	LYS	CD-CE	5.58	1.65	1.51
3	F	211	VAL	C-N	-5.58	1.21	1.34
2	E	15	ALA	C-O	5.58	1.33	1.23
2	E	209	SER	CB-OG	5.58	1.49	1.42
3	H	134	ALA	CA-CB	5.58	1.64	1.52
2	C	105	GLY	N-CA	5.57	1.54	1.46
2	C	140	CYS	C-N	-5.57	1.21	1.34
4	O	30	ALA	C-O	-5.57	1.12	1.23
1	Q	22	VAL	CB-CG2	5.57	1.64	1.52
1	S	34	VAL	C-O	5.57	1.33	1.23
2	G	51	LYS	CD-CE	5.57	1.65	1.51
3	D	60	TYR	CD2-CE2	5.57	1.47	1.39
2	C	13	VAL	CA-CB	-5.57	1.43	1.54
3	H	180	TYR	CE1-CZ	5.57	1.45	1.38
2	A	67	ARG	C-N	-5.57	1.21	1.34
3	H	71	SER	N-CA	-5.57	1.35	1.46
2	A	48	GLN	CA-CB	5.56	1.66	1.53
3	F	140	MET	C-O	5.56	1.33	1.23
2	C	86	ALA	N-CA	-5.56	1.35	1.46
3	D	69	ALA	N-CA	-5.56	1.35	1.46
2	E	104	PHE	CD1-CE1	5.56	1.50	1.39
2	G	124	PHE	C-O	-5.55	1.12	1.23
2	A	210	PRO	C-O	5.55	1.34	1.23
3	D	194	PRO	CA-CB	-5.55	1.42	1.53
4	L	18	LYS	CA-C	5.55	1.67	1.52
2	C	144	ASN	C-O	-5.55	1.12	1.23
3	D	21	SER	C-O	-5.55	1.12	1.23
3	D	20	ILE	C-N	5.55	1.46	1.34
4	M	39	PHE	CB-CG	5.55	1.60	1.51
3	D	94	TYR	CZ-OH	5.55	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	216	ASN	CB-CG	-5.55	1.38	1.51
3	H	157	VAL	C-N	-5.55	1.21	1.34
2	E	193	GLU	CD-OE1	-5.54	1.19	1.25
3	F	22	CYS	C-O	-5.54	1.12	1.23
4	N	30	ALA	CA-CB	5.54	1.64	1.52
2	C	91	VAL	CA-C	-5.54	1.38	1.52
3	H	171	PHE	CE1-CZ	5.54	1.47	1.37
2	A	215	PHE	CD1-CE1	-5.54	1.28	1.39
3	F	100	LEU	CA-C	5.54	1.67	1.52
3	B	123	PRO	C-N	-5.53	1.23	1.34
4	N	24	LYS	N-CA	-5.53	1.35	1.46
3	D	43	LYS	C-N	5.53	1.43	1.33
2	C	39	LEU	C-O	5.53	1.33	1.23
2	E	213	LYS	CA-C	-5.53	1.38	1.52
3	H	54	GLU	CB-CG	5.53	1.62	1.52
3	D	2	ILE	CB-CG1	5.53	1.69	1.54
3	D	18	VAL	CA-C	5.53	1.67	1.52
3	F	167	GLY	N-CA	-5.53	1.37	1.46
3	D	157	VAL	C-O	5.52	1.33	1.23
2	G	62	SER	CA-CB	5.52	1.61	1.52
3	H	64	PHE	CD2-CE2	5.52	1.50	1.39
3	H	88	ASN	C-O	-5.52	1.12	1.23
3	F	17	THR	CB-CG2	5.52	1.70	1.52
2	E	148	LYS	N-CA	5.52	1.57	1.46
1	S	35	TYR	C-O	5.52	1.33	1.23
2	E	39	LEU	CA-CB	-5.52	1.41	1.53
2	E	133	SER	C-N	5.52	1.43	1.33
2	E	190	ASP	CB-CG	5.52	1.63	1.51
3	F	104	TYR	N-CA	-5.52	1.35	1.46
1	S	43	ARG	CD-NE	5.52	1.55	1.46
3	H	64	PHE	CG-CD2	5.52	1.47	1.38
2	A	29	LEU	CG-CD1	5.51	1.72	1.51
3	D	82	GLN	CA-C	-5.51	1.38	1.52
2	E	218	ASN	CA-C	-5.51	1.38	1.52
2	C	103	THR	N-CA	5.51	1.57	1.46
3	F	193	TRP	CZ3-CH2	-5.51	1.31	1.40
3	H	127	TYR	CB-CG	5.51	1.59	1.51
3	D	191	SER	CB-OG	5.51	1.49	1.42
3	B	213	LYS	CE-NZ	5.51	1.62	1.49
2	C	195	HIS	CA-C	5.51	1.67	1.52
3	H	150	TYR	CE1-CZ	5.51	1.45	1.38
2	A	127	SER	CB-OG	5.50	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	56	TRP	CA-C	-5.50	1.38	1.52
4	O	66	ALA	N-CA	-5.50	1.35	1.46
2	A	2	ILE	CA-CB	-5.50	1.42	1.54
1	P	38	PRO	C-O	-5.50	1.12	1.23
2	A	35	ARG	CZ-NH1	-5.50	1.25	1.33
3	B	111	GLY	N-CA	5.50	1.54	1.46
2	E	177	SER	CA-CB	-5.50	1.44	1.52
2	C	52	VAL	CA-C	-5.50	1.38	1.52
3	H	48	MET	N-CA	5.50	1.57	1.46
1	P	24	PHE	CD2-CE2	5.50	1.50	1.39
2	C	93	TYR	CZ-OH	5.50	1.47	1.37
3	D	46	ASN	CB-CG	5.50	1.63	1.51
2	E	124	PHE	CA-CB	-5.50	1.41	1.53
2	G	71	ARG	C-N	5.50	1.43	1.33
4	O	63	GLU	CD-OE1	-5.50	1.19	1.25
4	L	34	ILE	CA-CB	-5.49	1.42	1.54
2	C	130	GLN	CD-OE1	5.49	1.36	1.24
3	H	34	MET	CB-CG	-5.49	1.33	1.51
3	H	161	SER	C-O	5.49	1.33	1.23
1	S	8	GLN	CB-CG	5.49	1.67	1.52
2	G	94	CYS	CB-SG	5.49	1.91	1.82
3	B	54	GLU	CG-CD	5.49	1.60	1.51
3	H	170	THR	CA-C	5.49	1.67	1.52
2	G	191	GLU	CG-CD	5.49	1.60	1.51
2	A	85	GLN	N-CA	-5.49	1.35	1.46
3	B	80	TYR	CG-CD2	5.49	1.46	1.39
3	B	155	VAL	C-O	5.49	1.33	1.23
1	Q	35	TYR	CZ-OH	-5.49	1.28	1.37
1	P	20	GLN	CA-CB	5.48	1.66	1.53
3	B	205	PRO	C-O	5.48	1.34	1.23
2	C	70	GLY	N-CA	5.48	1.54	1.46
3	H	119	ALA	CA-CB	-5.48	1.41	1.52
2	G	183	SER	CA-C	5.48	1.67	1.52
2	C	192	TYR	CD2-CE2	5.48	1.47	1.39
3	B	73	GLU	CB-CG	-5.48	1.41	1.52
3	H	201	ASN	C-O	-5.48	1.12	1.23
3	F	141	VAL	CB-CG1	-5.47	1.41	1.52
2	G	93	TYR	C-O	-5.47	1.12	1.23
2	G	98	TYR	CD1-CE1	-5.47	1.31	1.39
2	A	100	PRO	C-O	5.47	1.34	1.23
2	C	215	PHE	CA-CB	5.47	1.66	1.53
4	M	34	ILE	CB-CG2	5.47	1.69	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	116	VAL	C-O	5.47	1.33	1.23
3	D	131	PRO	CA-C	5.46	1.63	1.52
2	E	23	CYS	CA-CB	-5.46	1.42	1.53
2	C	201	GLU	CA-CB	5.46	1.66	1.53
3	B	21	SER	CA-C	-5.46	1.38	1.52
3	B	74	THR	CB-OG1	5.46	1.54	1.43
2	C	31	ASN	CB-CG	5.46	1.63	1.51
2	A	68	PHE	CG-CD1	-5.46	1.30	1.38
4	L	27	LEU	CG-CD2	-5.46	1.31	1.51
2	C	219	GLU	CD-OE2	-5.46	1.19	1.25
3	D	201	ASN	C-O	5.46	1.33	1.23
3	H	180	TYR	C-O	-5.46	1.12	1.23
3	F	62	ASP	C-O	-5.46	1.12	1.23
3	H	56	GLY	C-O	-5.45	1.15	1.23
2	A	192	TYR	CD2-CE2	5.45	1.47	1.39
3	B	116	VAL	C-O	-5.45	1.12	1.23
4	O	52	ARG	CG-CD	5.45	1.65	1.51
2	A	188	THR	N-CA	-5.45	1.35	1.46
2	E	191	GLU	C-O	-5.45	1.12	1.23
3	D	214	LYS	CB-CG	5.45	1.67	1.52
4	O	59	LYS	N-CA	-5.45	1.35	1.46
3	B	95	PHE	CA-CB	5.45	1.66	1.53
3	B	68	PHE	CD1-CE1	-5.45	1.28	1.39
3	B	163	SER	N-CA	-5.45	1.35	1.46
3	D	207	SER	C-O	-5.45	1.13	1.23
3	D	124	PRO	CA-C	-5.44	1.42	1.52
3	B	171	PHE	CB-CG	-5.44	1.42	1.51
3	F	121	THR	N-CA	5.44	1.57	1.46
3	F	147	VAL	CB-CG2	5.44	1.64	1.52
4	L	45	GLU	CD-OE2	5.44	1.31	1.25
2	E	6	GLN	N-CA	5.44	1.57	1.46
2	E	205	LYS	CA-CB	-5.44	1.42	1.53
3	H	70	PHE	CA-C	5.44	1.67	1.52
2	A	36	LYS	CA-CB	-5.44	1.42	1.53
3	B	31	ASP	CB-CG	-5.44	1.40	1.51
3	B	175	LEU	N-CA	-5.44	1.35	1.46
3	F	179	LEU	C-O	5.44	1.33	1.23
3	F	218	ARG	CA-C	5.44	1.67	1.52
3	H	54	GLU	CA-CB	5.44	1.66	1.53
3	F	196	GLU	CD-OE2	5.44	1.31	1.25
2	C	124	PHE	CA-CB	5.43	1.66	1.53
3	F	1	GLN	CA-C	5.43	1.67	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	39	LEU	CA-C	5.43	1.67	1.52
4	M	40	LYS	N-CA	5.43	1.57	1.46
2	C	201	GLU	CD-OE2	-5.43	1.19	1.25
1	Q	36	LEU	C-O	5.43	1.33	1.23
2	E	61	GLU	CD-OE1	-5.43	1.19	1.25
3	F	81	LEU	C-O	-5.43	1.13	1.23
2	G	36	LYS	CD-CE	5.43	1.64	1.51
2	A	137	SER	N-CA	-5.43	1.35	1.46
3	B	40	ALA	C-N	-5.43	1.24	1.34
1	S	17	ARG	CZ-NH1	5.43	1.40	1.33
2	G	202	ALA	CA-CB	-5.43	1.41	1.52
2	A	86	ALA	CA-C	-5.42	1.38	1.52
3	B	46	ASN	C-O	-5.42	1.13	1.23
3	H	135	ALA	CA-C	-5.42	1.38	1.52
3	H	216	VAL	CB-CG1	5.42	1.64	1.52
2	A	59	THR	CB-CG2	-5.42	1.34	1.52
2	A	95	LYS	CB-CG	5.42	1.67	1.52
3	D	172	PRO	C-O	5.42	1.34	1.23
2	E	53	LEU	CB-CG	5.42	1.68	1.52
2	A	145	PHE	CE2-CZ	-5.42	1.27	1.37
3	B	64	PHE	CE1-CZ	-5.42	1.27	1.37
2	A	141	PHE	CD2-CE2	-5.42	1.28	1.39
3	D	65	LYS	CG-CD	5.42	1.70	1.52
3	F	171	PHE	CE1-CZ	-5.42	1.27	1.37
3	F	140	MET	SD-CE	5.42	2.08	1.77
3	B	29	PHE	CB-CG	5.41	1.60	1.51
2	A	216	ASN	N-CA	5.41	1.57	1.46
3	D	47	TRP	CE3-CZ3	-5.41	1.29	1.38
3	D	104	TYR	CD1-CE1	5.41	1.47	1.39
2	G	5	SER	CA-CB	-5.41	1.44	1.52
2	A	7	SER	CA-CB	-5.41	1.44	1.52
2	C	61	GLU	CG-CD	5.41	1.60	1.51
3	D	27	TYR	CA-C	-5.41	1.38	1.52
3	D	145	CYS	CA-C	-5.41	1.38	1.52
2	A	147	PRO	CB-CG	-5.41	1.23	1.50
2	E	55	TYR	CZ-OH	-5.41	1.28	1.37
2	E	121	VAL	CA-C	5.41	1.67	1.52
2	E	194	ARG	CB-CG	5.41	1.67	1.52
4	L	73	ASN	CA-CB	5.40	1.67	1.53
2	C	17	GLU	CD-OE1	5.40	1.31	1.25
2	G	151	ASN	CB-CG	5.40	1.63	1.51
3	B	166	SER	C-O	-5.40	1.13	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Q	43	ARG	CG-CD	5.40	1.65	1.51
2	A	89	GLN	CD-OE1	-5.40	1.12	1.24
2	C	109	LYS	CB-CG	5.40	1.67	1.52
2	A	176	ASP	CA-CB	-5.39	1.42	1.53
3	F	1	GLN	CD-OE1	-5.39	1.12	1.24
3	H	159	TRP	CA-C	-5.39	1.39	1.52
3	H	108	TRP	CB-CG	-5.39	1.40	1.50
4	O	49	GLU	CB-CG	5.39	1.62	1.52
4	M	20	GLU	CD-OE1	5.39	1.31	1.25
2	G	44	GLN	CG-CD	-5.39	1.38	1.51
3	H	60	TYR	CE1-CZ	-5.39	1.31	1.38
3	D	123	PRO	CA-CB	-5.39	1.42	1.53
2	E	50	PRO	CA-C	-5.39	1.42	1.52
2	G	38	TYR	CD2-CE2	5.39	1.47	1.39
2	A	15	ALA	CA-CB	5.38	1.63	1.52
1	S	3	THR	CB-OG1	5.38	1.54	1.43
3	B	205	PRO	N-CD	-5.38	1.40	1.47
2	E	98	TYR	CA-C	-5.38	1.39	1.52
3	F	185	SER	CB-OG	5.38	1.49	1.42
3	D	83	ILE	C-O	-5.38	1.13	1.23
3	B	141	VAL	CB-CG2	5.37	1.64	1.52
2	G	133	SER	CA-C	-5.37	1.39	1.52
2	G	199	THR	C-O	-5.37	1.13	1.23
2	E	102	LEU	CB-CG	-5.37	1.36	1.52
3	D	6	GLN	CA-CB	5.37	1.65	1.53
3	B	2	ILE	CA-C	-5.37	1.39	1.52
4	L	71	GLY	CA-C	5.37	1.60	1.51
3	F	142	THR	CA-CB	5.37	1.67	1.53
3	B	157	VAL	CB-CG1	5.36	1.64	1.52
2	E	19	VAL	CA-C	5.36	1.66	1.52
3	B	120	LYS	C-O	-5.36	1.13	1.23
3	H	98	ARG	CB-CG	5.36	1.67	1.52
3	H	161	SER	CB-OG	5.36	1.49	1.42
2	E	22	SER	CB-OG	5.36	1.49	1.42
3	H	1	GLN	CD-OE1	5.36	1.35	1.24
2	E	67	ARG	NE-CZ	5.35	1.40	1.33
2	A	217	ARG	CZ-NH1	5.35	1.40	1.33
1	Q	4	ASN	CG-ND2	5.35	1.46	1.32
4	M	59	LYS	CG-CD	5.35	1.70	1.52
3	F	69	ALA	CA-C	-5.35	1.39	1.52
2	G	42	TYR	CB-CG	5.35	1.59	1.51
2	A	101	PRO	CA-C	-5.34	1.42	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	94	TYR	CE1-CZ	-5.34	1.31	1.38
2	C	194	ARG	C-O	5.34	1.33	1.23
2	A	149	ASP	C-O	5.34	1.33	1.23
4	N	77	ILE	CA-CB	5.34	1.67	1.54
3	H	163	SER	CA-C	5.34	1.66	1.52
2	A	15	ALA	N-CA	-5.34	1.35	1.46
3	D	181	THR	CA-CB	-5.34	1.39	1.53
3	D	15	GLY	N-CA	-5.33	1.38	1.46
2	G	186	THR	CA-C	5.33	1.66	1.52
3	D	202	VAL	CB-CG2	-5.33	1.41	1.52
2	E	125	PRO	C-O	-5.33	1.12	1.23
2	C	104	PHE	N-CA	-5.33	1.35	1.46
2	G	37	ASN	CB-CG	5.33	1.63	1.51
2	C	27	GLN	C-N	5.33	1.46	1.34
2	E	208	THR	CB-CG2	5.33	1.70	1.52
3	F	103	GLN	CA-CB	-5.33	1.42	1.53
2	G	30	LEU	CG-CD1	5.33	1.71	1.51
3	H	162	GLY	CA-C	-5.33	1.43	1.51
4	L	68	LEU	CG-CD2	5.32	1.71	1.51
2	C	129	GLU	CD-OE1	5.32	1.31	1.25
1	Q	24	PHE	CE2-CZ	5.32	1.47	1.37
2	E	51	LYS	CG-CD	5.32	1.70	1.52
2	G	45	LYS	CA-C	-5.32	1.39	1.52
3	B	23	LYS	CE-NZ	5.32	1.62	1.49
3	B	91	THR	CB-OG1	5.32	1.53	1.43
2	G	36	LYS	N-CA	5.32	1.56	1.46
3	B	211	VAL	N-CA	-5.32	1.35	1.46
4	M	79	PHE	CG-CD1	-5.32	1.30	1.38
2	G	80	THR	CA-C	5.32	1.66	1.52
2	C	81	ILE	C-N	-5.32	1.21	1.34
4	M	26	ASN	CB-CG	-5.32	1.38	1.51
2	E	68	PHE	CD2-CE2	-5.32	1.28	1.39
4	N	26	ASN	CG-OD1	5.32	1.35	1.24
4	O	55	ALA	C-O	-5.32	1.13	1.23
2	A	56	TRP	CE3-CZ3	-5.31	1.29	1.38
4	N	79	PHE	C-O	5.31	1.33	1.23
3	B	98	ARG	CB-CG	5.31	1.66	1.52
4	L	63	GLU	CB-CG	5.31	1.62	1.52
3	D	50	TRP	NE1-CE2	-5.31	1.30	1.37
4	O	32	GLY	CA-C	5.31	1.60	1.51
2	A	141	PHE	CE2-CZ	-5.31	1.27	1.37
3	B	43	LYS	N-CA	-5.30	1.35	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	78	THR	N-CA	-5.30	1.35	1.46
1	S	22	VAL	C-O	5.30	1.33	1.23
2	C	93	TYR	C-O	-5.30	1.13	1.23
2	C	147	PRO	N-CD	5.30	1.55	1.47
3	F	34	MET	CB-CG	-5.30	1.34	1.51
3	F	112	THR	CA-C	-5.30	1.39	1.52
4	N	50	ALA	CA-CB	5.30	1.63	1.52
4	O	51	TYR	CD1-CE1	5.30	1.47	1.39
3	B	47	TRP	CD2-CE3	-5.30	1.32	1.40
2	E	2	ILE	CA-CB	-5.30	1.42	1.54
3	F	32	PHE	CD2-CE2	-5.30	1.28	1.39
3	H	213	LYS	CE-NZ	5.30	1.62	1.49
2	C	41	TRP	CD2-CE3	-5.30	1.32	1.40
4	M	56	LEU	CA-C	-5.30	1.39	1.52
2	E	60	ARG	CB-CG	5.30	1.66	1.52
2	A	50	PRO	CA-C	5.30	1.63	1.52
3	F	75	SER	CA-CB	-5.29	1.45	1.52
2	C	39	LEU	CA-CB	5.29	1.66	1.53
1	Q	45	GLY	CA-C	5.29	1.60	1.51
2	E	50	PRO	N-CD	-5.29	1.40	1.47
3	F	43	LYS	CD-CE	5.29	1.64	1.51
3	H	196	GLU	CA-CB	5.29	1.65	1.53
3	B	197	THR	CA-C	5.29	1.66	1.52
4	N	25	VAL	CB-CG2	-5.29	1.41	1.52
2	G	124	PHE	CG-CD1	5.29	1.46	1.38
3	B	145	CYS	CA-C	5.28	1.66	1.52
2	C	157	ASP	CB-CG	-5.28	1.40	1.51
3	D	19	LYS	CB-CG	5.28	1.66	1.52
2	E	209	SER	CA-CB	5.28	1.60	1.52
3	F	159	TRP	CA-C	5.28	1.66	1.52
2	A	204	HIS	C-O	5.28	1.33	1.23
2	C	113	LYS	CA-C	-5.28	1.39	1.52
2	C	173	ASP	CB-CG	-5.28	1.40	1.51
3	D	18	VAL	C-O	5.28	1.33	1.23
3	H	166	SER	CA-CB	5.28	1.60	1.52
4	O	45	GLU	C-O	-5.28	1.13	1.23
2	A	50	PRO	CG-CD	-5.28	1.33	1.50
3	B	94	TYR	CE2-CZ	-5.28	1.31	1.38
4	L	43	PHE	CA-CB	-5.28	1.42	1.53
2	E	77	PHE	CD1-CE1	-5.28	1.28	1.39
2	G	33	ARG	N-CA	5.27	1.56	1.46
3	B	128	PRO	N-CA	-5.27	1.38	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	160	ASN	N-CA	-5.27	1.35	1.46
3	D	200	CYS	CA-C	-5.27	1.39	1.52
2	E	194	ARG	C-O	-5.27	1.13	1.23
3	B	215	ILE	CB-CG1	-5.27	1.39	1.54
3	F	28	THR	CB-CG2	5.27	1.69	1.52
3	B	130	ALA	CA-C	-5.26	1.39	1.52
3	D	64	PHE	CG-CD2	-5.26	1.30	1.38
3	B	80	TYR	CE1-CZ	5.26	1.45	1.38
3	D	125	SER	CB-OG	5.26	1.49	1.42
3	F	94	TYR	CD1-CE1	-5.26	1.31	1.39
2	A	211	ILE	CG1-CD1	5.26	1.86	1.50
2	E	62	SER	CA-C	-5.26	1.39	1.52
2	G	49	SER	CA-CB	5.26	1.60	1.52
3	F	33	SER	C-O	5.26	1.33	1.23
2	G	12	ALA	CA-CB	-5.26	1.41	1.52
2	G	212	VAL	CA-CB	-5.26	1.43	1.54
3	D	153	GLU	C-O	5.25	1.33	1.23
3	F	80	TYR	CE1-CZ	-5.25	1.31	1.38
4	N	32	GLY	N-CA	-5.25	1.38	1.46
4	O	34	ILE	N-CA	-5.25	1.35	1.46
2	E	167	ASN	CG-ND2	5.25	1.46	1.32
3	F	194	PRO	N-CA	-5.25	1.38	1.47
2	G	70	GLY	C-O	5.25	1.32	1.23
1	Q	30	ILE	C-O	5.25	1.33	1.23
2	A	110	LEU	CA-C	-5.25	1.39	1.52
3	B	182	LEU	CA-C	-5.25	1.39	1.52
3	F	34	MET	CA-CB	-5.25	1.42	1.53
2	G	89	GLN	C-O	-5.25	1.13	1.23
3	B	146	LEU	CA-CB	-5.25	1.41	1.53
3	B	214	LYS	N-CA	5.25	1.56	1.46
4	L	24	LYS	CD-CE	5.24	1.64	1.51
3	D	168	VAL	CA-C	-5.24	1.39	1.52
2	E	156	ILE	C-O	5.24	1.33	1.23
2	C	141	PHE	CG-CD2	5.24	1.46	1.38
3	D	160	ASN	C-O	-5.24	1.13	1.23
2	E	201	GLU	CD-OE1	-5.24	1.19	1.25
3	H	101	LEU	CB-CG	5.24	1.67	1.52
3	F	114	VAL	N-CA	-5.24	1.35	1.46
1	S	7	PRO	CB-CG	5.24	1.76	1.50
3	D	61	ALA	N-CA	-5.23	1.35	1.46
4	M	36	THR	C-O	5.23	1.33	1.23
3	H	193	TRP	CD2-CE3	-5.23	1.32	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Q	24	PHE	CB-CG	5.23	1.60	1.51
3	B	19	LYS	CE-NZ	-5.23	1.35	1.49
3	H	84	ASN	N-CA	-5.23	1.35	1.46
3	H	164	LEU	N-CA	-5.23	1.35	1.46
2	C	187	LEU	CA-CB	-5.23	1.41	1.53
3	D	213	LYS	CD-CE	5.23	1.64	1.51
1	Q	3	THR	C-O	5.23	1.33	1.23
3	H	45	LEU	CA-C	5.23	1.66	1.52
2	E	167	ASN	C-O	5.22	1.33	1.23
2	C	105	GLY	C-O	-5.22	1.15	1.23
2	E	130	GLN	CB-CG	5.22	1.66	1.52
3	B	176	GLN	CA-CB	-5.22	1.42	1.53
2	A	199	THR	CA-C	-5.22	1.39	1.52
3	B	150	TYR	C-O	-5.22	1.13	1.23
1	Q	18	ARG	CG-CD	5.22	1.65	1.51
4	N	77	ILE	C-O	-5.22	1.13	1.23
3	H	54	GLU	CD-OE1	5.22	1.31	1.25
4	L	44	GLU	CD-OE1	5.22	1.31	1.25
3	D	38	ASN	CB-CG	-5.22	1.39	1.51
2	G	212	VAL	C-O	-5.22	1.13	1.23
3	H	197	THR	CB-OG1	5.22	1.53	1.43
2	A	209	SER	C-O	-5.21	1.13	1.23
2	C	55	TYR	CG-CD1	-5.21	1.32	1.39
2	E	93	TYR	CD2-CE2	5.21	1.47	1.39
3	B	129	LEU	C-N	5.21	1.46	1.34
2	C	27	GLN	C-O	5.21	1.33	1.23
2	E	89	GLN	C-O	5.21	1.33	1.23
3	H	71	SER	CA-C	5.21	1.66	1.52
2	E	6	GLN	CD-NE2	5.21	1.45	1.32
3	H	70	PHE	CD2-CE2	-5.21	1.28	1.39
3	H	147	VAL	CA-CB	-5.21	1.43	1.54
2	C	67	ARG	C-O	5.21	1.33	1.23
4	N	74	HIS	CB-CG	5.21	1.59	1.50
2	E	99	ILE	C-N	-5.20	1.24	1.34
3	H	4	LEU	CA-CB	-5.20	1.41	1.53
2	A	140	CYS	C-O	-5.20	1.13	1.23
3	F	93	THR	CA-CB	-5.20	1.39	1.53
4	O	29	PHE	CE2-CZ	5.20	1.47	1.37
2	E	34	THR	CA-CB	-5.20	1.39	1.53
3	F	201	ASN	N-CA	-5.20	1.35	1.46
3	H	98	ARG	N-CA	-5.20	1.35	1.46
2	A	170	THR	CA-C	5.20	1.66	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	93	TYR	CE1-CZ	-5.20	1.31	1.38
4	M	47	THR	C-N	-5.20	1.22	1.34
3	F	14	PRO	N-CA	-5.20	1.38	1.47
4	N	20	GLU	CB-CG	5.20	1.62	1.52
2	C	69	THR	C-O	5.19	1.33	1.23
3	B	159	TRP	CA-C	5.19	1.66	1.52
3	D	109	GLY	C-O	-5.19	1.15	1.23
1	Q	24	PHE	CE1-CZ	5.19	1.47	1.37
2	E	45	LYS	C-N	-5.19	1.24	1.34
3	F	158	THR	CA-C	-5.19	1.39	1.52
2	E	34	THR	CA-C	5.18	1.66	1.52
3	F	102	ARG	C-O	-5.18	1.13	1.23
3	B	180	TYR	CD1-CE1	-5.18	1.31	1.39
2	G	175	LYS	CD-CE	5.18	1.64	1.51
2	A	194	ARG	N-CA	5.18	1.56	1.46
1	S	22	VAL	CA-C	5.18	1.66	1.52
2	A	104	PHE	CG-CD2	-5.18	1.30	1.38
2	E	199	THR	CA-C	-5.18	1.39	1.52
4	N	77	ILE	N-CA	-5.18	1.35	1.46
3	B	85	SER	CA-CB	-5.17	1.45	1.52
2	C	31	ASN	CG-ND2	5.17	1.45	1.32
2	A	147	PRO	CA-CB	-5.17	1.43	1.53
2	G	6	GLN	CA-C	-5.17	1.39	1.52
2	G	98	TYR	CG-CD1	-5.17	1.32	1.39
2	A	151	ASN	CG-OD1	-5.17	1.12	1.24
3	F	119	ALA	CA-CB	-5.17	1.41	1.52
1	Q	7	PRO	CA-CB	5.17	1.63	1.53
2	E	189	LYS	N-CA	5.17	1.56	1.46
4	N	20	GLU	CD-OE1	5.17	1.31	1.25
4	L	44	GLU	C-O	5.16	1.33	1.23
3	H	177	SER	CA-CB	5.16	1.60	1.52
3	B	217	PRO	CA-C	-5.16	1.42	1.52
3	F	199	THR	C-N	5.16	1.46	1.34
3	B	180	TYR	CZ-OH	5.16	1.46	1.37
2	G	188	THR	CB-CG2	-5.16	1.35	1.52
3	F	58	PRO	N-CA	-5.16	1.38	1.47
2	A	196	ASN	C-O	5.15	1.33	1.23
2	C	4	MET	CB-CG	5.15	1.67	1.51
3	B	10	GLU	N-CA	5.15	1.56	1.46
3	B	120	LYS	CG-CD	5.15	1.70	1.52
3	D	50	TRP	C-O	5.15	1.33	1.23
3	D	147	VAL	C-O	-5.15	1.13	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	165	VAL	C-O	5.15	1.33	1.23
3	F	177	SER	C-N	-5.15	1.22	1.34
2	C	213	LYS	CD-CE	5.15	1.64	1.51
3	D	215	ILE	N-CA	-5.15	1.36	1.46
3	D	60	TYR	CB-CG	5.14	1.59	1.51
2	A	110	LEU	CG-CD1	5.14	1.70	1.51
3	D	124	PRO	N-CD	-5.14	1.40	1.47
2	E	3	VAL	CB-CG2	-5.14	1.42	1.52
2	G	111	GLU	C-O	-5.14	1.13	1.23
2	C	96	GLN	CG-CD	5.14	1.62	1.51
3	D	26	GLY	C-O	5.14	1.31	1.23
2	E	111	GLU	C-O	-5.14	1.13	1.23
4	O	75	MET	CG-SD	-5.14	1.67	1.81
4	L	29	PHE	C-O	5.14	1.33	1.23
2	E	144	ASN	N-CA	-5.14	1.36	1.46
3	F	24	ALA	CA-CB	5.14	1.63	1.52
3	F	131	PRO	N-CA	5.14	1.55	1.47
3	H	200	CYS	CA-CB	5.14	1.65	1.53
4	O	21	VAL	CA-CB	5.14	1.65	1.54
2	C	1	ASP	N-CA	5.13	1.56	1.46
3	D	124	PRO	C-O	-5.13	1.12	1.23
1	Q	30	ILE	CB-CG2	5.13	1.68	1.52
2	G	182	SER	N-CA	-5.13	1.36	1.46
3	D	213	LYS	CG-CD	5.13	1.70	1.52
2	E	120	THR	CA-CB	-5.13	1.40	1.53
4	M	48	ALA	N-CA	-5.13	1.36	1.46
2	G	129	GLU	CD-OE2	-5.13	1.20	1.25
3	H	96	CYS	CB-SG	5.13	1.91	1.82
3	B	197	THR	CA-CB	5.13	1.66	1.53
2	A	161	ARG	CZ-NH2	5.13	1.39	1.33
4	N	58	ALA	N-CA	-5.13	1.36	1.46
2	C	146	TYR	CE2-CZ	-5.13	1.31	1.38
2	E	41	TRP	CD2-CE3	5.13	1.48	1.40
2	E	176	ASP	CA-CB	5.12	1.65	1.53
3	B	29	PHE	CG-CD2	-5.12	1.31	1.38
2	E	204	HIS	C-O	5.12	1.33	1.23
3	B	99	PHE	CA-CB	5.12	1.65	1.53
3	D	148	LYS	C-O	-5.12	1.13	1.23
3	D	150	TYR	CD1-CE1	-5.12	1.31	1.39
3	F	194	PRO	CG-CD	5.12	1.67	1.50
2	E	38	TYR	CB-CG	5.12	1.59	1.51
4	O	38	GLU	CD-OE2	5.12	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	49	GLY	CA-C	5.12	1.60	1.51
2	C	198	TYR	CE1-CZ	5.11	1.45	1.38
2	E	104	PHE	CA-CB	-5.11	1.42	1.53
3	B	112	THR	N-CA	-5.11	1.36	1.46
2	C	60	ARG	C-N	-5.11	1.22	1.34
2	A	104	PHE	CD1-CE1	5.11	1.49	1.39
2	C	144	ASN	CA-CB	-5.11	1.39	1.53
3	B	16	GLU	C-O	-5.10	1.13	1.23
3	F	44	GLY	C-O	5.10	1.31	1.23
4	N	74	HIS	CA-CB	5.10	1.65	1.53
2	G	179	TYR	N-CA	-5.10	1.36	1.46
2	C	73	SER	C-N	-5.10	1.23	1.33
3	H	116	VAL	CB-CG2	5.10	1.63	1.52
2	G	98	TYR	CZ-OH	5.10	1.46	1.37
3	H	184	SER	CA-C	-5.10	1.39	1.52
3	B	127	TYR	CZ-OH	-5.10	1.29	1.37
4	L	34	ILE	CG1-CD1	5.10	1.85	1.50
2	C	202	ALA	CA-C	-5.10	1.39	1.52
3	H	186	VAL	C-O	-5.10	1.13	1.23
3	B	8	GLY	CA-C	5.09	1.60	1.51
2	A	26	SER	C-O	-5.09	1.13	1.23
3	F	48	MET	N-CA	-5.09	1.36	1.46
3	F	161	SER	CA-C	5.09	1.66	1.52
2	A	6	GLN	CB-CG	5.09	1.66	1.52
3	F	49	GLY	CA-C	-5.09	1.43	1.51
4	N	31	ASP	N-CA	5.09	1.56	1.46
4	O	55	ALA	CA-CB	5.08	1.63	1.52
2	C	211	ILE	CA-CB	5.08	1.66	1.54
3	H	169	HIS	CA-CB	5.08	1.65	1.53
4	O	41	GLY	N-CA	5.08	1.53	1.46
4	O	79	PHE	CD2-CE2	5.08	1.49	1.39
2	C	3	VAL	C-O	-5.07	1.13	1.23
3	D	180	TYR	CE1-CZ	5.07	1.45	1.38
2	E	140	CYS	CA-CB	5.07	1.65	1.53
2	A	99	ILE	C-O	-5.07	1.13	1.23
3	B	208	SER	CA-CB	-5.07	1.45	1.52
3	H	125	SER	CA-C	-5.07	1.39	1.52
3	H	160	ASN	N-CA	5.07	1.56	1.46
3	B	41	PRO	CB-CG	-5.07	1.24	1.50
3	D	133	SER	C-O	5.07	1.32	1.23
4	M	25	VAL	CA-C	-5.07	1.39	1.52
4	M	38	GLU	CA-C	-5.07	1.39	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	63	GLU	CD-OE1	5.07	1.31	1.25
2	G	108	THR	CB-OG1	5.07	1.53	1.43
4	O	64	TRP	CD2-CE3	-5.07	1.32	1.40
4	M	53	TYR	CG-CD2	5.06	1.45	1.39
4	N	59	LYS	CG-CD	5.06	1.69	1.52
1	S	25	PRO	CA-C	5.06	1.62	1.52
2	G	165	VAL	CB-CG2	-5.06	1.42	1.52
3	H	123	PRO	CG-CD	5.06	1.67	1.50
2	A	162	GLN	CD-OE1	5.06	1.35	1.24
2	E	82	SER	CB-OG	-5.06	1.35	1.42
4	N	30	ALA	CA-C	-5.05	1.39	1.52
3	H	168	VAL	CB-CG1	5.05	1.63	1.52
3	H	171	PHE	CG-CD2	5.05	1.46	1.38
2	G	169	TRP	CE3-CZ3	5.05	1.47	1.38
3	B	6	GLN	CA-C	-5.05	1.39	1.52
2	E	51	LYS	CB-CG	5.05	1.66	1.52
3	F	56	GLY	CA-C	-5.05	1.43	1.51
2	G	77	PHE	CB-CG	5.05	1.59	1.51
2	E	56	TRP	CA-CB	-5.05	1.42	1.53
3	H	16	GLU	CG-CD	5.05	1.59	1.51
4	O	40	LYS	CA-C	-5.05	1.39	1.52
3	B	209	THR	CB-CG2	-5.05	1.35	1.52
2	C	199	THR	N-CA	-5.05	1.36	1.46
3	F	140	MET	CG-SD	-5.05	1.68	1.81
2	G	68	PHE	CE1-CZ	-5.04	1.27	1.37
2	G	77	PHE	CG-CD2	5.04	1.46	1.38
3	B	201	ASN	CG-ND2	-5.04	1.20	1.32
3	H	72	LEU	C-O	-5.04	1.13	1.23
3	D	9	PRO	N-CA	-5.04	1.38	1.47
4	N	45	GLU	N-CA	-5.04	1.36	1.46
2	G	92	TYR	CE1-CZ	5.04	1.45	1.38
3	H	19	LYS	CG-CD	5.04	1.69	1.52
2	C	190	ASP	CG-OD1	5.03	1.36	1.25
3	F	134	ALA	N-CA	-5.03	1.36	1.46
2	G	195	HIS	CB-CG	5.03	1.59	1.50
3	H	32	PHE	CD1-CE1	5.03	1.49	1.39
3	H	91	THR	CB-CG2	-5.03	1.35	1.52
3	B	125	SER	CB-OG	5.03	1.48	1.42
3	B	2	ILE	CG1-CD1	5.03	1.85	1.50
3	D	119	ALA	CA-C	-5.03	1.39	1.52
4	M	46	ALA	CA-CB	5.03	1.63	1.52
2	E	212	VAL	CB-CG2	5.03	1.63	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	47	TRP	N-CA	5.03	1.56	1.46
3	D	172	PRO	N-CD	-5.02	1.40	1.47
2	E	153	LYS	CE-NZ	5.02	1.61	1.49
3	F	124	PRO	CA-CB	-5.02	1.43	1.53
4	N	79	PHE	CD2-CE2	5.02	1.49	1.39
4	O	39	PHE	CD1-CE1	5.02	1.49	1.39
4	O	49	GLU	CG-CD	5.02	1.59	1.51
2	E	122	SER	N-CA	-5.02	1.36	1.46
4	N	29	PHE	N-CA	-5.02	1.36	1.46
2	E	104	PHE	CG-CD1	-5.02	1.31	1.38
2	A	97	ALA	C-O	-5.02	1.13	1.23
2	A	176	ASP	CB-CG	-5.02	1.41	1.51
3	B	62	ASP	N-CA	5.02	1.56	1.46
3	D	39	GLN	CD-NE2	-5.02	1.20	1.32
3	B	210	LYS	CB-CG	5.02	1.66	1.52
1	P	37	LEU	CB-CG	5.01	1.67	1.52
2	C	28	SER	CA-CB	5.01	1.60	1.52
3	D	41	PRO	CA-CB	5.01	1.63	1.53
2	E	124	PHE	CE2-CZ	-5.01	1.27	1.37
2	C	89	GLN	CA-C	-5.01	1.40	1.52
3	F	32	PHE	CB-CG	-5.01	1.42	1.51
4	M	79	PHE	CB-CG	5.01	1.59	1.51
2	G	33	ARG	CD-NE	5.01	1.54	1.46
3	H	118	SER	C-O	5.01	1.32	1.23
3	D	118	SER	C-N	-5.01	1.22	1.34
3	B	32	PHE	CE2-CZ	5.01	1.46	1.37
3	H	29	PHE	CE2-CZ	5.00	1.46	1.37
3	D	10	GLU	CD-OE2	-5.00	1.20	1.25
3	D	195	SER	CB-OG	5.00	1.48	1.42
2	A	98	TYR	C-O	5.00	1.32	1.23
3	D	159	TRP	CG-CD2	-5.00	1.35	1.43
4	M	29	PHE	CA-CB	-5.00	1.43	1.53
3	F	36	TRP	CA-CB	-5.00	1.43	1.53
2	G	125	PRO	CA-CB	5.00	1.63	1.53
3	H	44	GLY	CA-C	-5.00	1.43	1.51

All (717) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	60	ARG	NE-CZ-NH1	18.43	129.51	120.30
1	Q	40	ARG	NE-CZ-NH1	17.41	129.01	120.30
3	F	178	ASP	CB-CG-OD2	16.47	133.12	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	161	ARG	NE-CZ-NH2	-15.38	112.61	120.30
1	Q	13	ARG	NE-CZ-NH1	-15.12	112.74	120.30
2	C	60	ARG	NE-CZ-NH2	-14.77	112.92	120.30
3	B	98	ARG	NE-CZ-NH2	-14.73	112.94	120.30
1	S	6	LYS	C-N-CD	-13.69	90.49	120.60
2	E	60	ARG	NE-CZ-NH2	-13.39	113.60	120.30
1	P	40	ARG	NE-CZ-NH1	13.33	126.96	120.30
2	G	35	ARG	NE-CZ-NH2	13.01	126.81	120.30
2	E	217	ARG	NE-CZ-NH2	12.91	126.76	120.30
2	C	161	ARG	NE-CZ-NH1	12.91	126.75	120.30
3	F	178	ASP	CB-CG-OD1	-12.69	106.88	118.30
4	L	53	TYR	CB-CG-CD2	12.58	128.55	121.00
2	G	35	ARG	NE-CZ-NH1	-12.36	114.12	120.30
1	P	40	ARG	NE-CZ-NH2	-12.28	114.16	120.30
3	F	68	PHE	CB-CG-CD1	12.28	129.40	120.80
3	B	155	VAL	CG1-CB-CG2	-12.07	91.59	110.90
1	Q	17	ARG	NE-CZ-NH1	-11.80	114.40	120.30
2	C	35	ARG	NE-CZ-NH2	-11.75	114.42	120.30
4	L	52	ARG	NE-CZ-NH1	-11.32	114.64	120.30
3	D	127	TYR	CB-CG-CD2	10.94	127.56	121.00
3	F	98	ARG	NE-CZ-NH1	-10.86	114.87	120.30
2	E	192	TYR	CB-CG-CD1	10.86	127.51	121.00
2	G	114	ARG	NE-CZ-NH1	-10.74	114.93	120.30
3	B	99	PHE	CB-CG-CD1	-10.68	113.33	120.80
3	F	98	ARG	NE-CZ-NH2	10.55	125.58	120.30
2	A	149	ASP	CB-CG-OD2	10.48	127.73	118.30
3	B	151	PHE	CB-CG-CD1	10.46	128.12	120.80
4	M	31	ASP	CB-CG-OD1	-10.46	108.88	118.30
3	D	212	ASP	CB-CG-OD2	10.43	127.69	118.30
2	E	1	ASP	CB-CG-OD2	-10.30	109.03	118.30
2	A	42	TYR	CB-CG-CD1	-10.23	114.86	121.00
2	G	76	ASP	CB-CG-OD1	10.20	127.48	118.30
2	G	179	TYR	CB-CG-CD1	-10.19	114.89	121.00
2	A	149	ASP	CB-CG-OD1	-10.16	109.15	118.30
3	H	67	ARG	NE-CZ-NH1	-10.09	115.25	120.30
2	E	104	PHE	CB-CG-CD2	10.08	127.86	120.80
4	N	51	TYR	CB-CG-CD1	-10.06	114.96	121.00
2	E	114	ARG	NE-CZ-NH2	10.00	125.30	120.30
2	A	35	ARG	NE-CZ-NH2	9.96	125.28	120.30
2	G	192	TYR	CB-CG-CD1	9.92	126.95	121.00
2	E	66	ASP	CB-CG-OD2	9.73	127.06	118.30
4	M	79	PHE	CD1-CE1-CZ	9.71	131.75	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	M	79	PHE	CG-CD1-CE1	-9.70	110.13	120.80
2	C	145	PHE	CB-CG-CD1	-9.64	114.05	120.80
3	D	154	PRO	N-CD-CG	-9.60	88.80	103.20
3	B	29	PHE	CB-CG-CD1	9.56	127.50	120.80
3	B	54	GLU	OE1-CD-OE2	-9.48	111.93	123.30
2	G	53	LEU	CB-CG-CD2	-9.47	94.90	111.00
3	D	31	ASP	CB-CG-OD2	9.41	126.77	118.30
2	E	176	ASP	CB-CG-OD2	-9.41	109.83	118.30
2	E	49	SER	N-CA-CB	-9.39	96.41	110.50
3	D	180	TYR	CZ-CE2-CD2	-9.34	111.39	119.80
3	H	62	ASP	CB-CG-OD2	-9.34	109.90	118.30
2	C	93	TYR	CB-CG-CD2	9.32	126.59	121.00
2	E	93	TYR	CZ-CE2-CD2	9.24	128.12	119.80
3	D	143	LEU	CB-CG-CD2	9.24	126.70	111.00
1	Q	40	ARG	NH1-CZ-NH2	-9.22	109.26	119.40
2	E	157	ASP	CB-CG-OD2	9.21	126.59	118.30
3	D	98	ARG	NE-CZ-NH2	-9.20	115.70	120.30
2	G	98	TYR	CB-CA-C	-9.18	92.05	110.40
3	B	105	PHE	CB-CG-CD1	9.15	127.21	120.80
3	F	67	ARG	NE-CZ-NH1	9.09	124.84	120.30
2	E	71	ARG	NE-CZ-NH1	9.05	124.83	120.30
2	G	124	PHE	CB-CG-CD2	-9.03	114.48	120.80
3	H	18	VAL	CA-CB-CG1	-9.02	97.37	110.90
2	E	149	ASP	CB-CG-OD2	-9.01	110.19	118.30
1	S	40	ARG	NE-CZ-NH1	-8.99	115.81	120.30
2	G	92	TYR	CB-CG-CD2	-8.98	115.61	121.00
3	H	212	ASP	CB-CG-OD2	8.97	126.37	118.30
1	Q	37	LEU	CA-CB-CG	8.94	135.87	115.30
4	L	51	TYR	CG-CD2-CE2	8.94	128.45	121.30
3	D	145	CYS	CA-CB-SG	8.88	129.99	114.00
2	E	131	LEU	CB-CG-CD1	-8.79	96.05	111.00
2	C	217	ARG	NE-CZ-NH2	-8.79	115.90	120.30
2	A	176	ASP	CB-CG-OD1	8.75	126.17	118.30
2	E	88	ASP	CB-CG-OD1	-8.72	110.45	118.30
3	B	41	PRO	N-CD-CG	-8.67	90.20	103.20
2	E	157	ASP	CB-CG-OD1	-8.66	110.50	118.30
2	A	92	TYR	CG-CD2-CE2	8.64	128.22	121.30
2	C	64	VAL	CG1-CB-CG2	-8.64	97.08	110.90
2	G	145	PHE	CB-CG-CD2	8.63	126.84	120.80
2	G	198	TYR	CB-CG-CD1	-8.49	115.91	121.00
3	H	180	TYR	CG-CD2-CE2	8.48	128.09	121.30
2	A	192	TYR	CZ-CE2-CD2	8.47	127.42	119.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	190	ASP	CB-CG-OD2	8.46	125.91	118.30
3	B	70	PHE	CD1-CE1-CZ	8.45	130.24	120.10
2	A	217	ARG	NE-CZ-NH1	8.38	124.49	120.30
3	F	103	GLN	N-CA-C	8.38	133.62	111.00
4	M	38	GLU	OE1-CD-OE2	8.36	133.33	123.30
3	H	31	ASP	CB-CG-OD2	-8.36	110.78	118.30
2	E	179	TYR	CG-CD1-CE1	8.35	127.98	121.30
3	B	159	TRP	CD1-NE1-CE2	-8.32	101.51	109.00
3	B	80	TYR	CB-CG-CD2	8.28	125.97	121.00
4	L	25	VAL	CB-CA-C	-8.22	95.78	111.40
2	A	194	ARG	NE-CZ-NH2	-8.21	116.20	120.30
2	E	1	ASP	CB-CG-OD1	8.16	125.64	118.30
2	E	55	TYR	CB-CG-CD1	8.15	125.89	121.00
2	E	190	ASP	CB-CG-OD2	8.15	125.63	118.30
3	H	150	TYR	CB-CG-CD1	-8.12	116.13	121.00
4	M	77	ILE	CG1-CB-CG2	-8.10	93.58	111.40
2	E	66	ASP	CB-CG-OD1	-8.10	111.01	118.30
3	B	175	LEU	CB-CG-CD1	-8.08	97.26	111.00
2	A	1	ASP	CB-CG-OD2	8.07	125.56	118.30
2	C	93	TYR	CB-CG-CD1	-8.05	116.17	121.00
3	F	175	LEU	CB-CG-CD2	8.02	124.63	111.00
2	G	177	SER	O-C-N	8.01	135.52	122.70
3	F	212	ASP	CB-CG-OD2	8.01	125.50	118.30
4	M	39	PHE	CB-CG-CD1	7.98	126.39	120.80
2	A	121	VAL	CA-CB-CG2	-7.97	98.95	110.90
3	D	102	ARG	NE-CZ-NH1	7.94	124.27	120.30
2	G	152	VAL	CA-CB-CG2	-7.94	98.99	110.90
4	L	30	ALA	N-CA-CB	-7.93	99.00	110.10
2	A	29	LEU	CB-CG-CD1	-7.92	97.53	111.00
2	E	198	TYR	CZ-CE2-CD2	7.92	126.93	119.80
3	B	116	VAL	CG1-CB-CG2	-7.89	98.28	110.90
2	A	146	TYR	CB-CG-CD1	7.88	125.73	121.00
2	G	52	VAL	CA-CB-CG1	-7.88	99.08	110.90
4	O	39	PHE	CB-CG-CD1	7.87	126.31	120.80
4	N	67	ASP	CB-CG-OD1	-7.84	111.24	118.30
1	S	17	ARG	NE-CZ-NH1	7.82	124.21	120.30
3	D	186	VAL	CG1-CB-CG2	-7.81	98.40	110.90
2	A	67	ARG	NE-CZ-NH2	7.78	124.19	120.30
4	M	79	PHE	N-CA-C	7.77	131.98	111.00
3	D	127	TYR	CD1-CG-CD2	-7.76	109.36	117.90
3	F	106	ASP	CB-CG-OD1	-7.75	111.33	118.30
3	H	172	PRO	CA-N-CD	-7.73	100.67	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	89	GLU	OE1-CD-OE2	-7.72	114.04	123.30
3	F	110	ALA	N-CA-CB	-7.72	99.30	110.10
4	M	53	TYR	CD1-CE1-CZ	7.71	126.74	119.80
2	G	171	ASP	CB-CG-OD1	-7.68	111.39	118.30
3	H	180	TYR	CG-CD1-CE1	-7.68	115.16	121.30
4	N	74	HIS	N-CA-C	-7.67	90.29	111.00
2	C	110	LEU	CB-CG-CD2	-7.64	98.00	111.00
3	F	159	TRP	CD1-NE1-CE2	-7.63	102.13	109.00
2	E	82	SER	N-CA-CB	-7.62	99.07	110.50
2	A	92	TYR	CB-CG-CD1	7.61	125.57	121.00
2	E	170	THR	OG1-CB-CG2	-7.61	92.50	110.00
4	M	31	ASP	CB-CG-OD2	7.61	125.15	118.30
3	B	105	PHE	CD1-CE1-CZ	7.61	129.23	120.10
1	Q	13	ARG	NE-CZ-NH2	7.60	124.10	120.30
2	E	191	GLU	OE1-CD-OE2	7.60	132.42	123.30
2	C	189	LYS	CD-CE-NZ	7.57	129.12	111.70
3	F	218	ARG	NE-CZ-NH1	-7.57	116.52	120.30
2	E	71	ARG	NH1-CZ-NH2	-7.56	111.08	119.40
2	E	71	ARG	NE-CZ-NH2	7.56	124.08	120.30
2	G	141	PHE	CB-CG-CD1	-7.55	115.52	120.80
2	G	178	THR	OG1-CB-CG2	-7.50	92.74	110.00
2	G	91	VAL	CA-CB-CG2	-7.49	99.66	110.90
3	H	116	VAL	CG1-CB-CG2	7.48	122.87	110.90
4	O	43	PHE	CZ-CE2-CD2	-7.48	111.13	120.10
2	C	129	GLU	OE1-CD-OE2	7.47	132.26	123.30
2	E	104	PHE	CZ-CE2-CD2	7.46	129.06	120.10
3	F	218	ARG	NE-CZ-NH2	-7.45	116.57	120.30
2	C	104	PHE	CB-CG-CD1	-7.45	115.59	120.80
2	E	38	TYR	CB-CG-CD1	7.42	125.45	121.00
2	E	93	TYR	CB-CG-CD1	7.41	125.45	121.00
2	C	153	LYS	O-C-N	7.39	134.53	122.70
2	C	141	PHE	CB-CG-CD1	-7.38	115.64	120.80
2	G	27	GLN	N-CA-CB	-7.37	97.34	110.60
3	D	151	PHE	CB-CG-CD2	7.33	125.93	120.80
4	M	51	TYR	CD1-CE1-CZ	7.31	126.38	119.80
3	F	214	LYS	CD-CE-NZ	7.30	128.50	111.70
1	S	21	ASP	CB-CG-OD1	7.29	124.86	118.30
2	G	76	ASP	OD1-CG-OD2	-7.28	109.47	123.30
3	D	180	TYR	CG-CD2-CE2	7.27	127.12	121.30
2	E	141	PHE	CB-CG-CD2	-7.27	115.71	120.80
2	A	88	ASP	CB-CG-OD1	-7.25	111.78	118.30
2	C	198	TYR	CZ-CE2-CD2	-7.24	113.28	119.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	137	SER	N-CA-CB	-7.24	99.64	110.50
3	D	78	THR	CA-CB-CG2	-7.23	102.28	112.40
2	A	100	PRO	N-CA-C	-7.22	93.33	112.10
3	D	159	TRP	CD1-NE1-CE2	-7.22	102.50	109.00
4	M	79	PHE	N-CA-CB	-7.22	97.61	110.60
4	L	34	ILE	CG1-CB-CG2	-7.22	95.53	111.40
3	F	150	TYR	CG-CD2-CE2	-7.20	115.54	121.30
2	E	92	TYR	CD1-CE1-CZ	7.19	126.27	119.80
3	B	181	THR	CA-CB-CG2	-7.18	102.35	112.40
3	H	73	GLU	OE1-CD-OE2	-7.16	114.70	123.30
3	F	27	TYR	CB-CG-CD1	7.15	125.29	121.00
3	F	197	THR	OG1-CB-CG2	-7.15	93.55	110.00
2	C	122	SER	N-CA-CB	-7.15	99.78	110.50
3	D	14	PRO	CA-N-CD	-7.13	101.51	111.50
3	F	174	VAL	CG1-CB-CG2	-7.13	99.49	110.90
2	C	179	TYR	CZ-CE2-CD2	7.12	126.21	119.80
2	A	156	ILE	O-C-N	7.11	134.08	122.70
3	B	9	PRO	N-CA-C	-7.08	93.70	112.10
4	L	17	PRO	O-C-N	7.07	134.01	122.70
2	C	67	ARG	NE-CZ-NH2	7.06	123.83	120.30
2	A	187	LEU	CB-CG-CD2	-7.05	99.02	111.00
4	N	27	LEU	CB-CG-CD2	7.04	122.97	111.00
4	N	49	GLU	OE1-CD-OE2	7.04	131.75	123.30
4	L	79	PHE	CZ-CE2-CD2	-7.04	111.66	120.10
2	A	146	TYR	CG-CD1-CE1	7.03	126.93	121.30
2	G	184	THR	CA-CB-CG2	-7.03	102.56	112.40
3	F	200	CYS	CA-CB-SG	7.02	126.64	114.00
2	C	13	VAL	CG1-CB-CG2	7.01	122.12	110.90
4	O	33	LYS	N-CA-CB	-7.01	97.98	110.60
4	O	67	ASP	CB-CG-OD2	-7.01	111.99	118.30
3	H	68	PHE	CB-CG-CD1	-6.99	115.91	120.80
2	A	92	TYR	CD1-CE1-CZ	6.97	126.08	119.80
2	G	111	GLU	OE1-CD-OE2	6.97	131.66	123.30
3	F	149	GLY	N-CA-C	6.96	130.51	113.10
3	F	60	TYR	CG-CD1-CE1	-6.96	115.73	121.30
3	D	31	ASP	CB-CG-OD1	-6.95	112.04	118.30
2	E	91	VAL	CA-CB-CG2	-6.95	100.47	110.90
2	G	146	TYR	CD1-CE1-CZ	6.95	126.06	119.80
3	B	145	CYS	N-CA-C	-6.95	92.24	111.00
3	H	178	ASP	CB-CG-OD1	6.95	124.55	118.30
2	A	110	LEU	CB-CG-CD2	6.95	122.81	111.00
2	G	124	PHE	CB-CG-CD1	6.93	125.65	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	M	53	TYR	CG-CD1-CE1	-6.93	115.76	121.30
2	G	146	TYR	CG-CD1-CE1	-6.91	115.77	121.30
2	A	40	ALA	N-CA-CB	-6.89	100.45	110.10
3	H	172	PRO	N-CA-CB	6.89	111.57	103.30
3	D	211	VAL	CB-CA-C	-6.88	98.32	111.40
4	L	27	LEU	CB-CG-CD2	6.88	122.69	111.00
3	D	34	MET	CB-CA-C	-6.87	96.66	110.40
2	A	115	ALA	N-CA-CB	-6.87	100.48	110.10
3	F	31	ASP	CB-CG-OD2	6.83	124.45	118.30
3	F	60	TYR	CB-CG-CD1	-6.83	116.90	121.00
3	F	68	PHE	CB-CG-CD2	-6.82	116.02	120.80
3	F	218	ARG	NH1-CZ-NH2	6.81	126.89	119.40
2	G	153	LYS	CB-CA-C	-6.80	96.79	110.40
3	H	95	PHE	CB-CG-CD2	6.80	125.56	120.80
3	B	94	TYR	CZ-CE2-CD2	6.80	125.92	119.80
3	F	189	PRO	N-CD-CG	6.79	113.39	103.20
3	D	146	LEU	CB-CG-CD2	6.78	122.53	111.00
3	D	9	PRO	CA-N-CD	-6.78	102.01	111.50
2	A	33	ARG	NE-CZ-NH1	-6.78	116.91	120.30
2	E	217	ARG	NE-CZ-NH1	-6.77	116.92	120.30
3	H	101	LEU	CB-CG-CD1	6.76	122.49	111.00
2	C	1	ASP	CB-CG-OD2	6.75	124.37	118.30
2	E	88	ASP	N-CA-C	6.74	129.21	111.00
3	D	127	TYR	CZ-CE2-CD2	6.74	125.87	119.80
2	A	77	PHE	CB-CG-CD2	-6.73	116.09	120.80
4	O	80	ALA	CB-CA-C	6.70	120.16	110.10
3	D	35	HIS	N-CA-CB	6.70	122.66	110.60
3	F	45	LEU	CB-CG-CD2	-6.70	99.61	111.00
3	B	21	SER	CB-CA-C	-6.69	97.39	110.10
3	H	150	TYR	CG-CD2-CE2	6.69	126.65	121.30
3	H	170	THR	N-CA-CB	-6.68	97.60	110.30
3	B	10	GLU	OE1-CD-OE2	-6.66	115.31	123.30
2	A	38	TYR	CD1-CE1-CZ	-6.66	113.81	119.80
3	B	99	PHE	CB-CG-CD2	6.64	125.45	120.80
3	B	154	PRO	N-CA-CB	-6.64	95.29	102.60
3	B	145	CYS	O-C-N	-6.64	112.07	122.70
3	H	200	CYS	CA-CB-SG	6.64	125.94	114.00
2	A	173	ASP	CB-CG-OD2	6.63	124.27	118.30
4	N	70	ASP	CB-CG-OD1	6.63	124.27	118.30
4	L	29	PHE	CG-CD2-CE2	6.62	128.08	120.80
2	A	210	PRO	CA-N-CD	-6.61	102.24	111.50
1	S	18	ARG	N-CA-C	6.60	128.83	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Q	21	ASP	CB-CG-OD2	6.60	124.24	118.30
3	B	90	ASP	CB-CG-OD1	-6.59	112.36	118.30
2	E	100	PRO	N-CD-CG	-6.58	93.33	103.20
4	N	58	ALA	N-CA-CB	-6.58	100.88	110.10
3	D	174	VAL	CG1-CB-CG2	6.58	121.42	110.90
3	B	104	TYR	CB-CG-CD1	6.57	124.94	121.00
3	D	72	LEU	CB-CG-CD2	-6.57	99.83	111.00
4	L	51	TYR	CZ-CE2-CD2	-6.56	113.90	119.80
2	C	55	TYR	CB-CG-CD2	-6.56	117.07	121.00
2	A	122	SER	N-CA-CB	-6.54	100.69	110.50
2	E	44	GLN	O-C-N	-6.54	112.23	122.70
2	E	139	VAL	CB-CA-C	-6.54	98.97	111.40
2	A	120	THR	OG1-CB-CG2	-6.54	94.97	110.00
3	H	150	TYR	CB-CG-CD2	6.53	124.92	121.00
2	E	215	PHE	CB-CG-CD1	6.50	125.35	120.80
3	F	208	SER	CB-CA-C	6.50	122.45	110.10
2	C	57	ALA	N-CA-C	6.50	128.54	111.00
3	D	99	PHE	CG-CD2-CE2	6.50	127.95	120.80
2	E	131	LEU	CB-CG-CD2	6.49	122.03	111.00
3	F	77	SER	O-C-N	6.47	133.06	122.70
2	E	219	GLU	OE1-CD-OE2	-6.47	115.54	123.30
2	G	139	VAL	CG1-CB-CG2	-6.46	100.56	110.90
3	B	24	ALA	CB-CA-C	-6.46	100.41	110.10
2	G	33	ARG	NE-CZ-NH2	6.45	123.53	120.30
2	A	17	GLU	OE1-CD-OE2	-6.45	115.56	123.30
2	G	118	ALA	CB-CA-C	-6.44	100.43	110.10
2	A	71	ARG	NE-CZ-NH2	6.44	123.52	120.30
2	E	173	ASP	CB-CG-OD2	6.44	124.10	118.30
4	N	53	TYR	CZ-CE2-CD2	-6.44	114.00	119.80
3	D	45	LEU	CB-CG-CD2	-6.44	100.06	111.00
4	M	62	GLY	CA-C-O	-6.42	109.04	120.60
3	B	20	ILE	CG1-CB-CG2	-6.42	97.28	111.40
3	F	195	SER	N-CA-CB	-6.41	100.89	110.50
2	C	149	ASP	CB-CG-OD2	-6.40	112.54	118.30
3	H	131	PRO	N-CD-CG	-6.40	93.60	103.20
3	F	212	ASP	N-CA-C	-6.38	93.76	111.00
3	F	59	THR	CA-CB-CG2	-6.38	103.47	112.40
2	E	92	TYR	CG-CD1-CE1	-6.37	116.21	121.30
3	B	62	ASP	CB-CG-OD1	6.36	124.02	118.30
4	O	74	HIS	N-CA-CB	-6.35	99.16	110.60
3	B	144	GLY	N-CA-C	6.35	128.98	113.10
3	B	32	PHE	CB-CG-CD1	-6.34	116.36	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	112	LEU	CB-CG-CD1	-6.33	100.23	111.00
3	B	32	PHE	CD1-CE1-CZ	-6.32	112.52	120.10
2	A	42	TYR	CA-CB-CG	6.32	125.41	113.40
3	F	31	ASP	N-CA-C	6.32	128.06	111.00
4	L	53	TYR	CD1-CG-CD2	-6.29	110.98	117.90
2	G	62	SER	CB-CA-C	6.28	122.03	110.10
3	D	206	ALA	N-CA-CB	-6.27	101.33	110.10
4	M	68	LEU	CB-CG-CD1	6.27	121.65	111.00
3	F	94	TYR	CD1-CE1-CZ	-6.26	114.17	119.80
2	E	116	ASP	CB-CG-OD2	6.26	123.93	118.30
2	A	78	THR	CA-CB-CG2	-6.25	103.65	112.40
3	H	68	PHE	CD1-CG-CD2	6.23	126.40	118.30
3	D	159	TRP	NE1-CE2-CZ2	-6.23	123.55	130.40
4	O	35	GLN	N-CA-CB	-6.23	99.39	110.60
2	G	55	TYR	CZ-CE2-CD2	-6.22	114.20	119.80
3	H	168	VAL	CB-CA-C	-6.22	99.59	111.40
3	H	180	TYR	CB-CG-CD2	6.21	124.73	121.00
3	B	89	GLU	OE1-CD-OE2	6.20	130.74	123.30
2	G	173	ASP	CB-CG-OD1	-6.19	112.73	118.30
3	H	2	ILE	CG1-CB-CG2	-6.18	97.80	111.40
3	B	158	THR	CA-CB-CG2	-6.17	103.76	112.40
4	O	36	THR	N-CA-C	-6.17	94.33	111.00
3	F	52	ASN	N-CA-C	-6.17	94.33	111.00
3	H	197	THR	CB-CA-C	-6.16	94.96	111.60
4	L	39	PHE	CG-CD2-CE2	6.15	127.57	120.80
4	L	70	ASP	CB-CG-OD2	6.15	123.83	118.30
2	G	146	TYR	CB-CG-CD1	-6.14	117.32	121.00
2	C	79	LEU	CB-CG-CD1	-6.13	100.57	111.00
2	C	92	TYR	CD1-CE1-CZ	-6.13	114.28	119.80
2	E	185	LEU	CB-CG-CD1	6.12	121.41	111.00
2	G	38	TYR	CA-CB-CG	-6.12	101.77	113.40
4	M	81	GLY	CA-C-O	6.12	131.62	120.60
1	P	37	LEU	CA-CB-CG	6.12	129.37	115.30
2	E	30	LEU	CB-CG-CD2	6.11	121.39	111.00
2	G	1	ASP	CB-CG-OD2	6.11	123.80	118.30
2	E	60	ARG	NE-CZ-NH1	6.10	123.35	120.30
2	G	201	GLU	O-C-N	6.08	132.43	122.70
4	O	28	ILE	CG1-CB-CG2	-6.08	98.03	111.40
3	B	70	PHE	CB-CG-CD1	6.06	125.04	120.80
1	S	24	PHE	CB-CG-CD2	-6.06	116.56	120.80
3	H	15	GLY	CA-C-N	-6.05	103.88	117.20
3	H	98	ARG	CA-C-O	6.05	132.81	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Q	30	ILE	CB-CA-C	-6.05	99.50	111.60
2	C	93	TYR	CZ-CE2-CD2	-6.05	114.36	119.80
2	G	116	ASP	CB-CG-OD1	6.04	123.74	118.30
3	B	32	PHE	CZ-CE2-CD2	6.04	127.35	120.10
2	A	114	ARG	NE-CZ-NH2	6.04	123.32	120.30
3	F	80	TYR	CB-CG-CD2	6.04	124.62	121.00
2	A	171	ASP	CB-CG-OD2	6.03	123.73	118.30
3	D	193	TRP	CB-CA-C	-6.03	98.34	110.40
3	H	179	LEU	CB-CG-CD2	-6.03	100.75	111.00
4	M	24	LYS	N-CA-C	6.03	127.27	111.00
3	B	95	PHE	CB-CG-CD2	-6.01	116.59	120.80
2	E	198	TYR	CD1-CE1-CZ	-6.01	114.39	119.80
3	B	151	PHE	CD1-CG-CD2	-6.00	110.50	118.30
1	S	13	ARG	N-CA-C	5.99	127.16	111.00
3	H	18	VAL	CG1-CB-CG2	5.98	120.46	110.90
2	A	170	THR	CA-CB-CG2	5.98	120.77	112.40
3	H	64	PHE	CD1-CE1-CZ	5.96	127.26	120.10
2	G	105	GLY	N-CA-C	-5.96	98.20	113.10
3	F	175	LEU	CB-CG-CD1	-5.95	100.88	111.00
2	A	42	TYR	CD1-CE1-CZ	-5.95	114.44	119.80
4	L	52	ARG	NH1-CZ-NH2	5.94	125.94	119.40
2	A	42	TYR	CB-CG-CD2	5.93	124.56	121.00
2	E	159	SER	CB-CA-C	5.93	121.38	110.10
2	C	3	VAL	CB-CA-C	-5.93	100.13	111.40
3	B	166	SER	C-N-CA	-5.92	109.87	122.30
4	M	77	ILE	CB-CA-C	-5.91	99.78	111.60
3	F	95	PHE	CB-CG-CD2	5.91	124.94	120.80
2	G	66	ASP	CB-CG-OD1	5.91	123.62	118.30
4	M	67	ASP	CB-CG-OD1	5.90	123.61	118.30
3	F	180	TYR	CD1-CE1-CZ	5.90	125.11	119.80
2	E	76	ASP	CB-CG-OD2	-5.90	112.99	118.30
3	D	21	SER	N-CA-CB	5.89	119.34	110.50
4	M	49	GLU	OE1-CD-OE2	5.89	130.37	123.30
2	C	127	SER	CB-CA-C	-5.89	98.91	110.10
2	E	130	GLN	CA-CB-CG	5.89	126.35	113.40
3	H	126	VAL	CA-CB-CG2	-5.88	102.07	110.90
2	A	184	THR	CA-CB-CG2	-5.88	104.17	112.40
3	H	50	TRP	CA-C-N	-5.87	104.28	117.20
2	C	127	SER	N-CA-C	5.87	126.84	111.00
2	C	189	LYS	CB-CA-C	5.86	122.12	110.40
3	F	100	LEU	CB-CG-CD2	5.85	120.94	111.00
2	E	27	GLN	N-CA-CB	-5.84	100.09	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	211	VAL	CA-CB-CG1	-5.84	102.14	110.90
4	O	43	PHE	CB-CG-CD1	-5.84	116.71	120.80
3	F	29	PHE	CB-CG-CD1	-5.83	116.72	120.80
3	B	130	ALA	N-CA-C	-5.83	95.27	111.00
4	L	43	PHE	CB-CG-CD1	-5.83	116.72	120.80
3	B	91	THR	CA-CB-CG2	-5.82	104.25	112.40
3	F	4	LEU	CB-CG-CD1	-5.82	101.10	111.00
1	Q	17	ARG	NE-CZ-NH2	5.81	123.21	120.30
2	E	93	TYR	CE1-CZ-CE2	-5.81	110.50	119.80
2	G	36	LYS	CB-CA-C	-5.81	98.78	110.40
3	B	73	GLU	CA-C-N	-5.81	104.43	117.20
3	D	124	PRO	CA-N-CD	-5.80	103.37	111.50
2	E	146	TYR	CD1-CE1-CZ	-5.80	114.58	119.80
3	H	198	VAL	CG1-CB-CG2	-5.77	101.67	110.90
2	C	1	ASP	CB-CG-OD1	-5.76	113.12	118.30
3	F	90	ASP	CB-CG-OD2	-5.75	113.12	118.30
4	M	80	ALA	CB-CA-C	-5.75	101.47	110.10
2	A	198	TYR	CG-CD2-CE2	-5.74	116.71	121.30
2	C	33	ARG	CD-NE-CZ	5.74	131.64	123.60
2	E	3	VAL	CB-CA-C	-5.74	100.49	111.40
2	E	8	PRO	O-C-N	5.74	131.88	122.70
2	A	38	TYR	CG-CD1-CE1	5.73	125.88	121.30
3	F	175	LEU	CA-CB-CG	5.73	128.48	115.30
4	N	79	PHE	CB-CG-CD1	5.72	124.81	120.80
2	G	14	SER	CB-CA-C	-5.72	99.23	110.10
2	E	104	PHE	CD1-CG-CD2	-5.71	110.87	118.30
2	E	214	SER	N-CA-C	5.70	126.40	111.00
2	A	198	TYR	CZ-CE2-CD2	5.69	124.92	119.80
3	H	118	SER	N-CA-CB	5.68	119.03	110.50
3	B	211	VAL	O-C-N	-5.68	113.61	122.70
2	A	152	VAL	CG1-CB-CG2	-5.68	101.82	110.90
2	G	5	SER	CB-CA-C	-5.67	99.32	110.10
2	G	78	THR	CA-CB-CG2	-5.67	104.45	112.40
2	G	190	ASP	CB-CG-OD1	-5.67	113.19	118.30
2	G	192	TYR	CD1-CE1-CZ	5.67	124.91	119.80
3	F	125	SER	N-CA-C	-5.67	95.70	111.00
2	C	121	VAL	N-CA-CB	-5.66	99.04	111.50
2	G	52	VAL	CB-CA-C	-5.66	100.65	111.40
2	A	89	GLN	O-C-N	5.66	131.75	122.70
3	B	218	ARG	N-CA-CB	-5.66	100.42	110.60
3	F	94	TYR	N-CA-C	5.66	126.27	111.00
3	B	130	ALA	N-CA-CB	5.65	118.01	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	N	22	THR	CB-CA-C	-5.65	96.34	111.60
3	H	62	ASP	CB-CG-OD1	5.64	123.38	118.30
2	C	185	LEU	CB-CG-CD2	-5.64	101.41	111.00
1	S	9	ARG	NE-CZ-NH1	-5.64	117.48	120.30
2	E	192	TYR	CG-CD1-CE1	5.64	125.81	121.30
3	F	42	GLY	N-CA-C	-5.62	99.05	113.10
4	N	81	GLY	CA-C-O	-5.62	110.48	120.60
3	F	27	TYR	CD1-CE1-CZ	5.62	124.86	119.80
1	P	37	LEU	CB-CG-CD2	5.62	120.55	111.00
2	G	168	SER	CB-CA-C	-5.62	99.43	110.10
2	A	204	HIS	CB-CA-C	-5.61	99.18	110.40
3	D	81	LEU	CB-CA-C	-5.61	99.54	110.20
3	H	96	CYS	N-CA-CB	-5.61	100.51	110.60
3	H	5	VAL	CB-CA-C	-5.60	100.75	111.40
2	A	127	SER	CB-CA-C	-5.60	99.46	110.10
3	B	73	GLU	OE1-CD-OE2	5.60	130.02	123.30
2	E	157	ASP	N-CA-CB	-5.60	100.52	110.60
4	L	42	THR	OG1-CB-CG2	-5.59	97.14	110.00
3	B	57	GLU	OE1-CD-OE2	5.59	130.01	123.30
3	D	104	TYR	CD1-CE1-CZ	5.59	124.83	119.80
2	G	102	LEU	N-CA-C	-5.59	95.91	111.00
2	E	53	LEU	CB-CA-C	-5.58	99.59	110.20
3	H	51	VAL	CA-CB-CG2	-5.58	102.53	110.90
2	C	141	PHE	CG-CD1-CE1	-5.57	114.67	120.80
2	C	149	ASP	OD1-CG-OD2	5.57	133.89	123.30
3	F	41	PRO	N-CA-C	-5.57	97.62	112.10
2	G	1	ASP	OD1-CG-OD2	-5.56	112.73	123.30
2	A	30	LEU	CB-CG-CD1	5.56	120.45	111.00
3	F	137	THR	N-CA-C	-5.55	96.00	111.00
3	F	32	PHE	O-C-N	-5.55	113.82	122.70
2	E	18	LYS	N-CA-C	-5.55	96.02	111.00
3	F	94	TYR	N-CA-CB	-5.54	100.62	110.60
3	B	89	GLU	CG-CD-OE1	-5.54	107.22	118.30
3	B	122	THR	CA-CB-CG2	-5.54	104.64	112.40
4	L	47	THR	CA-CB-CG2	-5.54	104.65	112.40
2	E	3	VAL	CA-CB-CG2	-5.54	102.59	110.90
2	A	52	VAL	CA-CB-CG1	-5.54	102.60	110.90
3	D	78	THR	CA-CB-OG1	5.53	120.61	109.00
2	E	145	PHE	CD1-CE1-CZ	5.52	126.72	120.10
3	F	64	PHE	N-CA-C	5.52	125.90	111.00
4	L	55	ALA	N-CA-CB	5.52	117.82	110.10
3	H	178	ASP	CA-C-O	5.52	131.68	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	192	TYR	CD1-CE1-CZ	-5.51	114.84	119.80
4	M	43	PHE	CB-CG-CD1	5.51	124.66	120.80
2	A	47	GLY	N-CA-C	5.51	126.88	113.10
3	F	126	VAL	N-CA-C	5.51	125.87	111.00
3	B	13	LYS	N-CA-CB	5.50	120.50	110.60
2	E	114	ARG	CA-C-N	-5.50	105.10	117.20
3	F	183	SER	N-CA-C	5.49	125.82	111.00
3	B	172	PRO	N-CD-CG	-5.48	94.97	103.20
3	D	142	THR	O-C-N	5.48	131.47	122.70
2	G	186	THR	CA-CB-CG2	-5.48	104.72	112.40
3	F	18	VAL	CB-CA-C	-5.48	100.99	111.40
1	S	44	LEU	CB-CA-C	5.47	120.60	110.20
3	F	150	TYR	CD1-CE1-CZ	-5.47	114.87	119.80
3	D	14	PRO	CA-C-O	-5.47	107.07	120.20
3	D	68	PHE	CB-CG-CD2	-5.47	116.97	120.80
4	M	27	LEU	CB-CG-CD2	5.46	120.29	111.00
4	O	34	ILE	N-CA-CB	-5.46	98.23	110.80
3	H	104	TYR	CG-CD2-CE2	-5.46	116.93	121.30
2	G	161	ARG	NE-CZ-NH1	5.46	123.03	120.30
3	B	121	THR	CA-CB-OG1	5.46	120.46	109.00
3	H	195	SER	N-CA-C	-5.45	96.29	111.00
3	H	81	LEU	CB-CG-CD2	-5.45	101.74	111.00
3	D	45	LEU	CB-CG-CD1	5.44	120.25	111.00
2	E	181	MET	CG-SD-CE	5.43	108.89	100.20
2	E	74	GLY	O-C-N	-5.43	114.02	122.70
2	C	156	ILE	CB-CA-C	-5.43	100.75	111.60
2	E	187	LEU	CB-CG-CD1	-5.43	101.78	111.00
3	B	168	VAL	CG1-CB-CG2	-5.42	102.22	110.90
2	A	84	VAL	CB-CA-C	-5.42	101.09	111.40
4	L	49	GLU	OE1-CD-OE2	-5.42	116.79	123.30
1	Q	7	PRO	CA-CB-CG	-5.42	93.70	104.00
2	A	174	SER	N-CA-C	5.42	125.62	111.00
2	G	129	GLU	N-CA-CB	-5.42	100.85	110.60
2	E	2	ILE	CG1-CB-CG2	-5.41	99.49	111.40
3	F	79	ALA	CA-C-O	-5.41	108.73	120.10
2	E	121	VAL	CG1-CB-CG2	-5.41	102.24	110.90
4	O	45	GLU	N-CA-CB	5.41	120.33	110.60
2	G	146	TYR	CG-CD2-CE2	5.41	125.62	121.30
3	D	218	ARG	CA-C-O	-5.40	108.75	120.10
3	B	37	VAL	O-C-N	-5.40	114.06	122.70
2	G	77	PHE	CB-CG-CD1	-5.40	117.02	120.80
3	B	39	GLN	CA-CB-CG	5.40	125.27	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	93	TYR	CD1-CG-CD2	-5.39	111.97	117.90
3	B	5	VAL	CG1-CB-CG2	-5.39	102.27	110.90
3	H	41	PRO	N-CD-CG	-5.39	95.12	103.20
2	E	80	THR	CA-C-O	5.38	131.39	120.10
3	B	129	LEU	CA-C-O	-5.37	108.81	120.10
3	D	4	LEU	CB-CG-CD1	-5.37	101.86	111.00
3	D	210	LYS	N-CA-C	-5.37	96.50	111.00
2	E	39	LEU	CB-CG-CD1	-5.37	101.87	111.00
2	E	201	GLU	CA-CB-CG	5.37	125.21	113.40
3	H	105	PHE	CB-CG-CD1	5.37	124.56	120.80
1	P	30	ILE	CG1-CB-CG2	5.36	123.20	111.40
2	C	137	SER	N-CA-CB	-5.36	102.45	110.50
2	E	29	LEU	CB-CG-CD1	-5.36	101.88	111.00
2	C	179	TYR	CG-CD2-CE2	-5.36	117.01	121.30
4	M	69	GLU	N-CA-CB	-5.36	100.95	110.60
2	A	182	SER	N-CA-C	5.36	125.46	111.00
3	B	27	TYR	CZ-CE2-CD2	-5.36	114.98	119.80
2	A	121	VAL	CG1-CB-CG2	5.35	119.47	110.90
3	D	20	ILE	O-C-N	5.35	131.27	122.70
3	B	60	TYR	O-C-N	-5.35	114.14	122.70
3	D	5	VAL	N-CA-C	-5.35	96.56	111.00
3	D	191	SER	O-C-N	5.35	131.26	122.70
2	E	56	TRP	CD1-NE1-CE2	-5.35	104.19	109.00
1	P	31	VAL	CA-CB-CG1	5.35	118.92	110.90
2	A	5	SER	N-CA-CB	-5.34	102.48	110.50
2	A	179	TYR	CD1-CE1-CZ	5.34	124.61	119.80
2	A	17	GLU	CG-CD-OE1	5.33	128.97	118.30
4	N	24	LYS	N-CA-C	-5.33	96.61	111.00
4	L	68	LEU	CB-CG-CD2	5.33	120.06	111.00
3	F	100	LEU	CB-CG-CD1	-5.33	101.94	111.00
3	B	73	GLU	CB-CG-CD	-5.32	99.83	114.20
3	H	56	GLY	O-C-N	-5.32	114.18	122.70
3	D	30	THR	N-CA-C	-5.32	96.63	111.00
2	A	55	TYR	CZ-CE2-CD2	5.32	124.58	119.80
1	S	9	ARG	NE-CZ-NH2	5.31	122.96	120.30
3	D	1	GLN	CA-CB-CG	5.31	125.08	113.40
2	E	104	PHE	CE1-CZ-CE2	-5.31	110.44	120.00
3	F	89	GLU	CG-CD-OE2	-5.31	107.68	118.30
2	G	187	LEU	CA-CB-CG	-5.31	103.09	115.30
1	Q	23	LYS	CD-CE-NZ	5.31	123.91	111.70
2	G	111	GLU	CG-CD-OE1	-5.31	107.68	118.30
3	D	105	PHE	CZ-CE2-CD2	-5.30	113.73	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	L	79	PHE	CG-CD2-CE2	5.30	126.63	120.80
3	F	150	TYR	CB-CA-C	-5.30	99.81	110.40
3	F	101	LEU	N-CA-CB	-5.29	99.81	110.40
2	E	191	GLU	CB-CA-C	-5.29	99.82	110.40
3	H	64	PHE	CG-CD1-CE1	-5.29	114.98	120.80
3	B	109	GLY	CA-C-O	5.29	130.11	120.60
3	H	196	GLU	CA-CB-CG	5.28	125.02	113.40
3	D	158	THR	OG1-CB-CG2	-5.27	97.88	110.00
3	F	51	VAL	CB-CA-C	-5.27	101.39	111.40
3	H	145	CYS	CA-CB-SG	5.27	123.48	114.00
3	F	148	LYS	CD-CE-NZ	-5.27	99.59	111.70
3	B	54	GLU	CB-CA-C	-5.26	99.87	110.40
2	A	124	PHE	CB-CG-CD1	-5.26	117.12	120.80
3	B	129	LEU	O-C-N	5.26	131.11	122.70
1	Q	28	GLY	N-CA-C	5.26	126.24	113.10
2	G	67	ARG	N-CA-C	5.26	125.20	111.00
3	D	59	THR	OG1-CB-CG2	-5.26	97.91	110.00
2	C	149	ASP	CB-CG-OD1	-5.25	113.57	118.30
3	B	182	LEU	CB-CA-C	-5.25	100.23	110.20
2	C	146	TYR	CD1-CE1-CZ	-5.25	115.08	119.80
3	D	99	PHE	CZ-CE2-CD2	-5.25	113.81	120.10
3	D	172	PRO	CB-CA-C	-5.25	98.89	112.00
3	D	211	VAL	CG1-CB-CG2	5.25	119.29	110.90
2	C	92	TYR	CB-CG-CD1	5.24	124.15	121.00
2	G	127	SER	N-CA-C	5.24	125.15	111.00
2	E	8	PRO	N-CA-CB	5.24	109.59	103.30
2	E	213	LYS	O-C-N	5.24	131.08	122.70
2	C	51	LYS	N-CA-CB	5.24	120.03	110.60
4	O	74	HIS	CB-CA-C	5.24	120.88	110.40
2	C	198	TYR	CB-CG-CD2	-5.23	117.86	121.00
3	H	175	LEU	CD1-CG-CD2	5.23	126.20	110.50
2	A	166	LEU	CA-CB-CG	5.23	127.32	115.30
3	B	81	LEU	CB-CG-CD2	5.23	119.89	111.00
2	C	93	TYR	CG-CD2-CE2	5.23	125.48	121.30
3	F	137	THR	OG1-CB-CG2	-5.23	97.98	110.00
3	B	181	THR	CB-CA-C	-5.22	97.49	111.60
2	E	77	PHE	CB-CG-CD1	-5.22	117.14	120.80
2	E	91	VAL	CG1-CB-CG2	5.22	119.26	110.90
3	F	83	ILE	CG1-CB-CG2	-5.22	99.92	111.40
2	E	38	TYR	CG-CD2-CE2	5.22	125.47	121.30
3	F	101	LEU	O-C-N	-5.22	114.35	122.70
2	G	104	PHE	N-CA-CB	5.22	119.99	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	174	VAL	N-CA-C	-5.21	96.93	111.00
3	B	112	THR	CA-CB-CG2	-5.21	105.11	112.40
3	H	98	ARG	N-CA-CB	-5.21	101.22	110.60
3	B	63	ASP	CB-CG-OD2	5.20	122.98	118.30
1	Q	31	VAL	CG1-CB-CG2	-5.20	102.57	110.90
4	L	21	VAL	CB-CA-C	-5.19	101.53	111.40
2	E	103	THR	N-CA-CB	-5.19	100.44	110.30
2	G	38	TYR	N-CA-CB	-5.19	101.25	110.60
3	B	150	TYR	CD1-CG-CD2	-5.19	112.19	117.90
3	H	118	SER	O-C-N	5.18	131.00	122.70
3	B	90	ASP	N-CA-C	-5.18	97.01	111.00
3	B	204	HIS	CB-CA-C	-5.18	100.03	110.40
2	A	21	MET	CG-SD-CE	5.18	108.48	100.20
4	M	25	VAL	CG1-CB-CG2	-5.18	102.62	110.90
2	A	77	PHE	CB-CG-CD1	5.17	124.42	120.80
2	A	129	GLU	CA-CB-CG	5.17	124.79	113.40
2	C	200	CYS	CB-CA-C	-5.17	100.05	110.40
2	C	124	PHE	CB-CG-CD1	-5.17	117.18	120.80
2	A	192	TYR	CG-CD1-CE1	5.17	125.44	121.30
3	F	105	PHE	CB-CG-CD2	-5.17	117.18	120.80
1	S	20	GLN	N-CA-C	5.17	124.96	111.00
3	D	82	GLN	O-C-N	5.17	130.97	122.70
4	M	39	PHE	CE1-CZ-CE2	5.17	129.31	120.00
1	S	42	PRO	N-CD-CG	5.17	110.95	103.20
2	A	131	LEU	CB-CG-CD1	-5.17	102.22	111.00
3	H	53	THR	N-CA-CB	-5.17	100.49	110.30
2	G	166	LEU	CB-CG-CD1	5.16	119.78	111.00
2	G	173	ASP	CB-CG-OD2	5.16	122.95	118.30
3	H	185	SER	N-CA-C	5.16	124.94	111.00
2	G	193	GLU	CA-C-N	-5.16	105.85	117.20
2	A	102	LEU	CB-CA-C	5.16	120.00	110.20
3	F	104	TYR	CG-CD2-CE2	5.15	125.42	121.30
2	E	7	SER	N-CA-CB	-5.15	102.78	110.50
2	E	102	LEU	CD1-CG-CD2	-5.15	95.05	110.50
3	F	98	ARG	N-CA-C	-5.15	97.09	111.00
3	H	89	GLU	CB-CG-CD	5.15	128.10	114.20
3	D	202	VAL	CG1-CB-CG2	5.14	119.13	110.90
3	B	213	LYS	CA-C-O	5.14	130.90	120.10
3	D	101	LEU	CB-CG-CD1	5.14	119.73	111.00
3	D	157	VAL	CB-CA-C	-5.14	101.64	111.40
2	G	76	ASP	CB-CG-OD2	5.13	122.92	118.30
3	H	180	TYR	CD1-CE1-CZ	5.13	124.42	119.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	177	SER	CB-CA-C	-5.13	100.35	110.10
3	B	39	GLN	CB-CA-C	-5.13	100.14	110.40
4	M	60	VAL	CB-CA-C	-5.13	101.66	111.40
4	N	22	THR	CA-CB-CG2	-5.13	105.22	112.40
2	C	137	SER	O-C-N	-5.12	114.50	122.70
2	A	57	ALA	CB-CA-C	5.12	117.79	110.10
3	B	148	LYS	CB-CA-C	-5.12	100.16	110.40
2	C	41	TRP	CE2-CD2-CG	5.12	111.40	107.30
4	O	25	VAL	CB-CA-C	-5.12	101.67	111.40
3	B	10	GLU	CG-CD-OE1	5.12	128.54	118.30
4	O	51	TYR	CZ-CE2-CD2	5.12	124.41	119.80
4	M	53	TYR	CG-CD2-CE2	5.12	125.39	121.30
3	F	29	PHE	CD1-CG-CD2	5.12	124.95	118.30
2	C	218	ASN	N-CA-CB	-5.12	101.39	110.60
4	N	69	GLU	N-CA-C	-5.12	97.18	111.00
3	H	68	PHE	CD1-CE1-CZ	-5.11	113.97	120.10
4	O	49	GLU	OE1-CD-OE2	-5.11	117.17	123.30
3	B	72	LEU	CB-CG-CD1	-5.11	102.31	111.00
2	C	18	LYS	CB-CA-C	5.11	120.62	110.40
3	H	79	ALA	C-N-CA	-5.10	108.95	121.70
4	N	68	LEU	N-CA-C	5.10	124.77	111.00
2	G	93	TYR	CB-CG-CD2	5.10	124.06	121.00
4	M	64	TRP	CD1-NE1-CE2	-5.10	104.41	109.00
2	G	122	SER	N-CA-CB	-5.10	102.85	110.50
3	B	120	LYS	N-CA-C	5.09	124.75	111.00
2	C	80	THR	N-CA-C	5.09	124.75	111.00
3	F	114	VAL	CG1-CB-CG2	-5.09	102.76	110.90
2	C	188	THR	CA-CB-CG2	-5.09	105.28	112.40
3	F	154	PRO	O-C-N	5.09	130.84	122.70
2	A	181	MET	CA-C-O	-5.09	109.42	120.10
1	Q	42	PRO	CA-C-N	-5.09	106.01	117.20
1	Q	43	ARG	CA-C-N	-5.09	106.01	117.20
2	E	112	LEU	CB-CG-CD2	5.09	119.65	111.00
2	E	189	LYS	CA-C-N	-5.09	106.01	117.20
3	F	180	TYR	CG-CD1-CE1	-5.09	117.23	121.30
2	G	198	TYR	CD1-CG-CD2	5.09	123.50	117.90
2	A	55	TYR	CG-CD1-CE1	5.08	125.37	121.30
1	S	23	LYS	N-CA-C	5.08	124.72	111.00
2	E	11	LEU	CB-CA-C	-5.08	100.55	110.20
3	H	79	ALA	CB-CA-C	-5.08	102.48	110.10
2	A	155	LYS	CA-CB-CG	5.08	124.57	113.40
3	D	63	ASP	CB-CG-OD1	-5.08	113.73	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	66	ASP	N-CA-C	-5.08	97.29	111.00
3	D	169	HIS	N-CA-CB	-5.07	101.47	110.60
3	D	172	PRO	N-CD-CG	-5.07	95.59	103.20
3	B	117	SER	CB-CA-C	-5.07	100.46	110.10
3	D	95	PHE	CB-CG-CD2	-5.07	117.25	120.80
3	H	180	TYR	CZ-CE2-CD2	-5.07	115.24	119.80
2	A	4	MET	CG-SD-CE	5.07	108.31	100.20
3	B	125	SER	N-CA-C	-5.06	97.33	111.00
1	S	17	ARG	NH1-CZ-NH2	-5.06	113.83	119.40
3	B	172	PRO	CA-N-CD	-5.06	104.42	111.50
3	F	99	PHE	CB-CG-CD1	-5.05	117.26	120.80
3	H	92	ALA	N-CA-CB	-5.05	103.03	110.10
3	B	159	TRP	NE1-CE2-CZ2	-5.05	124.84	130.40
2	A	103	THR	CA-CB-CG2	-5.05	105.33	112.40
4	M	37	ALA	O-C-N	5.05	130.77	122.70
4	O	55	ALA	N-CA-CB	-5.04	103.04	110.10
3	D	98	ARG	N-CA-CB	-5.04	101.53	110.60
3	B	18	VAL	CG1-CB-CG2	5.04	118.96	110.90
2	C	118	ALA	N-CA-CB	5.04	117.16	110.10
3	F	34	MET	CB-CA-C	-5.04	100.33	110.40
2	G	110	LEU	CA-CB-CG	5.04	126.89	115.30
2	E	189	LYS	CD-CE-NZ	5.03	123.28	111.70
3	B	98	ARG	NH1-CZ-NH2	5.03	124.94	119.40
3	F	141	VAL	CG1-CB-CG2	-5.03	102.85	110.90
2	E	102	LEU	N-CA-C	-5.03	97.43	111.00
3	H	9	PRO	CB-CG-CD	-5.03	86.90	106.50
3	D	154	PRO	CA-CB-CG	-5.02	94.46	104.00
3	H	127	TYR	CG-CD2-CE2	5.02	125.31	121.30
1	P	28	GLY	CA-C-O	-5.01	111.57	120.60
3	B	120	LYS	CD-CE-NZ	-5.01	100.17	111.70
2	G	67	ARG	NE-CZ-NH2	-5.01	117.79	120.30
3	D	11	LEU	CB-CG-CD1	-5.01	102.48	111.00
2	E	189	LYS	O-C-N	5.01	130.72	122.70
2	E	86	ALA	O-C-N	5.01	130.72	122.70
3	F	113	THR	CA-CB-CG2	5.01	119.41	112.40
2	G	116	ASP	CB-CG-OD2	-5.01	113.79	118.30
2	E	63	GLY	O-C-N	5.01	130.71	122.70
2	C	124	PHE	CZ-CE2-CD2	-5.01	114.09	120.10
2	E	160	GLU	CG-CD-OE2	-5.01	108.29	118.30
3	B	9	PRO	N-CD-CG	-5.00	95.69	103.20
2	A	192	TYR	CB-CG-CD1	-5.00	118.00	121.00
3	D	200	CYS	CA-CB-SG	5.00	123.00	114.00

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	179	TYR	Sidechain
3	D	127	TYR	Sidechain
2	E	179	TYR	Sidechain
2	E	28	SER	Mainchain
2	E	55	TYR	Sidechain
3	F	102	ARG	Mainchain
2	G	146	TYR	Sidechain
2	G	98	TYR	Sidechain
3	H	94	TYR	Sidechain
4	L	53	TYR	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	P	167	0	162	39	0
1	Q	346	0	366	101	2
1	S	346	0	366	95	1
2	A	1708	0	1656	371	0
2	C	1708	0	1657	364	2
2	E	1708	0	1658	359	0
2	G	1701	0	1652	435	0
3	B	1660	0	1614	332	0
3	D	1660	0	1614	351	0
3	F	1660	0	1614	290	0
3	H	1660	0	1614	431	0
4	L	507	0	482	91	0
4	M	480	0	457	95	0
4	N	490	0	461	110	0
4	O	480	0	457	127	1
5	A	29	0	0	0	0
5	B	31	0	0	0	0
5	C	13	0	0	0	0
5	D	10	0	0	2	0
5	E	17	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	F	34	0	0	5	0
5	G	11	0	0	4	0
5	H	9	0	0	4	0
5	L	9	0	0	1	0
5	M	3	0	0	1	0
5	N	7	0	0	0	0
5	O	3	0	0	0	0
5	P	1	0	0	1	0
5	Q	6	0	0	1	0
5	S	3	0	0	0	0
All	All	16467	0	15830	3384	3

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 105.

All (3384) 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:Q:22:VAL:CB	1:Q:22:VAL:CA	1.75	1.65
1:S:3:THR:CG2	1:S:3:THR:CB	1.74	1.65
2:C:189:LYS:CA	2:C:189:LYS:CB	1.75	1.64
2:E:153:LYS:CG	2:E:153:LYS:CB	1.75	1.63
2:G:156:ILE:CB	2:G:156:ILE:CG2	1.77	1.63
1:S:7:PRO:CB	1:S:7:PRO:CG	1.76	1.63
1:Q:11:THR:CB	1:Q:11:THR:CA	1.75	1.63
2:E:71:ARG:CG	2:E:71:ARG:CB	1.74	1.63
3:F:101:LEU:CD2	3:F:101:LEU:CG	1.76	1.63
2:G:112:LEU:CD2	2:G:112:LEU:CG	1.77	1.63
3:B:98:ARG:CD	3:B:98:ARG:CG	1.76	1.63
4:L:33:LYS:CD	4:L:33:LYS:CG	1.76	1.62
4:O:33:LYS:CD	4:O:33:LYS:CG	1.77	1.62
2:G:153:LYS:CG	2:G:153:LYS:CD	1.74	1.62
2:C:56:TRP:CG	2:C:56:TRP:CB	1.81	1.62
3:D:197:THR:CA	3:D:197:THR:CB	1.78	1.62
2:C:161:ARG:CG	2:C:161:ARG:CD	1.77	1.62
2:A:118:ALA:CA	2:A:118:ALA:CB	1.76	1.61
3:H:99:PHE:CB	3:H:99:PHE:CA	1.76	1.61
1:Q:31:VAL:CB	1:Q:31:VAL:CA	1.78	1.61
3:H:188:VAL:CG2	3:H:188:VAL:CB	1.74	1.61
2:A:205:LYS:CG	2:A:205:LYS:CB	1.79	1.61
2:C:18:LYS:CG	2:C:18:LYS:CD	1.79	1.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:193:GLU:CG	2:G:193:GLU:CB	1.75	1.61
2:E:89:GLN:CB	2:E:89:GLN:CG	1.75	1.61
1:S:7:PRO:CD	1:S:7:PRO:CG	1.78	1.61
1:Q:23:LYS:CE	1:Q:23:LYS:CD	1.74	1.61
2:C:67:ARG:CG	2:C:67:ARG:CD	1.75	1.60
3:D:23:LYS:CB	3:D:23:LYS:CG	1.78	1.60
3:F:74:THR:CB	3:F:74:THR:CG2	1.80	1.60
2:E:41:TRP:CG	2:E:41:TRP:CB	1.77	1.60
3:D:210:LYS:CD	3:D:210:LYS:CE	1.77	1.60
2:G:109:LYS:CD	2:G:109:LYS:CG	1.77	1.60
4:O:58:ALA:CB	4:O:58:ALA:CA	1.78	1.59
3:B:126:VAL:CG2	3:B:126:VAL:CB	1.75	1.59
3:F:19:LYS:CG	3:F:19:LYS:CD	1.74	1.59
3:H:55:THR:CB	3:H:55:THR:CA	1.76	1.59
2:A:150:ILE:CG1	2:A:150:ILE:CD1	1.75	1.59
3:B:197:THR:CB	3:B:197:THR:CG2	1.75	1.59
3:F:100:LEU:CG	3:F:100:LEU:CD2	1.75	1.59
3:H:19:LYS:CG	3:H:19:LYS:CB	1.76	1.59
3:F:1:GLN:CG	3:F:1:GLN:CB	1.76	1.59
4:L:28:ILE:CB	4:L:28:ILE:CG2	1.76	1.59
2:C:30:LEU:CD1	2:C:30:LEU:CG	1.75	1.59
2:G:102:LEU:CG	2:G:102:LEU:CD1	1.78	1.59
4:M:28:ILE:CG1	4:M:28:ILE:CD1	1.78	1.59
4:N:28:ILE:CB	4:N:28:ILE:CG2	1.74	1.59
2:C:165:VAL:CG1	2:C:165:VAL:CB	1.77	1.58
2:A:33:ARG:CA	2:A:33:ARG:CB	1.77	1.58
3:H:175:LEU:CD1	3:H:175:LEU:CG	1.75	1.58
3:D:170:THR:CB	3:D:170:THR:CG2	1.82	1.58
4:L:55:ALA:CB	4:L:55:ALA:CA	1.76	1.58
4:O:59:LYS:CB	4:O:59:LYS:CG	1.79	1.58
2:G:54:ILE:CD1	2:G:54:ILE:CG1	1.81	1.57
1:Q:12:LYS:CE	1:Q:12:LYS:CD	1.74	1.57
3:B:113:THR:CG2	3:B:113:THR:CB	1.78	1.57
2:E:12:ALA:CB	2:E:12:ALA:CA	1.77	1.57
2:G:201:GLU:CB	2:G:201:GLU:CG	1.76	1.57
2:E:95:LYS:CE	2:E:95:LYS:CD	1.76	1.57
2:E:24:LYS:CD	2:E:24:LYS:CE	1.74	1.57
3:D:81:LEU:CD1	3:D:81:LEU:CG	1.79	1.57
2:G:205:LYS:CD	2:G:205:LYS:CE	1.78	1.57
2:G:166:LEU:CD1	2:G:166:LEU:CG	1.83	1.56
3:H:216:VAL:CA	3:H:216:VAL:CB	1.80	1.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:65:THR:CG2	4:N:65:THR:CB	1.80	1.56
3:F:120:LYS:CD	3:F:120:LYS:CE	1.76	1.56
2:C:108:THR:CG2	2:C:108:THR:CB	1.84	1.56
2:G:71:ARG:CD	2:G:71:ARG:CG	1.75	1.56
3:H:198:VAL:CB	3:H:198:VAL:CG2	1.79	1.56
4:O:52:ARG:CG	4:O:52:ARG:CB	1.78	1.56
2:G:175:LYS:CD	2:G:175:LYS:CG	1.75	1.56
2:C:51:LYS:NZ	2:C:51:LYS:CE	1.69	1.56
3:F:156:THR:CB	3:F:156:THR:CA	1.79	1.56
2:A:89:GLN:CB	2:A:89:GLN:CG	1.82	1.56
3:D:102:ARG:CD	3:D:102:ARG:CG	1.83	1.55
1:Q:23:LYS:CG	1:Q:23:LYS:CD	1.80	1.55
2:G:21:MET:CB	2:G:21:MET:CG	1.83	1.55
3:H:175:LEU:CG	3:H:175:LEU:CD2	1.83	1.55
1:P:30:ILE:CD1	1:P:30:ILE:CG1	1.84	1.55
3:H:164:LEU:CG	3:H:164:LEU:CD2	1.78	1.55
3:B:179:LEU:CD1	3:B:179:LEU:CG	1.76	1.55
2:C:129:GLU:CG	2:C:129:GLU:CB	1.77	1.55
3:H:86:LEU:CG	3:H:86:LEU:CD1	1.77	1.55
2:A:96:GLN:CG	2:A:96:GLN:CB	1.74	1.55
2:G:36:LYS:CG	2:G:36:LYS:CD	1.79	1.54
3:B:210:LYS:CG	3:B:210:LYS:CD	1.82	1.54
2:C:206:THR:CB	2:C:206:THR:CG2	1.76	1.54
2:G:67:ARG:CG	2:G:67:ARG:CD	1.82	1.54
4:N:33:LYS:CD	4:N:33:LYS:CE	1.74	1.54
4:O:26:ASN:HD22	4:O:76:ASN:ND2	1.04	1.54
3:D:197:THR:CB	3:D:197:THR:CG2	1.84	1.54
2:A:199:THR:CB	2:A:199:THR:CG2	1.81	1.54
4:L:34:ILE:CG1	4:L:34:ILE:CD1	1.85	1.54
3:B:119:ALA:CB	3:B:119:ALA:CA	1.82	1.53
1:Q:10:LYS:NZ	1:Q:10:LYS:CE	1.70	1.53
2:C:187:LEU:CG	2:C:187:LEU:CD1	1.80	1.53
3:B:2:ILE:CD1	3:B:2:ILE:CG1	1.85	1.53
3:D:124:PRO:CG	3:D:124:PRO:CD	1.76	1.53
4:M:24:LYS:CG	4:M:24:LYS:CB	1.82	1.52
1:S:37:LEU:CG	1:S:37:LEU:CD2	1.84	1.52
2:E:11:LEU:CD1	2:E:11:LEU:CG	1.77	1.52
3:F:131:PRO:CG	3:F:131:PRO:CD	1.77	1.52
2:E:194:ARG:CD	2:E:194:ARG:CG	1.82	1.52
3:D:41:PRO:CG	3:D:41:PRO:CD	1.77	1.52
3:H:9:PRO:CG	3:H:9:PRO:CD	1.83	1.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:175:LEU:CG	3:D:175:LEU:CD2	1.80	1.51
3:F:102:ARG:CG	3:F:102:ARG:CD	1.88	1.51
1:S:23:LYS:CE	1:S:23:LYS:NZ	1.73	1.51
4:N:68:LEU:CA	4:N:68:LEU:C	1.79	1.51
2:A:1:ASP:CB	2:A:1:ASP:CG	1.78	1.51
2:A:191:GLU:CA	2:A:191:GLU:N	1.69	1.50
3:B:218:ARG:C	3:B:218:ARG:CA	1.78	1.50
2:A:76:ASP:CG	2:A:76:ASP:CB	1.79	1.50
2:G:1:ASP:CG	2:G:1:ASP:CB	1.74	1.50
3:H:59:THR:CB	3:H:59:THR:CG2	1.85	1.50
4:O:73:ASN:C	4:O:73:ASN:CA	1.79	1.50
2:A:162:GLN:CG	2:A:162:GLN:CD	1.75	1.50
3:F:214:LYS:NZ	3:F:214:LYS:CE	1.75	1.50
2:A:211:ILE:CD1	2:A:211:ILE:CG1	1.86	1.49
3:H:172:PRO:CD	3:H:172:PRO:CG	1.83	1.49
3:D:103:GLN:CG	3:D:103:GLN:CD	1.77	1.49
2:E:155:LYS:NZ	2:E:155:LYS:CE	1.73	1.49
3:D:210:LYS:NZ	3:D:210:LYS:CE	1.69	1.49
2:G:213:LYS:NZ	2:G:213:LYS:CE	1.74	1.49
2:C:148:LYS:CD	2:C:148:LYS:CG	1.90	1.48
1:S:36:LEU:CD2	1:S:36:LEU:CG	1.90	1.48
3:F:120:LYS:CD	3:F:120:LYS:CG	1.88	1.48
2:A:36:LYS:NZ	2:A:36:LYS:CE	1.73	1.47
2:C:113:LYS:CE	2:C:113:LYS:NZ	1.74	1.47
4:N:33:LYS:CE	4:N:33:LYS:NZ	1.75	1.46
4:N:73:ASN:CB	4:N:73:ASN:CG	1.82	1.46
4:M:65:THR:CG2	4:M:65:THR:CB	1.92	1.46
3:F:48:MET:SD	3:F:48:MET:CG	2.02	1.45
3:H:89:GLU:CD	3:H:89:GLU:CG	1.83	1.44
1:S:31:VAL:CB	1:S:31:VAL:CG1	1.95	1.44
3:F:140:MET:CE	3:F:140:MET:SD	2.08	1.42
2:E:28:SER:OG	2:E:28:SER:CB	1.67	1.42
3:F:189:PRO:CG	3:F:189:PRO:CB	1.85	1.39
2:G:36:LYS:CE	2:G:36:LYS:NZ	1.87	1.37
4:O:26:ASN:ND2	4:O:76:ASN:HD21	1.19	1.36
2:E:31:ASN:ND2	2:E:34:THR:H	1.22	1.33
3:D:140:MET:SD	3:D:140:MET:CE	2.19	1.31
3:B:140:MET:SD	3:B:140:MET:CE	2.20	1.28
3:H:133:SER:CA	3:H:218:ARG:HD3	1.63	1.26
4:N:54:ALA:O	4:N:58:ALA:HB2	1.31	1.23
1:Q:9:ARG:CZ	1:Q:9:ARG:HB2	1.71	1.21

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:157:ASP:HA	2:A:197:SER:OG	1.37	1.19
3:H:160:ASN:HB2	3:H:163:SER:HB2	1.22	1.18
3:D:138:ASN:ND2	3:D:139:SER:H	1.40	1.17
3:B:129:LEU:HB2	3:B:144:GLY:HA3	1.27	1.17
2:A:19:VAL:O	2:A:80:THR:HG23	1.45	1.16
3:H:133:SER:HA	3:H:218:ARG:CD	1.75	1.16
4:N:55:ALA:O	4:N:58:ALA:HB3	1.44	1.14
3:F:211:VAL:HG22	3:F:212:ASP:N	1.60	1.14
2:A:3:VAL:HG22	2:A:26:SER:HB2	1.26	1.14
2:G:98:TYR:CE2	2:G:99:ILE:HD12	1.83	1.14
1:Q:33:GLY:HA2	1:Q:36:LEU:HB3	1.29	1.13
2:G:98:TYR:CE2	2:G:99:ILE:CD1	2.31	1.12
4:M:75:MET:HE3	4:M:77:ILE:HD11	1.28	1.12
3:B:17:THR:HG23	3:B:83:ILE:O	1.48	1.12
3:H:164:LEU:HD13	3:H:186:VAL:HG21	1.30	1.12
3:F:211:VAL:CG2	3:F:212:ASP:H	1.62	1.12
3:B:87:LYS:O	3:B:90:ASP:HB2	1.50	1.11
2:C:65:PRO:O	2:C:67:ARG:N	1.84	1.10
3:D:118:SER:O	3:D:119:ALA:O	1.71	1.09
4:N:68:LEU:HD12	4:N:68:LEU:H	0.93	1.09
2:G:182:SER:HB3	3:H:171:PHE:CE2	1.87	1.08
3:F:198:VAL:O	3:F:198:VAL:HG12	1.53	1.08
4:M:34:ILE:HG23	4:M:34:ILE:O	1.49	1.08
3:F:109:GLY:O	3:F:111:GLY:N	1.86	1.07
3:F:100:LEU:HD23	3:F:101:LEU:H	1.13	1.07
2:A:194:ARG:HG2	2:A:195:HIS:N	1.62	1.06
2:G:30:LEU:HA	2:G:38:TYR:CE1	1.89	1.06
3:B:209:THR:HG22	3:B:210:LYS:H	1.20	1.06
4:N:68:LEU:HD12	4:N:68:LEU:N	1.69	1.06
2:C:152:VAL:HG22	2:C:202:ALA:HA	1.33	1.05
2:G:121:VAL:HG12	2:G:213:LYS:HG3	1.36	1.05
2:E:31:ASN:ND2	2:E:34:THR:N	2.05	1.04
1:Q:44:LEU:HD13	1:Q:45:GLY:H	1.15	1.04
4:L:57:HIS:HB3	4:L:61:ASN:HD21	1.23	1.04
2:C:43:GLN:NE2	2:C:45:LYS:HZ2	1.55	1.04
3:B:6:GLN:NE2	3:B:111:GLY:H	1.56	1.04
4:M:25:VAL:HG22	4:M:26:ASN:H	1.20	1.04
3:H:148:LYS:HB2	3:H:181:THR:HB	1.41	1.03
2:E:153:LYS:HE3	2:E:160:GLU:CD	1.79	1.03
3:B:120:LYS:CD	3:B:120:LYS:H	1.72	1.02
2:A:166:LEU:HD11	3:B:176:GLN:HE22	1.24	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:68:LEU:CD1	4:N:68:LEU:H	1.72	1.02
1:S:13:ARG:HB2	1:S:13:ARG:NH1	1.74	1.02
3:H:182:LEU:HD12	3:H:183:SER:N	1.75	1.02
2:C:43:GLN:HE22	2:C:45:LYS:NZ	1.56	1.01
2:G:30:LEU:HA	2:G:38:TYR:HE1	1.20	1.01
3:B:143:LEU:HB3	3:B:215:ILE:HD12	1.40	1.01
1:S:13:ARG:C	2:G:62:SER:HB2	1.81	1.01
2:G:98:TYR:CZ	2:G:99:ILE:HD11	1.96	1.01
2:E:130:GLN:HE22	2:E:137:SER:N	1.57	1.01
2:A:176:ASP:OD2	2:A:178:THR:HG23	1.58	1.01
1:Q:9:ARG:HH11	1:Q:9:ARG:HG2	1.22	1.01
3:H:34:MET:O	3:H:51:VAL:HG22	1.60	1.01
2:C:191:GLU:OE2	2:C:195:HIS:NE2	1.94	1.00
2:E:39:LEU:O	2:E:39:LEU:HD13	1.62	1.00
3:F:40:ALA:HB1	3:F:41:PRO:HD2	1.43	1.00
3:D:20:ILE:HG22	3:D:112:THR:HG21	1.44	1.00
2:C:7:SER:HA	2:C:8:PRO:O	1.60	1.00
2:E:31:ASN:HD22	2:E:34:THR:H	1.06	1.00
2:E:19:VAL:HG12	2:E:81:ILE:O	1.62	1.00
3:F:11:LEU:HD13	3:F:11:LEU:O	1.59	1.00
3:D:182:LEU:HG	3:D:182:LEU:O	1.61	0.99
3:H:38:ASN:N	3:H:48:MET:HG3	1.77	0.99
3:B:129:LEU:HB2	3:B:144:GLY:CA	1.93	0.98
4:N:68:LEU:HD21	4:O:51:TYR:OH	1.63	0.98
2:G:145:PHE:CE2	2:G:180:SER:HA	1.98	0.98
3:B:175:LEU:HB2	3:B:180:TYR:CE1	1.98	0.98
3:H:189:PRO:HD2	3:H:192:THR:OG1	1.63	0.97
2:G:53:LEU:HB2	2:G:54:ILE:HD13	1.46	0.97
3:B:120:LYS:HD3	3:B:120:LYS:H	1.27	0.97
3:F:211:VAL:CG2	3:F:212:ASP:N	2.20	0.97
3:B:36:TRP:CZ2	3:B:81:LEU:HB2	1.98	0.97
3:B:144:GLY:O	3:B:145:CYS:HB2	1.62	0.97
2:G:113:LYS:HG2	2:G:146:TYR:OH	1.64	0.97
2:E:132:THR:O	2:E:133:SER:HB3	1.60	0.96
2:E:18:LYS:HA	2:E:82:SER:HA	1.48	0.96
2:C:217:ARG:HG2	2:C:218:ASN:HD21	1.29	0.96
2:C:65:PRO:C	2:C:67:ARG:H	1.65	0.96
3:D:18:VAL:HG11	3:D:114:VAL:HG21	1.45	0.96
2:A:8:PRO:HB3	4:L:39:PHE:CE2	2.00	0.96
4:O:75:MET:HG2	4:O:75:MET:O	1.63	0.96
4:M:25:VAL:HA	4:M:75:MET:HB3	1.45	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:53:LEU:CB	2:G:54:ILE:HD13	1.96	0.96
3:B:138:ASN:CG	3:B:139:SER:H	1.68	0.96
2:G:12:ALA:HB3	4:O:36:THR:HB	1.47	0.96
2:G:146:TYR:CD2	2:G:147:PRO:HA	2.00	0.95
3:H:151:PHE:CD1	3:H:151:PHE:O	2.19	0.95
1:Q:16:ASN:ND2	1:Q:17:ARG:HG3	1.81	0.95
2:A:130:GLN:HB2	3:B:127:TYR:CD1	2.00	0.95
2:A:141:PHE:CE2	3:B:185:SER:HB3	1.99	0.95
3:B:65:LYS:HA	3:B:65:LYS:NZ	1.81	0.95
2:A:28:SER:O	2:A:29:LEU:HD23	1.66	0.95
2:C:14:SER:HA	2:C:113:LYS:HB2	1.48	0.95
2:C:204:HIS:ND1	2:C:206:THR:HG23	1.81	0.95
2:C:95:LYS:NZ	3:D:104:TYR:HA	1.81	0.95
2:C:182:SER:HB2	3:D:171:PHE:CE2	2.02	0.95
2:E:188:THR:HG23	2:E:191:GLU:HB2	1.48	0.95
3:H:35:HIS:O	3:H:96:CYS:HA	1.66	0.95
4:O:27:LEU:HB2	4:O:35:GLN:HB2	1.47	0.94
2:G:167:ASN:H	2:G:167:ASN:ND2	1.60	0.94
3:H:155:VAL:HG12	3:H:156:THR:N	1.79	0.94
4:N:54:ALA:O	4:N:58:ALA:CB	2.15	0.94
3:B:38:ASN:OD1	3:B:39:GLN:N	1.99	0.94
2:G:137:SER:OG	2:G:186:THR:HA	1.68	0.94
2:A:130:GLN:HB2	3:B:127:TYR:CE1	2.01	0.94
3:H:45:LEU:HD22	3:H:45:LEU:H	1.31	0.94
3:H:106:ASP:OD2	3:H:107:VAL:N	2.00	0.94
4:L:23:ILE:O	4:L:23:ILE:HG22	1.68	0.93
2:C:71:ARG:HB2	2:C:78:THR:OG1	1.69	0.93
2:G:199:THR:HG22	2:G:214:SER:HA	1.51	0.93
3:H:61:ALA:C	3:H:63:ASP:H	1.69	0.93
4:M:49:GLU:HA	4:M:52:ARG:HB3	1.49	0.93
3:F:109:GLY:O	3:F:110:ALA:C	2.03	0.93
3:D:152:PRO:C	3:D:154:PRO:HD2	1.89	0.93
3:D:31:ASP:O	3:D:32:PHE:CD2	2.21	0.93
3:B:182:LEU:HD23	3:B:182:LEU:C	1.89	0.93
3:H:106:ASP:CG	3:H:107:VAL:H	1.72	0.92
3:B:193:TRP:CD1	3:B:194:PRO:HA	2.04	0.92
4:M:21:VAL:O	4:M:41:GLY:HA2	1.69	0.92
2:A:156:ILE:HG22	2:A:195:HIS:CD2	2.02	0.92
3:H:60:TYR:OH	3:H:69:ALA:HA	1.66	0.92
3:F:63:ASP:O	3:F:64:PHE:CD2	2.22	0.92
2:G:167:ASN:HB3	2:G:183:SER:HB2	1.48	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:150:ILE:HD13	2:G:151:ASN:H	1.34	0.92
4:O:55:ALA:O	4:O:57:HIS:N	2.03	0.92
2:G:39:LEU:HD13	2:G:40:ALA:H	1.32	0.91
2:A:37:ASN:HD21	2:A:74:GLY:H	1.18	0.91
4:N:31:ASP:OD2	4:N:33:LYS:HG2	1.69	0.91
2:A:186:THR:C	2:A:187:LEU:HD23	1.91	0.91
2:E:189:LYS:O	2:E:193:GLU:HG3	1.71	0.91
3:D:20:ILE:HG12	3:D:81:LEU:O	1.71	0.91
2:G:172:GLN:HG2	2:G:179:TYR:CE2	2.06	0.91
3:D:81:LEU:C	3:D:81:LEU:HD23	1.90	0.91
2:G:145:PHE:HE2	2:G:180:SER:HA	1.30	0.91
2:G:152:VAL:HG13	2:G:201:GLU:O	1.71	0.91
2:A:198:TYR:HB2	2:A:215:PHE:CD2	2.06	0.90
4:N:56:LEU:HD12	4:N:56:LEU:O	1.70	0.90
2:A:157:ASP:HA	2:A:197:SER:HG	1.36	0.90
2:E:150:ILE:HD13	2:E:151:ASN:N	1.86	0.90
2:G:204:HIS:CG	2:G:205:LYS:H	1.86	0.90
3:H:160:ASN:CB	3:H:163:SER:HB2	2.01	0.90
3:B:6:GLN:HE21	3:B:109:GLY:HA3	1.35	0.90
2:C:155:LYS:CD	2:C:158:GLY:O	2.19	0.90
3:D:112:THR:O	3:D:113:THR:C	2.08	0.90
3:F:211:VAL:HG22	3:F:212:ASP:H	1.24	0.90
2:E:44:GLN:HG3	2:E:50:PRO:HG3	1.51	0.90
4:N:68:LEU:CD1	4:N:68:LEU:N	2.33	0.90
3:B:126:VAL:CG2	3:B:126:VAL:CG1	2.50	0.90
2:E:95:LYS:HD3	2:E:104:PHE:CZ	2.05	0.90
3:F:165:SER:O	3:F:168:VAL:HG23	1.72	0.90
2:G:30:LEU:HD12	2:G:36:LYS:H	1.33	0.90
2:A:82:SER:O	2:A:83:SER:C	2.09	0.90
3:D:193:TRP:CG	3:D:194:PRO:HA	2.05	0.90
3:F:196:GLU:O	3:F:197:THR:HG23	1.71	0.90
3:H:207:SER:C	3:H:209:THR:H	1.67	0.90
3:D:198:VAL:O	3:D:215:ILE:HD12	1.72	0.90
3:D:1:GLN:OE1	1:Q:13:ARG:HD2	1.70	0.90
3:H:151:PHE:CD1	3:H:151:PHE:C	2.36	0.89
3:B:160:ASN:HB2	3:B:163:SER:HB3	1.54	0.89
4:L:54:ALA:C	4:L:56:LEU:H	1.73	0.89
2:E:34:THR:HG22	2:E:36:LYS:HB2	1.52	0.89
2:E:128:SER:O	2:E:130:GLN:N	2.05	0.89
3:F:82:GLN:HG2	3:F:84:ASN:OD1	1.72	0.89
3:B:128:PRO:C	3:B:129:LEU:HD12	1.93	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:19:VAL:CG1	2:G:81:ILE:HB	2.03	0.89
2:G:130:GLN:O	2:G:133:SER:HB3	1.73	0.89
2:G:146:TYR:CG	2:G:147:PRO:HA	2.08	0.89
3:D:178:ASP:OD2	5:D:224:HOH:O	1.91	0.89
1:S:39:ARG:O	1:S:40:ARG:HB3	1.72	0.89
2:C:81:ILE:HG21	2:C:84:VAL:HG12	1.55	0.88
2:C:95:LYS:HD2	2:C:102:LEU:HD23	1.54	0.88
2:C:167:ASN:ND2	2:C:183:SER:OG	2.06	0.88
3:F:40:ALA:HB1	3:F:41:PRO:CD	2.03	0.88
2:G:122:SER:HA	2:G:213:LYS:HE3	1.55	0.88
1:P:40:ARG:HE	3:F:98:ARG:HH12	1.18	0.88
2:G:152:VAL:HG12	2:G:153:LYS:N	1.87	0.88
1:S:13:ARG:HB2	1:S:13:ARG:HH11	1.36	0.88
2:G:155:LYS:HE2	2:G:201:GLU:OE1	1.74	0.88
2:G:168:SER:OG	3:H:172:PRO:HD2	1.74	0.88
3:B:19:LYS:HE2	3:B:80:TYR:HD1	1.38	0.88
3:F:148:LYS:HA	3:F:181:THR:HG23	1.55	0.88
2:E:153:LYS:HE3	2:E:160:GLU:OE2	1.74	0.88
4:N:43:PHE:O	4:N:46:ALA:N	2.06	0.88
3:D:158:THR:OG1	3:D:201:ASN:ND2	2.06	0.88
3:F:27:TYR:CE1	3:F:98:ARG:HD3	2.09	0.88
4:O:34:ILE:C	4:O:35:GLN:HG2	1.92	0.88
3:F:171:PHE:HD1	3:F:171:PHE:H	1.20	0.87
2:A:37:ASN:ND2	2:A:74:GLY:H	1.71	0.87
2:C:65:PRO:C	2:C:67:ARG:N	2.21	0.87
4:M:34:ILE:CG2	4:M:34:ILE:O	2.21	0.87
2:A:88:ASP:O	2:A:90:ALA:N	2.08	0.87
2:E:128:SER:O	2:E:129:GLU:C	2.11	0.87
2:E:1:ASP:C	2:E:2:ILE:HD12	1.95	0.87
2:E:49:SER:O	2:E:50:PRO:O	1.92	0.87
2:E:16:GLY:O	2:E:83:SER:HA	1.74	0.87
2:E:60:ARG:CZ	2:E:66:ASP:HA	2.04	0.87
3:B:31:ASP:O	3:B:32:PHE:CG	2.27	0.87
2:E:7:SER:HA	2:E:8:PRO:O	1.75	0.87
4:O:26:ASN:ND2	4:O:76:ASN:ND2	1.89	0.87
4:M:48:ALA:O	4:M:52:ARG:HB2	1.75	0.86
2:G:56:TRP:O	2:G:57:ALA:HB3	1.75	0.86
4:O:27:LEU:O	4:O:34:ILE:HA	1.75	0.86
2:A:45:LYS:HB3	2:A:46:PRO:HD2	1.57	0.86
3:H:188:VAL:HB	3:H:189:PRO:CD	2.06	0.86
2:E:102:LEU:C	2:E:103:THR:HG23	1.95	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:52:ASN:CG	3:B:55:THR:HB	1.95	0.86
2:G:196:ASN:HD22	2:G:217:ARG:N	1.73	0.86
3:H:152:PRO:O	3:H:154:PRO:HD2	1.75	0.86
2:C:82:SER:O	2:C:83:SER:HB3	1.76	0.86
3:D:138:ASN:ND2	3:D:139:SER:N	2.24	0.86
3:H:168:VAL:HG12	3:H:169:HIS:N	1.91	0.86
3:D:140:MET:HA	3:D:190:SER:OG	1.74	0.86
2:G:137:SER:HG	2:G:186:THR:HA	1.40	0.86
2:G:27:GLN:O	2:G:28:SER:O	1.93	0.86
2:G:2:ILE:O	2:G:4:MET:N	2.08	0.86
1:P:24:PHE:HB3	1:P:25:PRO:HD2	1.58	0.86
3:D:198:VAL:H	3:D:214:LYS:HE2	1.41	0.85
2:G:3:VAL:HB	2:G:26:SER:HB3	1.56	0.85
1:Q:12:LYS:O	1:Q:13:ARG:HG2	1.76	0.85
3:B:209:THR:HG22	3:B:210:LYS:N	1.92	0.85
2:A:176:ASP:CG	2:A:178:THR:HG23	1.95	0.85
3:B:37:VAL:HG21	3:B:108:TRP:HZ3	1.42	0.85
3:B:48:MET:HA	3:B:64:PHE:CE1	2.11	0.85
2:C:152:VAL:CG2	2:C:202:ALA:HA	2.05	0.85
3:F:100:LEU:HD23	3:F:101:LEU:N	1.90	0.85
2:A:194:ARG:HG2	2:A:195:HIS:H	1.39	0.85
3:H:36:TRP:HA	3:H:95:PHE:O	1.74	0.85
2:A:184:THR:O	2:A:186:THR:HG23	1.74	0.85
2:A:12:ALA:HB3	4:L:36:THR:HB	1.58	0.85
4:N:77:ILE:HG22	4:N:79:PHE:CE1	2.11	0.85
3:B:48:MET:HA	3:B:64:PHE:CD1	2.11	0.85
3:F:7:SER:HB3	3:F:20:ILE:HG13	1.57	0.85
3:B:100:LEU:HD11	3:B:106:ASP:OD1	1.77	0.84
3:D:188:VAL:HB	3:D:189:PRO:CD	2.07	0.84
3:F:189:PRO:O	3:F:192:THR:N	2.10	0.84
3:D:142:THR:HA	3:D:187:THR:HA	1.59	0.84
1:S:22:VAL:O	1:S:22:VAL:HG12	1.77	0.84
2:A:10:SER:O	2:A:11:LEU:HG	1.77	0.84
2:E:188:THR:HG23	2:E:191:GLU:CB	2.08	0.84
4:M:43:PHE:O	4:M:45:GLU:N	2.10	0.84
4:N:66:ALA:HB3	4:O:68:LEU:HD23	1.57	0.84
2:G:84:VAL:HA	2:G:88:ASP:OD1	1.76	0.84
1:S:23:LYS:O	1:S:24:PHE:HD1	1.58	0.84
2:E:60:ARG:HD3	2:E:64:VAL:O	1.77	0.84
1:S:39:ARG:O	1:S:40:ARG:CB	2.24	0.84
2:C:2:ILE:HD13	2:C:96:GLN:OE1	1.78	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:112:LEU:CB	2:G:112:LEU:CD2	2.56	0.84
3:D:215:ILE:HD12	3:D:215:ILE:H	1.43	0.84
3:H:168:VAL:CG1	3:H:169:HIS:N	2.41	0.84
2:A:121:VAL:HA	2:A:141:PHE:O	1.78	0.83
3:H:13:LYS:HA	3:H:117:SER:O	1.77	0.83
4:N:22:THR:HG22	4:N:23:ILE:N	1.93	0.83
2:A:156:ILE:HG22	2:A:195:HIS:HD2	1.40	0.83
2:A:193:GLU:O	2:A:217:ARG:NH2	2.11	0.83
3:D:160:ASN:HD21	3:D:198:VAL:HA	1.42	0.83
2:C:176:ASP:HB2	2:C:178:THR:OG1	1.79	0.83
2:E:16:GLY:C	2:E:83:SER:HA	1.98	0.83
2:E:176:ASP:O	2:E:177:SER:OG	1.96	0.83
1:S:16:ASN:HD22	1:S:16:ASN:N	1.74	0.83
3:F:157:VAL:O	3:F:157:VAL:HG12	1.77	0.83
2:G:199:THR:HA	2:G:213:LYS:O	1.79	0.83
2:G:199:THR:HG22	2:G:214:SER:CA	2.09	0.83
2:A:130:GLN:O	2:A:131:LEU:C	2.15	0.83
2:G:56:TRP:HB2	2:G:59:THR:OG1	1.79	0.83
3:H:198:VAL:CG1	3:H:198:VAL:CG2	2.56	0.83
2:G:98:TYR:CG	2:G:99:ILE:HG13	2.13	0.83
3:H:207:SER:C	3:H:209:THR:N	2.27	0.83
3:F:182:LEU:HD23	3:F:183:SER:N	1.93	0.83
2:C:142:LEU:HD11	2:C:152:VAL:HG21	1.60	0.82
2:G:196:ASN:ND2	2:G:216:ASN:HB3	1.94	0.82
4:M:25:VAL:HG22	4:M:26:ASN:N	1.91	0.82
1:S:30:ILE:HD11	1:S:35:TYR:O	1.78	0.82
2:A:102:LEU:HD12	3:B:47:TRP:NE1	1.94	0.82
2:G:121:VAL:HG12	2:G:213:LYS:CG	2.09	0.82
2:G:155:LYS:HG2	2:G:160:GLU:HB2	1.59	0.82
3:B:35:HIS:O	3:B:96:CYS:HA	1.80	0.82
3:H:156:THR:OG1	3:H:203:ALA:HB3	1.79	0.82
2:A:112:LEU:HD23	2:A:113:LYS:N	1.95	0.82
3:H:12:LYS:HE2	3:H:12:LYS:HA	1.60	0.82
3:H:129:LEU:HD21	3:H:146:LEU:HB2	1.61	0.82
3:H:182:LEU:HD12	3:H:182:LEU:C	1.99	0.82
4:M:79:PHE:N	4:M:79:PHE:CD1	2.48	0.82
3:D:78:THR:HG22	3:D:79:ALA:N	1.94	0.82
3:H:61:ALA:O	3:H:63:ASP:N	2.12	0.82
2:C:155:LYS:HD2	2:C:158:GLY:O	1.80	0.82
3:D:188:VAL:HB	3:D:189:PRO:HD2	1.61	0.82
2:G:131:LEU:O	2:G:133:SER:N	2.13	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:36:LYS:CG	2:G:36:LYS:CE	2.58	0.82
2:C:130:GLN:NE2	2:C:137:SER:OG	2.13	0.82
3:F:143:LEU:HB2	3:F:186:VAL:HG13	1.62	0.82
2:G:127:SER:C	2:G:129:GLU:N	2.31	0.82
4:M:65:THR:O	4:M:66:ALA:HB2	1.80	0.82
4:O:64:TRP:CE3	4:O:66:ALA:HB2	2.15	0.82
3:H:179:LEU:HG	3:H:180:TYR:H	1.44	0.81
2:E:101:PRO:O	2:E:103:THR:HG23	1.79	0.81
4:N:35:GLN:O	4:N:36:THR:OG1	1.97	0.81
3:H:61:ALA:C	3:H:63:ASP:N	2.31	0.81
3:F:31:ASP:O	3:F:32:PHE:CG	2.33	0.81
4:M:26:ASN:N	4:M:75:MET:O	2.14	0.81
1:Q:9:ARG:NH1	1:Q:9:ARG:HG2	1.96	0.81
2:A:65:PRO:O	2:A:67:ARG:N	2.13	0.81
3:B:209:THR:O	3:B:210:LYS:HB2	1.80	0.81
2:G:52:VAL:HG13	2:G:52:VAL:O	1.74	0.81
4:N:68:LEU:O	4:N:69:GLU:O	1.98	0.81
2:A:144:ASN:OD1	3:B:169:HIS:NE2	2.14	0.81
3:D:48:MET:CE	3:D:81:LEU:HD11	2.11	0.81
2:E:31:ASN:HB3	2:E:34:THR:HB	1.62	0.81
2:G:6:GLN:OE1	2:G:107:GLY:HA2	1.81	0.81
2:C:43:GLN:HE22	2:C:45:LYS:HZ2	0.82	0.81
3:D:3:GLN:O	3:D:4:LEU:HD23	1.80	0.81
3:H:199:THR:HG22	3:H:214:LYS:HA	1.61	0.81
3:H:38:ASN:H	3:H:48:MET:HG3	1.40	0.81
2:G:29:LEU:CD2	2:G:29:LEU:O	2.29	0.81
2:A:151:ASN:O	2:A:152:VAL:HG23	1.80	0.81
2:C:126:PRO:HG3	2:C:137:SER:O	1.80	0.81
3:F:54:GLU:OE2	3:F:55:THR:N	2.14	0.81
3:H:133:SER:HA	3:H:218:ARG:HD3	0.83	0.80
1:S:7:PRO:CA	1:S:7:PRO:CG	2.59	0.80
3:B:75:SER:C	3:B:77:SER:H	1.85	0.80
3:D:112:THR:O	3:D:114:VAL:N	2.14	0.80
3:D:3:GLN:HG2	3:D:4:LEU:H	1.46	0.80
2:A:166:LEU:HD11	3:B:176:GLN:NE2	1.96	0.80
3:D:180:TYR:O	3:D:181:THR:HG23	1.81	0.80
3:H:207:SER:O	3:H:209:THR:N	2.14	0.80
3:D:210:LYS:C	3:D:211:VAL:HG12	2.02	0.80
3:D:149:GLY:H	3:D:181:THR:HG22	1.47	0.80
3:F:129:LEU:HD12	3:F:145:CYS:N	1.96	0.80
3:F:60:TYR:OH	3:F:69:ALA:HA	1.81	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:9:ARG:CG	1:Q:9:ARG:HH11	1.95	0.80
2:A:199:THR:HA	2:A:214:SER:HA	1.63	0.80
2:A:89:GLN:OE1	2:A:172:GLN:NE2	2.14	0.80
4:N:22:THR:HG22	4:N:23:ILE:H	1.45	0.80
4:O:34:ILE:O	4:O:35:GLN:HG2	1.82	0.80
1:Q:7:PRO:HB2	1:Q:9:ARG:HH21	1.44	0.80
1:P:30:ILE:HD11	5:P:167:HOH:O	1.83	0.79
3:D:64:PHE:HB3	3:D:68:PHE:CD2	2.17	0.79
3:H:151:PHE:HB3	3:H:152:PRO:HD3	1.64	0.79
3:H:198:VAL:O	3:H:198:VAL:HG12	1.82	0.79
1:Q:30:ILE:O	1:Q:30:ILE:HG13	1.82	0.79
3:B:214:LYS:HE2	3:B:216:VAL:HG22	1.63	0.79
2:C:130:GLN:HB2	3:D:127:TYR:CD1	2.16	0.79
2:E:137:SER:HB3	2:E:186:THR:HG23	1.64	0.79
1:S:14:ASN:N	2:G:62:SER:HB2	1.97	0.79
3:H:72:LEU:HD21	3:H:74:THR:OG1	1.83	0.79
2:C:11:LEU:HD23	4:M:37:ALA:HB2	1.63	0.79
2:C:152:VAL:HG13	2:C:201:GLU:C	2.03	0.79
2:C:37:ASN:O	2:C:56:TRP:CA	2.31	0.79
2:C:71:ARG:O	2:C:78:THR:N	2.14	0.79
4:N:62:GLY:HA3	4:N:80:ALA:H	1.47	0.79
2:E:39:LEU:C	2:E:39:LEU:HD13	2.03	0.79
3:F:161:SER:H	3:F:201:ASN:HD21	1.29	0.79
2:A:55:TYR:O	2:A:57:ALA:N	2.16	0.79
3:F:52:ASN:HD22	3:F:57:GLU:HB2	1.48	0.79
3:H:50:TRP:HE1	3:H:59:THR:HB	1.48	0.79
3:D:53:THR:HG22	3:D:72:LEU:HD21	1.62	0.79
3:D:60:TYR:HE1	3:D:70:PHE:CD1	2.00	0.79
2:G:127:SER:O	2:G:129:GLU:N	2.14	0.79
3:H:164:LEU:CB	3:H:164:LEU:CD2	2.60	0.79
1:Q:5:PRO:O	1:Q:6:LYS:HG3	1.81	0.79
2:C:31:ASN:HB2	2:C:98:TYR:CE1	2.17	0.78
3:F:7:SER:CB	3:F:21:SER:H	1.96	0.78
2:C:33:ARG:O	2:C:34:THR:HG23	1.82	0.78
2:G:150:ILE:HD13	2:G:151:ASN:N	1.98	0.78
3:H:175:LEU:HD12	3:H:175:LEU:O	1.82	0.78
1:Q:40:ARG:NH1	1:Q:40:ARG:HB3	1.98	0.78
2:A:139:VAL:HG22	2:A:184:THR:HG23	1.66	0.78
2:C:19:VAL:CG1	2:C:81:ILE:HB	2.14	0.78
2:C:62:SER:CA	1:Q:11:THR:O	2.31	0.78
3:D:156:THR:HG23	3:D:203:ALA:HB3	1.63	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:52:ASN:O	3:D:54:GLU:N	2.17	0.78
2:E:156:ILE:HA	2:E:197:SER:O	1.82	0.78
3:F:211:VAL:HG23	3:F:212:ASP:H	1.48	0.78
2:A:215:PHE:CG	2:A:215:PHE:O	2.35	0.78
3:F:146:LEU:HG	3:F:146:LEU:O	1.83	0.78
2:G:29:LEU:HD11	2:G:39:LEU:HD23	1.64	0.78
2:G:54:ILE:HG22	2:G:60:ARG:HA	1.62	0.78
3:H:129:LEU:HD12	3:H:144:GLY:HA3	1.64	0.78
4:M:42:THR:HB	4:M:45:GLU:HB2	1.66	0.78
2:C:31:ASN:ND2	1:Q:33:GLY:O	2.17	0.78
2:C:29:LEU:HD12	2:C:77:PHE:CZ	2.19	0.78
3:D:189:PRO:HB2	3:D:192:THR:HG23	1.65	0.78
3:F:63:ASP:O	3:F:64:PHE:HD2	1.67	0.78
2:G:127:SER:O	2:G:128:SER:C	2.19	0.78
4:O:55:ALA:C	4:O:57:HIS:H	1.86	0.78
2:C:1:ASP:N	2:C:27:GLN:NE2	2.31	0.78
4:O:58:ALA:O	4:O:60:VAL:N	2.15	0.78
1:Q:36:LEU:HD23	1:Q:36:LEU:O	1.84	0.78
2:A:89:GLN:NE2	2:A:172:GLN:HB3	1.99	0.78
2:C:157:ASP:HB2	2:C:196:ASN:H	1.49	0.78
3:H:68:PHE:CE1	3:H:83:ILE:HD12	2.18	0.78
3:D:17:THR:HG22	3:D:84:ASN:HA	1.65	0.78
2:C:121:VAL:HG12	2:C:122:SER:H	1.49	0.78
2:C:88:ASP:O	2:C:92:TYR:OH	2.01	0.78
2:E:156:ILE:N	2:E:159:SER:O	2.15	0.78
2:E:36:LYS:HE2	2:E:37:ASN:H	1.49	0.78
3:H:11:LEU:HD11	3:H:151:PHE:HE2	1.48	0.78
2:A:95:LYS:HB3	2:A:95:LYS:HZ2	1.48	0.77
2:G:130:GLN:HB2	3:H:127:TYR:CD2	2.18	0.77
1:S:23:LYS:O	1:S:24:PHE:CD1	2.38	0.77
3:B:157:VAL:HA	3:B:201:ASN:O	1.83	0.77
2:G:201:GLU:HG2	2:G:212:VAL:HG11	1.65	0.77
2:G:130:GLN:HB2	3:H:127:TYR:CE2	2.20	0.77
2:C:39:LEU:HD22	2:C:40:ALA:N	2.00	0.77
2:G:29:LEU:HD13	2:G:77:PHE:CZ	2.20	0.77
3:H:4:LEU:HD23	3:H:24:ALA:HA	1.65	0.77
2:C:7:SER:CA	2:C:8:PRO:O	2.31	0.77
3:D:177:SER:O	3:D:177:SER:OG	1.95	0.77
1:Q:30:ILE:HD11	1:Q:36:LEU:HB2	1.66	0.77
2:A:31:ASN:HD22	2:A:31:ASN:C	1.85	0.77
2:C:157:ASP:OD2	2:C:196:ASN:HB2	1.85	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:36:TRP:HA	3:D:95:PHE:O	1.85	0.77
3:F:198:VAL:O	3:F:198:VAL:CG1	2.25	0.77
3:B:141:VAL:HG12	3:B:188:VAL:O	1.85	0.77
2:E:130:GLN:NE2	2:E:137:SER:N	2.31	0.77
2:G:8:PRO:HB3	4:O:39:PHE:CE2	2.20	0.77
2:A:156:ILE:CG2	2:A:195:HIS:HD2	1.97	0.77
3:H:11:LEU:HD11	3:H:151:PHE:CE2	2.19	0.77
4:O:64:TRP:HE3	4:O:66:ALA:HB2	1.49	0.76
1:Q:9:ARG:CG	1:Q:9:ARG:NH1	2.46	0.76
2:A:168:SER:OG	3:B:172:PRO:HD2	1.85	0.76
2:E:215:PHE:C	2:E:215:PHE:CD1	2.59	0.76
2:G:131:LEU:C	2:G:133:SER:H	1.88	0.76
1:S:7:PRO:N	1:S:7:PRO:CG	2.48	0.76
2:A:105:GLY:C	2:A:107:GLY:H	1.86	0.76
3:B:11:LEU:HD13	3:B:11:LEU:C	2.05	0.76
3:H:155:VAL:HG12	3:H:156:THR:H	1.50	0.76
2:A:31:ASN:HD22	2:A:32:SER:N	1.84	0.76
2:A:43:GLN:HB3	2:A:53:LEU:HD21	1.67	0.76
3:D:160:ASN:ND2	3:D:198:VAL:HA	2.01	0.76
2:E:12:ALA:HB3	2:E:113:LYS:HZ3	1.50	0.76
2:G:201:GLU:HG2	2:G:212:VAL:CG1	2.15	0.76
4:L:77:ILE:HD12	4:L:77:ILE:H	1.51	0.76
1:P:24:PHE:HB3	1:P:25:PRO:CD	2.16	0.76
3:F:7:SER:HB3	3:F:21:SER:H	1.49	0.76
4:N:46:ALA:C	4:N:48:ALA:H	1.88	0.76
2:A:112:LEU:HD23	2:A:113:LYS:H	1.49	0.76
2:A:126:PRO:HG2	2:A:136:ALA:HB1	1.68	0.76
2:A:198:TYR:HB2	2:A:215:PHE:O	1.86	0.76
3:B:193:TRP:CG	3:B:194:PRO:HA	2.20	0.76
2:C:43:GLN:NE2	2:C:45:LYS:NZ	2.25	0.76
3:H:50:TRP:NE1	3:H:59:THR:HB	2.01	0.76
2:G:98:TYR:CE2	2:G:99:ILE:HD11	2.12	0.76
4:N:68:LEU:C	4:N:68:LEU:CB	2.54	0.76
2:C:100:PRO:HB3	1:Q:31:VAL:HG11	1.66	0.76
2:A:105:GLY:O	2:A:107:GLY:N	2.18	0.76
2:G:68:PHE:CE1	2:G:81:ILE:HG23	2.21	0.76
1:S:29:GLN:NE2	3:H:52:ASN:HA	2.01	0.76
2:G:17:GLU:O	2:G:82:SER:O	2.04	0.76
3:H:38:ASN:H	3:H:48:MET:CG	1.99	0.76
1:S:29:GLN:HE21	3:H:53:THR:N	1.84	0.76
2:A:58:SER:HA	2:A:70:GLY:O	1.86	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:175:LEU:HD13	3:F:180:TYR:CE1	2.21	0.76
3:H:175:LEU:CD1	3:H:175:LEU:HG	2.12	0.76
4:L:55:ALA:CB	4:L:55:ALA:HA	2.11	0.76
2:A:151:ASN:OD1	2:A:152:VAL:N	2.17	0.75
2:E:185:LEU:HD12	2:E:186:THR:N	2.01	0.75
3:F:67:ARG:CB	3:F:67:ARG:HH11	1.98	0.75
3:H:51:VAL:O	3:H:52:ASN:HB2	1.84	0.75
1:S:35:TYR:O	1:S:36:LEU:HB2	1.85	0.75
3:B:40:ALA:HB3	3:B:43:LYS:HB2	1.69	0.75
2:C:173:ASP:OD1	2:C:175:LYS:HB2	1.87	0.75
3:D:30:THR:HG23	3:D:31:ASP:OD1	1.85	0.75
2:G:172:GLN:HG2	2:G:179:TYR:CZ	2.22	0.75
3:H:6:GLN:NE2	3:H:111:GLY:HA2	2.01	0.75
1:Q:40:ARG:CZ	1:Q:40:ARG:HB3	2.16	0.75
2:C:217:ARG:HG2	2:C:218:ASN:ND2	2.01	0.75
3:F:100:LEU:CD1	3:F:100:LEU:CD2	2.62	0.75
2:E:12:ALA:CB	2:E:12:ALA:C	2.52	0.75
2:G:39:LEU:CD1	2:G:40:ALA:H	1.99	0.75
3:B:52:ASN:O	3:B:54:GLU:N	2.18	0.75
3:D:31:ASP:O	3:D:32:PHE:CG	2.40	0.75
3:F:192:THR:HB	3:F:196:GLU:OE2	1.87	0.75
3:F:75:SER:OG	3:F:76:ALA:N	2.19	0.75
1:P:40:ARG:HE	3:F:98:ARG:NH1	1.83	0.75
2:A:125:PRO:HD2	3:B:218:ARG:HH21	1.52	0.75
3:B:91:THR:HG23	3:B:115:THR:HA	1.68	0.75
2:C:97:ALA:HB3	3:D:103:GLN:HB3	1.69	0.75
3:D:151:PHE:HB3	3:D:152:PRO:HD3	1.67	0.75
3:D:37:VAL:HG22	3:D:47:TRP:HA	1.69	0.75
2:C:188:THR:O	2:C:189:LYS:C	2.24	0.75
3:F:161:SER:H	3:F:201:ASN:ND2	1.83	0.75
1:S:30:ILE:CG2	3:H:101:LEU:HB3	2.16	0.75
1:P:36:LEU:O	1:P:37:LEU:HB3	1.86	0.75
2:A:198:TYR:CB	2:A:215:PHE:CD2	2.70	0.75
3:D:19:LYS:HG3	3:D:82:GLN:HG3	1.68	0.75
2:G:40:ALA:O	2:G:94:CYS:HA	1.87	0.75
4:O:32:GLY:O	4:O:33:LYS:HG3	1.87	0.75
3:B:19:LYS:HE2	3:B:80:TYR:CD1	2.22	0.74
2:C:23:CYS:HB2	2:C:41:TRP:CH2	2.22	0.74
3:D:108:TRP:CD1	3:D:108:TRP:N	2.54	0.74
3:H:87:LYS:HE3	5:H:227:HOH:O	1.87	0.74
4:M:42:THR:HB	4:M:45:GLU:CB	2.17	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:8:PRO:HB2	4:O:38:GLU:O	1.86	0.74
3:H:155:VAL:CG1	3:H:156:THR:N	2.47	0.74
3:H:189:PRO:O	3:H:192:THR:OG1	2.05	0.74
3:D:99:PHE:CZ	3:D:103:GLN:HA	2.22	0.74
2:G:30:LEU:HD12	2:G:36:LYS:N	2.01	0.74
3:D:193:TRP:CD1	3:D:194:PRO:HA	2.23	0.74
3:D:93:THR:O	3:D:94:TYR:HB2	1.85	0.74
3:B:6:GLN:NE2	3:B:111:GLY:N	2.33	0.74
2:C:37:ASN:ND2	2:C:74:GLY:H	1.85	0.74
2:E:55:TYR:CD1	3:F:104:TYR:CE2	2.75	0.74
2:G:167:ASN:HA	2:G:183:SER:HA	1.69	0.74
4:O:53:TYR:O	4:O:56:LEU:HB3	1.86	0.74
2:G:204:HIS:CG	2:G:205:LYS:N	2.55	0.74
3:H:67:ARG:HG3	3:H:68:PHE:CE2	2.22	0.74
2:C:45:LYS:O	2:C:48:GLN:HB2	1.87	0.74
2:E:55:TYR:O	2:E:57:ALA:N	2.21	0.74
3:F:190:SER:O	3:F:192:THR:N	2.21	0.74
2:G:6:GLN:CD	2:G:107:GLY:HA2	2.08	0.74
2:C:95:LYS:HZ1	3:D:104:TYR:HA	1.49	0.74
2:E:201:GLU:HG2	2:E:212:VAL:CG2	2.17	0.74
3:F:38:ASN:C	3:F:38:ASN:OD1	2.22	0.74
2:G:124:PHE:HE1	2:G:141:PHE:CD2	2.06	0.74
2:C:152:VAL:HG13	2:C:201:GLU:O	1.87	0.74
2:E:114:ARG:HG3	2:E:115:ALA:O	1.87	0.74
2:G:167:ASN:H	2:G:167:ASN:HD22	1.34	0.74
4:L:28:ILE:CA	4:L:28:ILE:CG2	2.66	0.74
3:F:109:GLY:C	3:F:111:GLY:H	1.90	0.74
2:C:185:LEU:HG	2:C:185:LEU:O	1.88	0.73
2:G:148:LYS:HB3	2:G:179:TYR:CD1	2.23	0.73
1:S:31:VAL:HA	3:H:99:PHE:HE1	1.53	0.73
3:D:152:PRO:O	3:D:154:PRO:CD	2.37	0.73
3:D:154:PRO:CG	3:D:205:PRO:HG2	2.18	0.73
4:N:68:LEU:CD2	4:O:51:TYR:OH	2.36	0.73
2:A:6:GLN:HE21	2:A:105:GLY:C	1.91	0.73
3:B:73:GLU:C	3:B:73:GLU:OE1	2.26	0.73
2:A:96:GLN:HG3	2:A:103:THR:OG1	1.88	0.73
2:C:38:TYR:CE2	2:C:56:TRP:NE1	2.55	0.73
2:C:46:PRO:HD3	2:C:90:ALA:HA	1.70	0.73
2:E:132:THR:O	2:E:133:SER:CB	2.27	0.73
3:H:121:THR:HG23	3:H:152:PRO:HG2	1.68	0.73
2:C:206:THR:CA	2:C:206:THR:CG2	2.67	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:20:ILE:HD11	3:D:81:LEU:HB3	1.69	0.73
3:F:58:PRO:O	3:F:58:PRO:HG2	1.86	0.73
2:G:202:ALA:O	2:G:210:PRO:HB3	1.89	0.73
2:A:118:ALA:N	2:A:206:THR:HG21	2.03	0.73
2:A:3:VAL:HG13	2:A:26:SER:OG	1.88	0.73
2:G:30:LEU:CD1	2:G:36:LYS:N	2.51	0.73
3:D:175:LEU:HD13	3:D:180:TYR:CE1	2.23	0.73
3:D:91:THR:HG22	3:D:91:THR:O	1.87	0.73
3:H:186:VAL:C	3:H:187:THR:HG22	2.09	0.73
4:N:47:THR:HG23	4:N:47:THR:O	1.87	0.73
2:C:105:GLY:O	2:C:106:ALA:O	2.07	0.73
3:B:204:HIS:O	3:B:205:PRO:C	2.24	0.73
2:C:39:LEU:HD22	2:C:40:ALA:H	1.52	0.73
3:D:78:THR:CG2	3:D:79:ALA:N	2.52	0.73
2:E:150:ILE:HD13	2:E:151:ASN:H	1.52	0.73
3:H:175:LEU:CD1	3:H:175:LEU:CB	2.67	0.73
3:D:20:ILE:CG1	3:D:81:LEU:O	2.36	0.72
3:B:204:HIS:O	3:B:206:ALA:N	2.22	0.72
3:D:138:ASN:CG	3:D:139:SER:H	1.88	0.72
2:G:102:LEU:CD2	2:G:102:LEU:CD1	2.65	0.72
2:G:29:LEU:O	2:G:29:LEU:HD22	1.89	0.72
3:H:188:VAL:CG2	3:H:188:VAL:CG1	2.67	0.72
2:C:123:ILE:HD12	2:C:139:VAL:O	1.89	0.72
2:C:8:PRO:HG2	2:C:108:THR:CG2	2.20	0.72
3:D:154:PRO:HG2	3:D:205:PRO:HG2	1.69	0.72
2:E:172:GLN:HE21	2:E:177:SER:HB2	1.52	0.72
2:E:27:GLN:O	2:E:28:SER:O	2.07	0.72
3:F:100:LEU:HG	3:F:100:LEU:CD2	2.14	0.72
2:G:152:VAL:CG1	2:G:153:LYS:N	2.52	0.72
2:G:52:VAL:HG22	2:G:53:LEU:N	2.04	0.72
2:A:12:ALA:O	2:A:113:LYS:HG3	1.90	0.72
3:F:52:ASN:HB3	3:F:55:THR:OG1	1.89	0.72
3:H:122:THR:O	3:H:150:TYR:HA	1.89	0.72
3:H:160:ASN:O	3:H:163:SER:N	2.22	0.72
4:L:67:ASP:OD1	4:L:76:ASN:HB2	1.87	0.72
4:O:25:VAL:O	4:O:25:VAL:HG13	1.89	0.72
1:S:18:ARG:HB3	1:S:19:PRO:HD3	1.70	0.72
1:P:36:LEU:CD2	3:B:102:ARG:HH22	2.01	0.72
1:P:36:LEU:HD21	3:B:102:ARG:HH22	1.55	0.72
3:B:73:GLU:O	3:B:75:SER:N	2.23	0.72
3:D:81:LEU:HD23	3:D:82:GLN:N	2.03	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:78:LYS:HE3	5:L:83:HOH:O	1.89	0.72
2:G:98:TYR:CD2	2:G:99:ILE:HG13	2.24	0.72
3:H:133:SER:O	3:H:218:ARG:NH1	2.21	0.72
2:A:112:LEU:CB	2:A:172:GLN:HE22	2.02	0.72
3:D:138:ASN:HD22	3:D:139:SER:H	1.34	0.72
2:C:217:ARG:C	2:C:218:ASN:CG	2.46	0.72
2:E:18:LYS:HG2	2:E:19:VAL:N	2.04	0.72
2:G:167:ASN:HB3	2:G:183:SER:CB	2.20	0.72
2:G:200:CYS:HB3	2:G:213:LYS:HB2	1.70	0.72
3:H:88:ASN:O	3:H:90:ASP:N	2.22	0.72
4:N:49:GLU:OE1	4:N:49:GLU:O	2.08	0.72
4:N:79:PHE:CD1	4:N:79:PHE:N	2.54	0.72
3:B:6:GLN:HE22	3:B:111:GLY:H	1.36	0.72
3:F:61:ALA:O	3:F:65:LYS:HG3	1.90	0.72
3:H:152:PRO:C	3:H:154:PRO:HD2	2.08	0.72
4:N:21:VAL:HG13	4:N:22:THR:N	2.04	0.72
2:A:130:GLN:C	2:A:132:THR:N	2.37	0.71
2:A:216:ASN:O	2:A:218:ASN:N	2.22	0.71
2:A:33:ARG:C	2:A:33:ARG:CB	2.57	0.71
3:B:65:LYS:HZ2	3:B:65:LYS:HA	1.53	0.71
2:C:36:LYS:HD3	2:C:56:TRP:CE3	2.25	0.71
2:C:30:LEU:HG	2:C:37:ASN:HD21	1.55	0.71
2:E:153:LYS:HG3	2:E:160:GLU:OE1	1.89	0.71
2:E:191:GLU:OE2	2:E:194:ARG:NH1	2.23	0.71
3:F:159:TRP:CZ2	3:F:186:VAL:HG12	2.24	0.71
3:H:152:PRO:O	3:H:154:PRO:CD	2.37	0.71
1:Q:31:VAL:CG1	1:Q:31:VAL:CA	2.67	0.71
3:B:86:LEU:HB3	3:B:116:VAL:HG21	1.71	0.71
3:D:84:ASN:O	3:D:85:SER:C	2.23	0.71
2:E:130:GLN:NE2	2:E:136:ALA:HA	2.05	0.71
3:F:190:SER:C	3:F:192:THR:H	1.93	0.71
2:G:201:GLU:HA	2:G:212:VAL:HG12	1.71	0.71
3:H:152:PRO:C	3:H:154:PRO:CD	2.59	0.71
4:M:27:LEU:O	4:M:34:ILE:HD13	1.90	0.71
2:A:43:GLN:NE2	2:A:92:TYR:OH	2.19	0.71
2:C:32:SER:O	2:C:34:THR:N	2.22	0.71
2:C:71:ARG:N	2:C:78:THR:O	2.23	0.71
2:G:102:LEU:HD23	3:H:105:PHE:CZ	2.26	0.71
2:G:176:ASP:O	2:G:178:THR:HG23	1.90	0.71
3:H:70:PHE:HE2	3:H:81:LEU:HD23	1.55	0.71
4:M:28:ILE:O	4:M:78:LYS:HA	1.88	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:21:VAL:HG13	4:N:22:THR:H	1.54	0.71
3:H:70:PHE:CE2	3:H:81:LEU:HD23	2.26	0.71
3:B:18:VAL:HG22	3:B:19:LYS:N	2.04	0.71
2:C:37:ASN:ND2	2:C:74:GLY:N	2.38	0.71
2:G:19:VAL:HG13	2:G:81:ILE:HB	1.73	0.71
2:A:130:GLN:O	2:A:132:THR:N	2.23	0.71
2:A:151:ASN:CG	2:A:152:VAL:H	1.93	0.71
2:C:146:TYR:CG	2:C:147:PRO:HA	2.26	0.71
2:C:155:LYS:HD2	2:C:158:GLY:C	2.10	0.71
3:D:159:TRP:HZ3	3:D:215:ILE:HD11	1.54	0.71
2:E:214:SER:OG	2:E:215:PHE:N	2.23	0.71
3:H:106:ASP:CG	3:H:107:VAL:N	2.43	0.71
4:M:43:PHE:C	4:M:45:GLU:H	1.92	0.71
3:D:72:LEU:O	3:D:74:THR:N	2.21	0.71
2:E:95:LYS:HB2	2:E:104:PHE:CD2	2.26	0.71
2:E:7:SER:HB2	2:E:8:PRO:HA	1.70	0.71
2:E:45:LYS:HG2	2:E:90:ALA:HB2	1.73	0.71
2:G:98:TYR:CZ	2:G:99:ILE:CD1	2.64	0.71
1:P:22:VAL:HA	1:P:24:PHE:CE2	2.26	0.71
1:Q:44:LEU:HD13	1:Q:45:GLY:N	1.99	0.71
1:S:11:THR:HG21	1:S:12:LYS:NZ	2.05	0.71
4:L:21:VAL:HG12	4:L:22:THR:N	2.06	0.71
1:S:29:GLN:HE21	3:H:53:THR:H	1.35	0.71
2:A:3:VAL:HG22	2:A:26:SER:CB	2.14	0.70
2:A:6:GLN:HE22	2:A:93:TYR:HA	1.55	0.70
2:C:122:SER:O	2:C:140:CYS:HA	1.91	0.70
2:E:39:LEU:HD22	2:E:40:ALA:N	2.06	0.70
2:A:48:GLN:H	2:A:48:GLN:NE2	1.88	0.70
3:D:146:LEU:HD12	3:D:147:VAL:N	2.06	0.70
3:D:210:LYS:C	3:D:211:VAL:CG1	2.59	0.70
1:S:29:GLN:NE2	3:H:53:THR:N	2.40	0.70
2:A:143:ASN:HA	2:A:180:SER:HB3	1.74	0.70
2:A:89:GLN:NE2	2:A:172:GLN:HG2	2.06	0.70
3:D:111:GLY:O	3:D:112:THR:OG1	2.08	0.70
3:D:180:TYR:C	3:D:181:THR:HG23	2.10	0.70
3:F:17:THR:HG23	3:F:84:ASN:OD1	1.91	0.70
4:N:62:GLY:HA3	4:N:80:ALA:N	2.06	0.70
3:B:11:LEU:HD22	3:B:12:LYS:N	2.07	0.70
3:D:211:VAL:HG23	3:D:212:ASP:N	2.07	0.70
3:D:29:PHE:CE1	3:D:53:THR:HG21	2.26	0.70
2:G:196:ASN:ND2	2:G:217:ARG:N	2.39	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:62:SER:OG	1:Q:14:ASN:ND2	2.25	0.70
2:E:11:LEU:HD23	4:N:37:ALA:HB2	1.72	0.70
2:E:190:ASP:O	2:E:194:ARG:HB2	1.92	0.70
3:F:171:PHE:N	3:F:171:PHE:CD1	2.55	0.70
2:G:98:TYR:CD1	2:G:98:TYR:O	2.44	0.70
2:A:43:GLN:CB	2:A:53:LEU:HD21	2.21	0.70
2:A:60:ARG:HH12	2:A:68:PHE:H	1.39	0.70
2:A:89:GLN:OE1	2:A:177:SER:HA	1.90	0.70
2:C:37:ASN:O	2:C:56:TRP:HA	1.91	0.70
2:C:67:ARG:CB	2:C:67:ARG:CD	2.66	0.70
3:F:103:GLN:OE1	3:F:103:GLN:N	2.25	0.70
3:F:19:LYS:CB	3:F:19:LYS:CD	2.69	0.70
2:A:105:GLY:C	2:A:107:GLY:N	2.35	0.70
3:B:52:ASN:C	3:B:54:GLU:H	1.95	0.70
2:E:157:ASP:CG	2:E:195:HIS:HB3	2.11	0.70
2:G:12:ALA:CB	4:O:36:THR:HB	2.22	0.70
2:E:130:GLN:NE2	2:E:136:ALA:CA	2.55	0.70
3:F:34:MET:HG3	3:F:35:HIS:N	2.05	0.70
3:B:36:TRP:CH2	3:B:81:LEU:HB2	2.27	0.70
2:C:112:LEU:HB3	2:C:172:GLN:OE1	1.92	0.70
2:G:102:LEU:HB2	3:H:47:TRP:CD1	2.26	0.70
2:G:196:ASN:HD21	2:G:216:ASN:HB3	1.54	0.70
2:G:125:PRO:HB3	2:G:215:PHE:CZ	2.26	0.70
2:G:20:THR:HB	2:G:80:THR:HG22	1.74	0.70
4:L:56:LEU:HG	4:L:57:HIS:H	1.55	0.70
1:P:40:ARG:NE	3:F:98:ARG:HH12	1.90	0.70
2:A:94:CYS:O	2:A:104:PHE:HA	1.92	0.69
3:D:165:SER:O	3:D:168:VAL:HG21	1.91	0.69
3:H:155:VAL:CG1	3:H:156:THR:H	2.05	0.69
3:H:45:LEU:N	3:H:45:LEU:HD22	2.06	0.69
2:E:172:GLN:NE2	2:E:177:SER:HB2	2.07	0.69
2:E:24:LYS:HE3	2:E:76:ASP:OD1	1.92	0.69
3:F:91:THR:HG23	3:F:115:THR:HA	1.73	0.69
1:S:29:GLN:O	1:S:30:ILE:HB	1.92	0.69
2:G:156:ILE:HD12	2:G:161:ARG:CG	2.21	0.69
3:H:175:LEU:CB	3:H:175:LEU:CD2	2.69	0.69
4:O:55:ALA:C	4:O:57:HIS:N	2.37	0.69
1:Q:37:LEU:HB3	1:Q:38:PRO:HD3	1.74	0.69
1:S:11:THR:HG21	1:S:12:LYS:HZ3	1.56	0.69
2:A:190:ASP:O	2:A:192:TYR:N	2.26	0.69
3:B:150:TYR:O	3:B:151:PHE:HB2	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:60:TYR:CE1	3:D:70:PHE:CD1	2.80	0.69
3:F:153:GLU:OE1	3:F:173:ALA:HB3	1.92	0.69
2:G:110:LEU:O	2:G:111:GLU:O	2.09	0.69
2:G:56:TRP:O	2:G:57:ALA:CB	2.41	0.69
2:G:85:GLN:O	2:G:88:ASP:HB2	1.92	0.69
2:C:55:TYR:CD1	2:C:55:TYR:N	2.60	0.69
3:B:126:VAL:CA	3:B:126:VAL:CG2	2.67	0.69
2:C:55:TYR:HD1	2:C:55:TYR:N	1.91	0.69
2:C:6:GLN:OE1	2:C:107:GLY:HA2	1.93	0.69
3:D:81:LEU:C	3:D:81:LEU:CD2	2.53	0.69
2:G:156:ILE:HD12	2:G:161:ARG:HG2	1.73	0.69
2:G:167:ASN:ND2	2:G:167:ASN:N	2.31	0.69
3:H:217:PRO:O	3:H:217:PRO:HG2	1.91	0.69
1:P:22:VAL:HA	1:P:24:PHE:CZ	2.28	0.69
2:C:188:THR:O	2:C:189:LYS:O	2.09	0.69
3:H:40:ALA:HB3	3:H:43:LYS:HG3	1.72	0.69
3:H:52:ASN:HB3	3:H:55:THR:HB	1.72	0.69
4:O:25:VAL:HG11	4:O:39:PHE:HE1	1.57	0.69
1:Q:9:ARG:O	1:Q:10:LYS:O	2.09	0.69
1:S:34:VAL:HG23	2:G:31:ASN:HB2	1.73	0.69
2:E:130:GLN:NE2	2:E:136:ALA:C	2.46	0.69
3:F:99:PHE:HD2	3:F:105:PHE:CE1	2.09	0.69
2:G:102:LEU:CD1	2:G:102:LEU:CB	2.69	0.69
2:A:45:LYS:HG2	2:A:90:ALA:HB2	1.75	0.69
2:C:52:VAL:HG21	3:D:104:TYR:CD1	2.28	0.69
3:D:140:MET:CA	3:D:190:SER:OG	2.41	0.69
2:E:28:SER:HA	2:E:74:GLY:O	1.93	0.69
3:F:158:THR:OG1	3:F:159:TRP:N	2.23	0.69
3:H:72:LEU:HD23	3:H:73:GLU:N	2.07	0.69
4:N:28:ILE:CA	4:N:28:ILE:CG2	2.69	0.69
4:O:70:ASP:HB3	4:O:73:ASN:HB3	1.75	0.69
2:A:142:LEU:N	2:A:142:LEU:HD23	2.07	0.69
2:C:148:LYS:O	2:C:149:ASP:C	2.31	0.69
3:D:175:LEU:HG	3:D:176:GLN:H	1.58	0.69
3:F:64:PHE:O	3:F:65:LYS:C	2.31	0.69
3:H:114:VAL:HG22	3:H:115:THR:N	2.06	0.69
4:O:42:THR:O	4:O:43:PHE:C	2.31	0.69
3:B:179:LEU:CD1	3:B:179:LEU:CB	2.70	0.69
3:D:129:LEU:HB2	3:D:144:GLY:C	2.14	0.69
2:E:139:VAL:HG12	2:E:184:THR:HG23	1.75	0.69
2:E:75:THR:HG23	2:E:76:ASP:OD2	1.91	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:155:LYS:HA	2:G:160:GLU:HA	1.73	0.69
4:L:77:ILE:O	4:L:77:ILE:HG22	1.92	0.69
1:S:13:ARG:CB	1:S:13:ARG:HH11	2.06	0.69
3:B:37:VAL:HG21	3:B:108:TRP:CZ3	2.28	0.68
2:E:185:LEU:C	2:E:185:LEU:HD12	2.12	0.68
4:L:21:VAL:HG12	4:L:22:THR:H	1.56	0.68
4:L:54:ALA:C	4:L:56:LEU:N	2.46	0.68
4:O:21:VAL:CG1	4:O:22:THR:N	2.56	0.68
4:O:59:LYS:CA	4:O:59:LYS:CG	2.69	0.68
3:B:153:GLU:HB3	3:B:154:PRO:HA	1.75	0.68
3:B:161:SER:H	3:B:201:ASN:ND2	1.90	0.68
3:B:54:GLU:O	3:B:55:THR:C	2.31	0.68
2:C:130:GLN:NE2	2:C:137:SER:H	1.90	0.68
3:F:32:PHE:CE1	3:F:100:LEU:HG	2.28	0.68
5:G:224:HOH:O	3:H:167:GLY:HA3	1.92	0.68
3:D:152:PRO:O	3:D:154:PRO:HD2	1.92	0.68
2:E:60:ARG:HG2	2:E:61:GLU:O	1.94	0.68
3:H:12:LYS:HG3	3:H:18:VAL:HB	1.76	0.68
1:Q:31:VAL:CB	1:Q:31:VAL:HA	2.13	0.68
2:A:34:THR:CG2	2:A:36:LYS:HB2	2.24	0.68
2:E:201:GLU:HG2	2:E:212:VAL:HG22	1.75	0.68
2:E:68:PHE:CD1	2:E:81:ILE:HG12	2.28	0.68
2:G:14:SER:OG	2:G:15:ALA:N	2.13	0.68
2:G:196:ASN:O	2:G:216:ASN:HA	1.93	0.68
2:A:185:LEU:HD12	2:A:186:THR:N	2.07	0.68
2:A:198:TYR:CB	2:A:215:PHE:HD2	2.07	0.68
3:B:116:VAL:O	3:B:116:VAL:HG13	1.91	0.68
3:B:182:LEU:CD2	3:B:182:LEU:C	2.53	0.68
2:C:62:SER:HB3	1:Q:11:THR:O	1.93	0.68
4:N:58:ALA:O	4:N:60:VAL:N	2.26	0.68
3:B:119:ALA:CB	3:B:119:ALA:C	2.61	0.68
3:B:11:LEU:HD22	3:B:12:LYS:H	1.58	0.68
3:B:55:THR:HG22	3:B:57:GLU:HB2	1.76	0.68
2:C:204:HIS:CE1	2:C:206:THR:HG23	2.28	0.68
2:C:29:LEU:N	2:C:29:LEU:HD23	2.07	0.68
3:F:94:TYR:CD2	3:F:94:TYR:N	2.60	0.68
2:E:153:LYS:CE	2:E:160:GLU:CD	2.60	0.68
2:E:83:SER:O	2:E:84:VAL:C	2.30	0.68
2:E:95:LYS:CG	2:E:95:LYS:CE	2.71	0.68
3:H:60:TYR:OH	3:H:70:PHE:N	2.26	0.68
1:Q:11:THR:CB	1:Q:11:THR:HA	2.14	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:102:LEU:C	2:A:103:THR:HG23	2.13	0.68
3:B:215:ILE:HG22	3:B:215:ILE:O	1.94	0.68
3:H:214:LYS:HG2	3:H:215:ILE:H	1.57	0.68
3:H:34:MET:O	3:H:51:VAL:CG2	2.40	0.68
3:B:182:LEU:HG	3:B:183:SER:N	2.07	0.68
3:B:55:THR:HG23	2:E:99:ILE:HD12	1.76	0.68
2:C:189:LYS:HA	2:C:189:LYS:CB	2.13	0.68
2:C:56:TRP:O	2:C:57:ALA:HB3	1.93	0.68
2:E:11:LEU:CD2	2:E:11:LEU:CD1	2.68	0.68
3:F:190:SER:C	3:F:192:THR:N	2.44	0.68
2:G:131:LEU:C	2:G:133:SER:N	2.43	0.68
4:L:64:TRP:HE3	4:L:66:ALA:H	1.39	0.68
4:M:24:LYS:CG	4:M:24:LYS:CA	2.70	0.68
2:A:112:LEU:HB3	2:A:172:GLN:HE22	1.57	0.68
2:A:128:SER:O	2:A:129:GLU:C	2.32	0.68
2:A:3:VAL:CG2	2:A:26:SER:HB2	2.17	0.68
2:C:188:THR:HG23	2:C:191:GLU:CB	2.24	0.68
2:C:189:LYS:CB	2:C:189:LYS:N	2.56	0.68
2:G:23:CYS:N	2:G:77:PHE:O	2.24	0.68
4:N:56:LEU:HD12	4:N:56:LEU:C	2.14	0.68
3:D:210:LYS:O	3:D:211:VAL:HG12	1.94	0.67
3:D:74:THR:O	3:D:75:SER:C	2.32	0.67
3:H:65:LYS:C	3:H:67:ARG:H	1.98	0.67
4:L:57:HIS:CB	4:L:61:ASN:HD21	2.03	0.67
4:M:62:GLY:HA3	4:M:80:ALA:HB3	1.76	0.67
2:G:203:THR:HA	2:G:210:PRO:HB3	1.76	0.67
3:H:72:LEU:CD2	3:H:74:THR:H	2.07	0.67
2:C:167:ASN:HD22	2:C:183:SER:CB	2.08	0.67
2:E:102:LEU:O	2:E:103:THR:HG23	1.94	0.67
2:G:98:TYR:CD2	2:G:99:ILE:HD12	2.28	0.67
3:H:6:GLN:CD	3:H:111:GLY:H	1.97	0.67
4:M:23:ILE:HG22	4:M:23:ILE:O	1.94	0.67
1:Q:9:ARG:NH1	1:Q:9:ARG:CB	2.57	0.67
1:S:43:ARG:HH21	1:S:43:ARG:HA	1.59	0.67
2:E:89:GLN:CA	2:E:89:GLN:CG	2.69	0.67
2:G:102:LEU:HD22	3:H:47:TRP:NE1	2.08	0.67
3:H:10:GLU:O	3:H:115:THR:N	2.28	0.67
4:M:21:VAL:HG12	4:M:22:THR:H	1.59	0.67
2:C:142:LEU:CD1	2:C:152:VAL:HG21	2.23	0.67
2:E:6:GLN:NE2	2:E:41:TRP:HZ3	1.92	0.67
4:O:75:MET:SD	4:O:77:ILE:HD11	2.34	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:31:ASN:ND2	2:A:31:ASN:C	2.46	0.67
3:B:182:LEU:CG	3:B:183:SER:N	2.57	0.67
2:C:145:PHE:O	2:C:145:PHE:CD1	2.48	0.67
3:H:19:LYS:CD	3:H:19:LYS:CB	2.72	0.67
3:B:11:LEU:HB2	3:B:152:PRO:HG3	1.77	0.67
3:B:188:VAL:HB	3:B:189:PRO:CD	2.25	0.67
3:B:65:LYS:HA	3:B:65:LYS:HZ3	1.57	0.67
2:C:30:LEU:CD1	2:C:30:LEU:CB	2.71	0.67
2:E:55:TYR:O	2:E:56:TRP:C	2.33	0.67
2:G:148:LYS:HD3	2:G:179:TYR:CZ	2.30	0.67
2:G:98:TYR:CD2	2:G:99:ILE:CD1	2.78	0.67
3:H:55:THR:HG22	3:H:57:GLU:HB2	1.76	0.67
2:E:110:LEU:HG	2:E:110:LEU:O	1.95	0.67
3:F:32:PHE:CE2	3:F:98:ARG:NH2	2.63	0.67
2:G:166:LEU:HD12	2:G:186:THR:OG1	1.95	0.67
4:L:28:ILE:CG1	4:L:28:ILE:CG2	2.71	0.67
2:C:65:PRO:O	2:C:66:ASP:C	2.32	0.67
3:D:199:THR:HA	3:D:214:LYS:HA	1.76	0.67
2:E:128:SER:O	2:E:131:LEU:N	2.28	0.67
2:G:138:VAL:O	2:G:185:LEU:N	2.27	0.67
2:G:211:ILE:HD12	2:G:212:VAL:H	1.60	0.67
4:L:25:VAL:HG22	4:L:26:ASN:H	1.59	0.67
2:A:54:ILE:CD1	2:A:70:GLY:N	2.57	0.67
3:B:87:LYS:O	3:B:90:ASP:CB	2.35	0.67
2:G:67:ARG:NH2	2:G:85:GLN:HG3	2.10	0.67
4:L:25:VAL:HG22	4:L:26:ASN:N	2.09	0.67
2:G:67:ARG:HD2	2:G:68:PHE:CZ	2.30	0.66
2:G:68:PHE:HE1	2:G:81:ILE:HG23	1.59	0.66
2:A:191:GLU:N	2:A:191:GLU:C	2.48	0.66
3:B:18:VAL:CG2	3:B:19:LYS:N	2.58	0.66
3:B:60:TYR:HB2	3:B:65:LYS:HZ1	1.60	0.66
2:C:152:VAL:CG1	2:C:153:LYS:N	2.57	0.66
2:C:173:ASP:CG	2:C:175:LYS:HB2	2.14	0.66
3:D:211:VAL:HG23	3:D:212:ASP:O	1.94	0.66
2:E:187:LEU:HD22	2:E:191:GLU:OE1	1.95	0.66
3:F:20:ILE:HD12	3:F:112:THR:HB	1.75	0.66
4:M:27:LEU:HD12	4:M:35:GLN:HB2	1.77	0.66
2:A:118:ALA:HB1	2:A:119:PRO:HD2	1.77	0.66
2:A:37:ASN:HD21	2:A:74:GLY:N	1.93	0.66
2:E:55:TYR:HD2	2:E:56:TRP:HB2	1.60	0.66
2:E:7:SER:C	2:E:8:PRO:O	2.33	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:51:VAL:O	3:F:53:THR:N	2.29	0.66
3:H:209:THR:O	3:H:210:LYS:HB2	1.95	0.66
4:L:62:GLY:HA3	4:L:81:GLY:N	2.11	0.66
2:A:128:SER:HA	2:A:131:LEU:HD12	1.77	0.66
2:E:123:ILE:HA	2:E:140:CYS:HA	1.78	0.66
2:E:60:ARG:NH1	2:E:66:ASP:HA	2.10	0.66
2:G:151:ASN:C	2:G:152:VAL:HG23	2.15	0.66
3:H:188:VAL:HB	3:H:189:PRO:HD2	1.77	0.66
4:N:50:ALA:O	4:N:51:TYR:C	2.34	0.66
3:F:20:ILE:HG12	3:F:21:SER:N	2.10	0.66
3:H:207:SER:OG	3:H:209:THR:HG23	1.94	0.66
4:L:21:VAL:CG1	4:L:22:THR:H	2.07	0.66
4:O:75:MET:CG	4:O:75:MET:O	2.33	0.66
2:A:130:GLN:CB	3:B:127:TYR:CE1	2.77	0.66
2:A:190:ASP:C	2:A:192:TYR:H	1.99	0.66
3:B:87:LYS:O	3:B:90:ASP:N	2.27	0.66
2:C:37:ASN:HD21	2:C:74:GLY:N	1.92	0.66
2:A:118:ALA:CA	2:A:206:THR:HG21	2.26	0.66
2:A:89:GLN:HE22	2:A:172:GLN:HG2	1.61	0.66
2:G:20:THR:CG2	5:G:221:HOH:O	2.44	0.66
2:G:121:VAL:CG1	2:G:213:LYS:HG3	2.21	0.66
2:A:60:ARG:NH1	2:A:65:PRO:O	2.29	0.66
2:E:204:HIS:ND1	2:E:205:LYS:N	2.43	0.66
3:H:69:ALA:O	3:H:82:GLN:N	2.26	0.66
3:H:6:GLN:NE2	3:H:111:GLY:CA	2.58	0.66
4:L:25:VAL:HG12	4:L:37:ALA:O	1.96	0.66
2:A:201:GLU:HG2	2:A:212:VAL:HG13	1.78	0.66
3:B:194:PRO:O	3:B:196:GLU:N	2.30	0.66
2:C:19:VAL:HG11	2:C:81:ILE:HB	1.78	0.66
2:E:55:TYR:CE2	2:E:59:THR:HB	2.30	0.66
4:O:26:ASN:HB2	4:O:76:ASN:ND2	2.10	0.66
3:B:40:ALA:HB1	3:B:41:PRO:CD	2.25	0.65
2:C:141:PHE:HE1	2:C:182:SER:HG	1.43	0.65
2:C:43:GLN:HG2	2:C:44:GLN:N	2.10	0.65
3:D:193:TRP:CG	3:D:194:PRO:CA	2.78	0.65
2:A:114:ARG:HD3	2:A:177:SER:O	1.96	0.65
3:F:50:TRP:NE1	3:F:59:THR:HB	2.11	0.65
2:A:52:VAL:HG13	2:A:52:VAL:O	1.94	0.65
3:B:196:GLU:HA	3:B:196:GLU:OE1	1.95	0.65
3:B:207:SER:O	3:B:208:SER:C	2.28	0.65
2:E:102:LEU:O	2:E:103:THR:CG2	2.44	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:68:PHE:HE1	2:E:81:ILE:HD11	1.62	0.65
3:B:153:GLU:CB	3:B:154:PRO:HA	2.24	0.65
2:C:173:ASP:OD1	2:C:175:LYS:HD3	1.96	0.65
2:C:55:TYR:O	2:C:59:THR:CB	2.44	0.65
3:D:1:GLN:CD	1:Q:13:ARG:HD2	2.16	0.65
2:E:153:LYS:CB	2:E:153:LYS:CD	2.70	0.65
4:N:34:ILE:HG22	4:N:35:GLN:N	2.10	0.65
3:B:6:GLN:NE2	3:B:109:GLY:HA3	2.09	0.65
3:D:186:VAL:O	3:D:186:VAL:HG13	1.96	0.65
3:F:54:GLU:OE2	3:F:54:GLU:C	2.35	0.65
4:N:28:ILE:HD12	4:N:28:ILE:H	1.61	0.65
1:Q:9:ARG:CZ	1:Q:9:ARG:CB	2.48	0.65
1:S:30:ILE:O	1:S:30:ILE:HG13	1.95	0.65
2:A:89:GLN:NE2	2:A:172:GLN:CG	2.60	0.65
2:C:95:LYS:HB3	2:C:104:PHE:CE2	2.32	0.65
3:F:182:LEU:C	3:F:182:LEU:HD23	2.16	0.65
2:A:169:TRP:NE1	2:A:181:MET:HE3	2.12	0.65
2:A:34:THR:HG22	2:A:36:LYS:HB2	1.78	0.65
3:B:138:ASN:CG	3:B:139:SER:N	2.38	0.65
3:D:19:LYS:HE2	3:D:80:TYR:CD1	2.32	0.65
2:E:138:VAL:N	2:E:185:LEU:O	2.30	0.65
3:F:57:GLU:N	3:F:57:GLU:OE2	2.30	0.65
2:G:150:ILE:CD1	2:G:151:ASN:N	2.59	0.65
4:M:25:VAL:HG13	4:M:26:ASN:N	2.12	0.65
2:E:34:THR:CG2	2:E:36:LYS:HB2	2.26	0.65
3:F:27:TYR:CD1	3:F:98:ARG:HD3	2.31	0.65
2:G:14:SER:HB3	2:G:17:GLU:CD	2.17	0.65
2:G:27:GLN:O	2:G:28:SER:C	2.34	0.65
3:H:199:THR:HG22	3:H:214:LYS:CA	2.25	0.65
3:H:6:GLN:HE22	3:H:111:GLY:HA2	1.59	0.65
4:N:79:PHE:HD1	4:N:79:PHE:N	1.95	0.65
1:Q:44:LEU:CD1	1:Q:45:GLY:H	1.99	0.65
2:A:89:GLN:NE2	2:A:172:GLN:CB	2.60	0.65
3:D:197:THR:HA	3:D:214:LYS:CE	2.27	0.65
3:H:182:LEU:HD12	3:H:183:SER:CA	2.26	0.65
1:P:20:GLN:HE22	3:B:2:ILE:HD13	1.61	0.65
1:Q:16:ASN:ND2	1:Q:17:ARG:CG	2.58	0.65
1:S:3:THR:OG1	1:S:4:ASN:N	2.28	0.65
2:E:88:ASP:C	2:E:90:ALA:H	1.99	0.65
3:F:126:VAL:HG21	3:F:202:VAL:HG21	1.79	0.65
2:G:56:TRP:HB2	2:G:59:THR:HG1	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:189:PRO:O	3:H:192:THR:N	2.30	0.65
4:L:43:PHE:O	4:L:47:THR:HB	1.96	0.65
2:A:6:GLN:HE21	2:A:105:GLY:CA	2.10	0.64
3:D:135:ALA:C	3:D:137:THR:H	2.01	0.64
3:D:210:LYS:CG	3:D:210:LYS:CE	2.75	0.64
3:D:72:LEU:HD12	3:D:79:ALA:HA	1.77	0.64
2:G:199:THR:CG2	2:G:214:SER:HA	2.24	0.64
3:B:98:ARG:NE	3:B:98:ARG:CG	2.59	0.64
2:C:145:PHE:C	2:C:145:PHE:CD1	2.70	0.64
2:E:68:PHE:HA	2:E:80:THR:O	1.96	0.64
2:A:2:ILE:HG22	2:A:2:ILE:O	1.97	0.64
2:A:6:GLN:NE2	2:A:93:TYR:HA	2.12	0.64
3:D:117:SER:OG	3:D:118:SER:N	2.29	0.64
2:E:68:PHE:CE1	2:E:81:ILE:HD11	2.32	0.64
2:G:121:VAL:CG1	2:G:213:LYS:CG	2.76	0.64
2:G:55:TYR:CZ	2:G:59:THR:HG21	2.32	0.64
3:H:164:LEU:HD13	3:H:186:VAL:CG2	2.18	0.64
3:H:91:THR:HG22	3:H:91:THR:O	1.97	0.64
1:P:20:GLN:NE2	3:B:2:ILE:HD13	2.12	0.64
3:B:146:LEU:HG	3:B:146:LEU:O	1.95	0.64
3:B:168:VAL:HG22	3:B:186:VAL:HG12	1.79	0.64
2:C:61:GLU:H	2:C:64:VAL:HG21	1.62	0.64
3:D:41:PRO:O	3:D:43:LYS:NZ	2.30	0.64
2:G:36:LYS:HD3	2:G:56:TRP:CD1	2.33	0.64
3:H:98:ARG:HB3	3:H:106:ASP:OD2	1.98	0.64
3:B:75:SER:O	3:B:77:SER:N	2.29	0.64
3:B:91:THR:O	3:B:92:ALA:HB2	1.96	0.64
2:C:37:ASN:C	2:C:56:TRP:HA	2.18	0.64
2:E:12:ALA:CB	2:E:113:LYS:HZ3	2.11	0.64
3:F:67:ARG:HD2	3:F:84:ASN:O	1.98	0.64
3:H:160:ASN:O	3:H:162:GLY:N	2.30	0.64
2:A:215:PHE:CD2	2:A:215:PHE:O	2.51	0.64
3:B:141:VAL:HG22	3:B:142:THR:H	1.62	0.64
2:C:112:LEU:HD13	2:C:113:LYS:O	1.98	0.64
2:C:165:VAL:CG1	2:C:165:VAL:CG2	2.73	0.64
2:C:187:LEU:CB	2:C:187:LEU:CD1	2.74	0.64
2:C:77:PHE:CD2	2:C:77:PHE:N	2.64	0.64
3:D:23:LYS:CG	3:D:23:LYS:CA	2.74	0.64
2:E:175:LYS:HG3	2:E:175:LYS:O	1.97	0.64
2:E:92:TYR:CD1	2:E:92:TYR:N	2.66	0.64
2:A:36:LYS:HD2	2:A:56:TRP:CG	2.32	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:144:ASN:H	3:B:169:HIS:HE1	1.44	0.64
3:D:180:TYR:O	3:D:181:THR:CG2	2.45	0.64
2:E:143:ASN:O	2:E:144:ASN:C	2.30	0.64
2:E:165:VAL:C	2:E:166:LEU:HD12	2.17	0.64
2:E:41:TRP:CA	2:E:41:TRP:CG	2.76	0.64
3:F:93:THR:OG1	3:F:113:THR:HG22	1.98	0.64
2:G:86:ALA:C	2:G:88:ASP:H	1.99	0.64
3:H:88:ASN:O	3:H:89:GLU:C	2.33	0.64
4:O:25:VAL:CG2	4:O:77:ILE:HG13	2.28	0.64
2:A:218:ASN:N	2:A:218:ASN:OD1	2.28	0.64
2:A:6:GLN:HB3	2:A:22:SER:O	1.97	0.64
2:E:7:SER:CA	2:E:8:PRO:O	2.45	0.64
3:H:216:VAL:HG23	3:H:217:PRO:HD2	1.79	0.64
1:Q:44:LEU:HD22	1:Q:45:GLY:N	2.13	0.64
3:B:73:GLU:CA	3:B:73:GLU:OE1	2.45	0.64
3:D:151:PHE:CB	3:D:152:PRO:HD3	2.28	0.64
1:Q:9:ARG:HB2	1:Q:9:ARG:NH1	2.13	0.64
1:S:29:GLN:C	1:S:30:ILE:HG22	2.16	0.64
2:C:69:THR:O	2:C:80:THR:HG22	1.98	0.64
3:D:91:THR:HG23	3:D:115:THR:HA	1.79	0.64
3:F:142:THR:OG1	3:F:187:THR:HG23	1.97	0.64
3:F:189:PRO:O	3:F:192:THR:OG1	2.15	0.64
3:F:199:THR:HG22	3:F:214:LYS:CB	2.28	0.64
3:F:67:ARG:CG	3:F:67:ARG:HH11	2.10	0.64
3:B:112:THR:HG22	3:B:114:VAL:H	1.62	0.63
2:C:7:SER:HA	2:C:8:PRO:C	2.19	0.63
2:E:60:ARG:HG2	2:E:61:GLU:N	2.11	0.63
3:H:176:GLN:C	3:H:178:ASP:N	2.45	0.63
3:H:1:GLN:HG2	3:H:2:ILE:H	1.62	0.63
4:O:25:VAL:HG23	4:O:75:MET:O	1.98	0.63
4:M:65:THR:CA	4:M:65:THR:CG2	2.75	0.63
4:N:55:ALA:O	4:N:58:ALA:CB	2.34	0.63
3:B:144:GLY:O	3:B:215:ILE:HD11	1.99	0.63
3:B:75:SER:C	3:B:77:SER:N	2.52	0.63
2:E:31:ASN:HD22	2:E:31:ASN:C	2.01	0.63
2:G:208:THR:O	2:G:210:PRO:HD3	1.98	0.63
3:H:126:VAL:O	3:H:127:TYR:CD1	2.52	0.63
4:M:27:LEU:HD12	4:M:35:GLN:CB	2.29	0.63
1:S:13:ARG:CZ	1:S:13:ARG:HB2	2.29	0.63
2:A:204:HIS:ND1	2:A:206:THR:HG23	2.12	0.63
2:C:81:ILE:CG2	2:C:84:VAL:HG12	2.26	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:152:PRO:O	3:D:153:GLU:C	2.36	0.63
3:D:214:LYS:HD3	3:D:215:ILE:O	1.98	0.63
2:E:24:LYS:HE3	2:E:76:ASP:CG	2.19	0.63
2:G:59:THR:O	2:G:59:THR:HG22	1.98	0.63
4:N:33:LYS:CG	4:N:33:LYS:CE	2.75	0.63
2:C:152:VAL:HG12	2:C:153:LYS:N	2.13	0.63
3:D:97:ALA:HB2	3:D:108:TRP:HA	1.79	0.63
2:G:68:PHE:CD1	2:G:81:ILE:HD12	2.34	0.63
2:C:12:ALA:N	4:M:36:THR:O	2.31	0.63
3:B:162:GLY:O	3:B:163:SER:C	2.37	0.63
2:C:16:GLY:HA2	2:C:83:SER:C	2.18	0.63
3:F:182:LEU:HD23	3:F:183:SER:CA	2.29	0.63
2:G:152:VAL:HG22	2:G:203:THR:H	1.64	0.63
4:M:39:PHE:O	4:M:40:LYS:O	2.17	0.63
1:Q:12:LYS:CG	1:Q:12:LYS:CE	2.75	0.63
2:A:141:PHE:CE2	3:B:185:SER:CB	2.79	0.63
2:A:151:ASN:CG	2:A:152:VAL:N	2.51	0.63
2:A:216:ASN:HB2	2:A:219:GLU:OE2	1.98	0.63
3:B:120:LYS:CD	3:B:120:LYS:N	2.51	0.63
3:B:209:THR:CG2	3:B:210:LYS:H	2.05	0.63
3:B:73:GLU:C	3:B:75:SER:H	2.02	0.63
4:L:77:ILE:CD1	4:L:77:ILE:H	2.11	0.63
1:S:29:GLN:HB3	3:H:33:SER:OG	1.98	0.63
3:B:1:GLN:HG3	3:B:2:ILE:H	1.64	0.63
3:B:28:THR:O	3:B:29:PHE:C	2.37	0.63
2:E:31:ASN:CB	2:E:34:THR:HB	2.28	0.63
2:G:81:ILE:HG21	2:G:84:VAL:HG12	1.80	0.63
1:S:23:LYS:CD	1:S:24:PHE:HB2	2.28	0.63
2:A:72:GLY:HA3	2:A:77:PHE:CD1	2.33	0.63
2:C:55:TYR:O	2:C:59:THR:OG1	2.16	0.63
2:E:143:ASN:HA	2:E:180:SER:HB3	1.79	0.63
2:E:88:ASP:O	2:E:90:ALA:N	2.32	0.63
2:E:96:GLN:NE2	2:E:98:TYR:H	1.96	0.63
3:H:9:PRO:HG2	3:H:205:PRO:HB2	1.80	0.63
3:H:60:TYR:HH	3:H:69:ALA:HA	1.63	0.63
4:O:21:VAL:HG12	4:O:22:THR:N	2.13	0.63
2:C:155:LYS:NZ	2:C:158:GLY:O	2.27	0.62
3:D:153:GLU:N	3:D:154:PRO:HD2	2.10	0.62
2:E:165:VAL:HG13	5:E:225:HOH:O	1.98	0.62
2:E:175:LYS:O	2:E:176:ASP:HB3	1.98	0.62
2:E:71:ARG:CG	2:E:71:ARG:CA	2.75	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:173:ALA:HB1	3:H:180:TYR:CD1	2.34	0.62
3:H:214:LYS:HG2	3:H:215:ILE:N	2.13	0.62
3:H:40:ALA:O	3:H:43:LYS:HB2	1.98	0.62
2:G:93:TYR:CZ	3:H:45:LEU:CD2	2.82	0.62
2:A:54:ILE:HD12	2:A:70:GLY:N	2.14	0.62
2:E:45:LYS:O	2:E:46:PRO:C	2.36	0.62
3:F:148:LYS:HZ2	3:F:149:GLY:N	1.98	0.62
1:Q:37:LEU:H	1:Q:38:PRO:HD2	1.64	0.62
1:S:11:THR:CG2	1:S:12:LYS:NZ	2.61	0.62
3:B:65:LYS:CA	3:B:65:LYS:HZ3	2.12	0.62
2:C:63:GLY:N	1:Q:11:THR:O	2.33	0.62
3:D:97:ALA:CB	3:D:108:TRP:HA	2.29	0.62
3:F:6:GLN:HG2	3:F:22:CYS:HA	1.81	0.62
3:H:207:SER:O	3:H:208:SER:HB2	1.99	0.62
4:O:73:ASN:CB	4:O:73:ASN:C	2.65	0.62
1:P:38:PRO:HG2	3:F:32:PHE:CE1	2.34	0.62
2:A:187:LEU:N	2:A:187:LEU:HD23	2.13	0.62
2:A:155:LYS:NZ	2:A:201:GLU:OE1	2.25	0.62
3:B:31:ASP:O	3:B:32:PHE:CD1	2.52	0.62
3:D:48:MET:HE1	3:D:81:LEU:HD11	1.79	0.62
3:D:48:MET:HE2	3:D:81:LEU:HD11	1.81	0.62
2:E:143:ASN:O	2:E:144:ASN:O	2.16	0.62
2:G:21:MET:CB	2:G:21:MET:SD	2.87	0.62
4:M:79:PHE:N	4:M:79:PHE:HD1	1.95	0.62
2:C:1:ASP:N	2:C:27:GLN:HE22	1.98	0.62
3:F:13:LYS:O	3:F:16:GLU:HB2	1.99	0.62
3:F:71:SER:O	3:F:72:LEU:HD23	2.00	0.62
3:F:23:LYS:HG3	3:F:78:THR:OG1	2.00	0.62
3:H:129:LEU:HG	3:H:145:CYS:N	2.15	0.62
4:N:62:GLY:CA	4:N:80:ALA:H	2.13	0.62
3:H:73:GLU:O	3:H:73:GLU:HG3	2.00	0.62
2:E:145:PHE:O	2:E:179:TYR:N	2.31	0.62
3:F:67:ARG:HB2	3:F:67:ARG:HH11	1.65	0.62
3:H:64:PHE:C	3:H:68:PHE:CD2	2.72	0.62
4:L:44:GLU:O	4:L:48:ALA:N	2.26	0.62
3:B:6:GLN:HE22	3:B:111:GLY:N	1.94	0.62
3:D:175:LEU:CD2	3:D:175:LEU:CB	2.74	0.62
3:D:188:VAL:CB	3:D:189:PRO:CD	2.77	0.62
3:D:81:LEU:CD1	3:D:81:LEU:CD2	2.71	0.62
3:F:98:ARG:HB3	3:F:107:VAL:CG1	2.30	0.62
3:B:120:LYS:O	3:B:120:LYS:HG2	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:54:ILE:HA	2:C:59:THR:O	2.00	0.62
2:C:60:ARG:HD2	2:C:64:VAL:HB	1.80	0.62
3:F:175:LEU:HB2	3:F:180:TYR:CE1	2.35	0.62
2:G:21:MET:CA	2:G:21:MET:CG	2.77	0.62
4:M:49:GLU:HG3	4:M:52:ARG:HD3	1.80	0.62
3:H:153:GLU:OE2	3:H:173:ALA:HB2	1.99	0.62
3:H:72:LEU:HD23	3:H:74:THR:H	1.64	0.62
2:A:190:ASP:O	2:A:193:GLU:N	2.32	0.61
2:E:191:GLU:HG2	2:E:194:ARG:NH1	2.14	0.61
4:L:21:VAL:CG1	4:L:22:THR:N	2.63	0.61
4:O:30:ALA:H	4:O:61:ASN:ND2	1.97	0.61
2:C:144:ASN:N	2:C:144:ASN:ND2	2.45	0.61
3:D:197:THR:C	3:D:197:THR:CB	2.63	0.61
2:E:130:GLN:HG3	3:F:127:TYR:CE2	2.36	0.61
3:F:168:VAL:HG12	3:F:169:HIS:N	2.15	0.61
2:G:124:PHE:HE1	2:G:141:PHE:HD2	1.47	0.61
2:G:142:LEU:HD12	2:G:181:MET:HB3	1.82	0.61
3:H:45:LEU:CD2	3:H:45:LEU:H	2.07	0.61
4:L:68:LEU:HB3	4:L:72:GLY:HA2	1.82	0.61
1:S:16:ASN:ND2	1:S:16:ASN:N	2.45	0.61
1:S:29:GLN:O	1:S:30:ILE:CB	2.48	0.61
2:C:204:HIS:CG	2:C:206:THR:HG23	2.35	0.61
2:C:55:TYR:O	2:C:59:THR:HB	2.01	0.61
3:D:13:LYS:HB2	3:D:16:GLU:OE1	2.00	0.61
3:F:171:PHE:HD1	3:F:171:PHE:N	1.91	0.61
3:F:214:LYS:O	3:F:216:VAL:HG23	2.00	0.61
2:G:176:ASP:O	2:G:177:SER:C	2.38	0.61
2:G:98:TYR:CD2	2:G:99:ILE:CG1	2.83	0.61
3:H:149:GLY:O	3:H:150:TYR:O	2.17	0.61
3:H:18:VAL:CG1	3:H:86:LEU:HD21	2.30	0.61
3:B:73:GLU:C	3:B:75:SER:N	2.53	0.61
3:D:20:ILE:CD1	3:D:81:LEU:HB3	2.30	0.61
2:E:41:TRP:CE2	2:E:79:LEU:HB2	2.35	0.61
2:G:167:ASN:CA	2:G:183:SER:HA	2.30	0.61
4:O:53:TYR:O	4:O:57:HIS:CE1	2.53	0.61
2:A:89:GLN:CD	2:A:172:GLN:NE2	2.53	0.61
2:C:37:ASN:HB2	2:C:57:ALA:HB2	1.81	0.61
2:C:8:PRO:HG2	2:C:108:THR:HG23	1.81	0.61
3:D:40:ALA:O	3:D:43:LYS:HB2	2.01	0.61
2:E:170:THR:OG1	2:E:171:ASP:N	2.33	0.61
3:F:156:THR:CB	3:F:156:THR:N	2.55	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:148:LYS:HD2	3:F:181:THR:HG21	1.81	0.61
3:H:150:TYR:CE2	3:H:180:TYR:HB3	2.35	0.61
3:H:69:ALA:O	3:H:81:LEU:HA	2.01	0.61
2:A:89:GLN:CD	2:A:172:GLN:HE21	2.02	0.61
2:A:65:PRO:C	2:A:67:ARG:H	2.04	0.61
3:F:176:GLN:HA	3:F:176:GLN:HE21	1.65	0.61
3:H:153:GLU:O	3:H:155:VAL:HG23	2.00	0.61
2:G:182:SER:CB	3:H:171:PHE:CE2	2.74	0.61
4:M:58:ALA:O	4:M:61:ASN:N	2.34	0.61
1:S:13:ARG:O	1:S:14:ASN:OD1	2.18	0.61
2:A:2:ILE:O	2:A:4:MET:HG2	2.01	0.61
3:H:132:GLY:O	3:H:135:ALA:HB3	1.99	0.61
3:H:164:LEU:HA	3:H:164:LEU:HD23	1.81	0.61
4:N:24:LYS:HE3	4:N:38:GLU:OE1	2.01	0.61
2:C:121:VAL:HG13	2:C:142:LEU:HD23	1.81	0.61
2:C:42:TYR:HH	3:D:104:TYR:HB2	1.65	0.61
2:G:13:VAL:HG23	2:G:14:SER:N	2.16	0.61
2:G:23:CYS:C	2:G:24:LYS:HD3	2.21	0.61
3:H:164:LEU:CD1	3:H:186:VAL:HG21	2.20	0.61
3:H:30:THR:HA	3:H:53:THR:HB	1.82	0.61
4:L:30:ALA:HB2	4:L:79:PHE:O	2.01	0.61
4:O:61:ASN:HD22	4:O:79:PHE:HD2	1.48	0.61
2:E:124:PHE:CD1	2:E:124:PHE:N	2.66	0.61
3:F:140:MET:CE	3:F:140:MET:CG	2.79	0.61
3:F:158:THR:HG23	3:F:201:ASN:HB2	1.81	0.61
2:G:98:TYR:O	2:G:99:ILE:HG13	2.01	0.61
3:H:37:VAL:HA	3:H:48:MET:H	1.65	0.61
4:N:77:ILE:HG22	4:N:79:PHE:CZ	2.35	0.61
1:Q:7:PRO:HB2	1:Q:9:ARG:NH2	2.13	0.61
2:C:112:LEU:HD13	2:C:113:LYS:N	2.16	0.61
3:D:98:ARG:NH1	3:D:106:ASP:OD1	2.32	0.61
3:D:132:GLY:O	3:D:134:ALA:N	2.34	0.61
3:D:129:LEU:HB2	3:D:144:GLY:CA	2.31	0.61
3:D:81:LEU:CD1	3:D:81:LEU:CB	2.76	0.61
2:G:112:LEU:HD23	2:G:177:SER:OG	2.00	0.61
3:H:38:ASN:N	3:H:48:MET:CG	2.57	0.61
2:A:189:LYS:O	2:A:193:GLU:N	2.30	0.60
3:B:36:TRP:HA	3:B:95:PHE:O	2.01	0.60
2:C:14:SER:HA	2:C:113:LYS:CB	2.29	0.60
3:D:156:THR:CG2	3:D:203:ALA:HB3	2.31	0.60
2:C:182:SER:HB2	3:D:171:PHE:CD2	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:166:LEU:HD21	3:H:176:GLN:OE1	2.01	0.60
4:L:25:VAL:O	4:L:25:VAL:CG1	2.45	0.60
4:N:51:TYR:OH	4:O:51:TYR:OH	2.07	0.60
4:O:64:TRP:CE3	4:O:66:ALA:CB	2.83	0.60
2:A:129:GLU:O	2:A:130:GLN:C	2.39	0.60
3:D:93:THR:O	3:D:94:TYR:CB	2.49	0.60
2:G:6:GLN:NE2	2:G:108:THR:N	2.50	0.60
3:H:175:LEU:HD13	3:H:180:TYR:CE2	2.36	0.60
1:S:31:VAL:HA	3:H:99:PHE:CE1	2.35	0.60
4:N:60:VAL:HG22	4:N:60:VAL:O	2.01	0.60
2:C:121:VAL:HG12	2:C:122:SER:N	2.16	0.60
2:E:204:HIS:CE1	2:E:206:THR:HG23	2.37	0.60
2:E:68:PHE:CE1	2:E:81:ILE:CD1	2.84	0.60
4:L:53:TYR:CZ	4:L:57:HIS:CE1	2.90	0.60
3:B:149:GLY:CA	3:B:179:LEU:HD22	2.31	0.60
2:C:18:LYS:O	4:M:35:GLN:OE1	2.19	0.60
3:D:153:GLU:O	3:D:154:PRO:C	2.37	0.60
2:G:102:LEU:CD2	3:H:105:PHE:CZ	2.84	0.60
2:C:10:SER:OG	4:M:38:GLU:HB2	2.01	0.60
1:S:23:LYS:HD2	1:S:24:PHE:HB2	1.81	0.60
2:A:105:GLY:O	2:A:106:ALA:C	2.32	0.60
2:A:114:ARG:HE	2:A:146:TYR:CB	2.14	0.60
3:B:167:GLY:O	3:B:186:VAL:HA	2.00	0.60
2:C:126:PRO:HG3	2:C:137:SER:C	2.22	0.60
2:G:196:ASN:HD22	2:G:217:ARG:H	1.46	0.60
3:B:116:VAL:O	3:B:116:VAL:CG1	2.49	0.60
2:C:171:ASP:O	2:C:172:GLN:C	2.39	0.60
3:D:141:VAL:HG22	3:D:142:THR:H	1.66	0.60
2:E:190:ASP:HA	2:E:193:GLU:HB2	1.83	0.60
3:F:143:LEU:HD22	3:F:215:ILE:HG21	1.83	0.60
4:O:25:VAL:CG1	4:O:25:VAL:O	2.50	0.60
2:C:199:THR:HB	2:C:214:SER:CB	2.32	0.60
3:D:189:PRO:CB	3:D:192:THR:HG23	2.31	0.60
3:D:7:SER:O	3:D:8:GLY:O	2.19	0.60
4:M:57:HIS:O	4:M:58:ALA:O	2.20	0.60
4:O:30:ALA:H	4:O:61:ASN:HD21	1.48	0.60
4:N:66:ALA:CB	4:O:68:LEU:HD23	2.30	0.60
2:C:18:LYS:CG	2:C:18:LYS:CE	2.73	0.60
2:G:194:ARG:O	2:G:194:ARG:CD	2.50	0.60
3:H:148:LYS:CB	3:H:181:THR:HB	2.24	0.60
4:O:31:ASP:OD1	4:O:33:LYS:HD3	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:O:54:ALA:O	4:O:55:ALA:C	2.38	0.60
3:B:159:TRP:CZ3	3:B:200:CYS:HB3	2.37	0.60
3:B:36:TRP:HE3	3:B:95:PHE:O	1.84	0.60
3:D:207:SER:C	3:D:209:THR:H	2.03	0.60
2:E:130:GLN:HE22	2:E:136:ALA:C	2.02	0.60
2:E:188:THR:CG2	2:E:191:GLU:HB2	2.28	0.60
2:G:166:LEU:HG	2:G:166:LEU:CD1	2.20	0.60
3:H:169:HIS:HB3	3:H:171:PHE:CE1	2.36	0.60
3:H:209:THR:O	3:H:210:LYS:CB	2.47	0.60
3:H:17:THR:HA	3:H:86:LEU:CD1	2.32	0.60
3:H:86:LEU:CD1	3:H:86:LEU:CD2	2.75	0.60
4:O:27:LEU:HB2	4:O:35:GLN:CB	2.29	0.60
2:C:1:ASP:H3	2:C:27:GLN:NE2	1.98	0.60
2:E:50:PRO:HB2	3:F:108:TRP:CZ2	2.37	0.60
2:G:52:VAL:CG1	2:G:52:VAL:O	2.45	0.60
3:H:199:THR:CG2	3:H:214:LYS:HA	2.30	0.60
1:P:29:GLN:O	1:P:30:ILE:HB	2.00	0.60
3:D:15:GLY:O	3:D:16:GLU:O	2.20	0.59
3:F:13:LYS:O	3:F:14:PRO:O	2.19	0.59
2:A:166:LEU:O	2:A:183:SER:HA	2.02	0.59
3:B:129:LEU:CB	3:B:144:GLY:HA3	2.18	0.59
2:C:152:VAL:CG1	2:C:153:LYS:H	2.15	0.59
2:C:157:ASP:OD2	2:C:196:ASN:N	2.35	0.59
2:E:56:TRP:O	2:E:57:ALA:HB3	2.00	0.59
4:M:60:VAL:HG13	4:M:61:ASN:ND2	2.16	0.59
4:N:53:TYR:CE2	4:N:57:HIS:ND1	2.69	0.59
1:Q:25:PRO:HG3	1:Q:39:ARG:HD3	1.83	0.59
2:C:31:ASN:HB2	2:C:98:TYR:HE1	1.65	0.59
3:D:182:LEU:O	3:D:182:LEU:CG	2.33	0.59
2:E:156:ILE:O	2:E:159:SER:N	2.36	0.59
2:A:8:PRO:HB3	4:L:39:PHE:HE2	1.61	0.59
2:G:98:TYR:CG	2:G:98:TYR:O	2.44	0.59
4:L:56:LEU:C	4:L:58:ALA:H	2.05	0.59
2:A:36:LYS:HB3	2:A:56:TRP:CD1	2.37	0.59
2:C:112:LEU:HD13	2:C:113:LYS:H	1.67	0.59
2:E:10:SER:O	4:N:37:ALA:HA	2.02	0.59
2:E:109:LYS:HG2	2:E:110:LEU:N	2.16	0.59
2:G:79:LEU:HD12	2:G:80:THR:N	2.17	0.59
4:N:77:ILE:O	4:N:79:PHE:HE1	1.85	0.59
2:A:204:HIS:CG	2:A:205:LYS:N	2.65	0.59
2:A:95:LYS:HB3	2:A:95:LYS:NZ	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:43:GLN:N	2:C:51:LYS:O	2.33	0.59
3:D:1:GLN:NE2	1:Q:13:ARG:HD2	2.17	0.59
2:E:85:GLN:C	2:E:87:GLU:H	2.06	0.59
3:F:6:GLN:OE1	3:F:20:ILE:HD11	2.03	0.59
3:H:141:VAL:O	3:H:141:VAL:HG13	2.03	0.59
3:H:214:LYS:C	3:H:215:ILE:HG13	2.21	0.59
3:H:216:VAL:CG2	3:H:217:PRO:HD2	2.32	0.59
1:Q:32:GLY:O	1:Q:36:LEU:HB3	2.02	0.59
2:A:96:GLN:CD	2:A:96:GLN:CB	2.68	0.59
3:D:175:LEU:HD13	3:D:180:TYR:CZ	2.37	0.59
4:N:58:ALA:C	4:N:60:VAL:H	2.06	0.59
2:A:188:THR:OG1	2:A:191:GLU:HB2	2.03	0.59
2:C:122:SER:OG	2:C:141:PHE:HB2	2.03	0.59
3:D:175:LEU:CD2	3:D:175:LEU:CD1	2.76	0.59
3:D:36:TRP:C	3:D:37:VAL:HG23	2.23	0.59
2:E:172:GLN:HG2	2:E:177:SER:HA	1.85	0.59
2:E:31:ASN:ND2	2:E:33:ARG:N	2.51	0.59
2:G:169:TRP:CD2	2:G:169:TRP:N	2.71	0.59
2:G:152:VAL:CG2	2:G:202:ALA:HA	2.33	0.59
3:H:125:SER:HB3	3:H:127:TYR:CZ	2.38	0.59
3:H:191:SER:O	3:H:195:SER:HB2	2.02	0.59
4:L:68:LEU:H	4:L:68:LEU:HD12	1.66	0.59
1:S:17:ARG:HG2	1:S:17:ARG:O	2.02	0.59
2:E:128:SER:OG	2:E:129:GLU:OE2	2.19	0.59
2:G:165:VAL:O	2:G:165:VAL:HG13	2.03	0.59
2:G:36:LYS:HD3	2:G:56:TRP:CG	2.38	0.59
2:G:52:VAL:CG2	2:G:53:LEU:N	2.65	0.59
3:H:161:SER:H	3:H:201:ASN:HD21	1.50	0.59
2:A:114:ARG:HE	2:A:146:TYR:HB3	1.66	0.59
2:A:45:LYS:HB3	2:A:46:PRO:CD	2.29	0.59
3:B:129:LEU:N	3:B:129:LEU:HD12	2.17	0.59
2:C:155:LYS:HD3	2:C:158:GLY:O	2.03	0.59
2:E:28:SER:HG	2:E:28:SER:CB	2.10	0.59
2:G:77:PHE:C	2:G:78:THR:CG2	2.70	0.59
3:H:159:TRP:HB2	3:H:164:LEU:HB2	1.84	0.59
4:L:43:PHE:O	4:L:44:GLU:C	2.42	0.59
2:A:19:VAL:HG11	2:A:81:ILE:HD12	1.84	0.58
2:G:112:LEU:CD2	2:G:112:LEU:HG	2.19	0.58
2:G:175:LYS:CB	2:G:175:LYS:CD	2.78	0.58
2:G:155:LYS:CE	2:G:201:GLU:OE1	2.47	0.58
2:A:11:LEU:HD23	4:L:37:ALA:HB2	1.83	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:42:TYR:HE1	2:C:95:LYS:HG2	1.68	0.58
3:D:170:THR:O	3:D:170:THR:HG22	2.03	0.58
3:H:168:VAL:CG1	3:H:169:HIS:H	2.16	0.58
4:L:62:GLY:HA3	4:L:81:GLY:CA	2.34	0.58
4:M:27:LEU:HB2	4:M:35:GLN:HB2	1.85	0.58
4:M:58:ALA:O	4:M:60:VAL:N	2.36	0.58
4:O:70:ASP:HB2	4:O:74:HIS:H	1.68	0.58
3:B:136:GLN:NE2	3:B:136:GLN:H	2.00	0.58
3:B:17:THR:CG2	3:B:83:ILE:O	2.39	0.58
3:D:83:ILE:HG22	3:D:86:LEU:CD2	2.33	0.58
2:G:77:PHE:C	2:G:78:THR:HG23	2.22	0.58
1:P:38:PRO:HB2	3:F:31:ASP:O	2.02	0.58
2:A:10:SER:O	2:A:11:LEU:CG	2.51	0.58
3:B:106:ASP:OD2	3:B:107:VAL:HG12	2.04	0.58
3:B:28:THR:O	3:B:30:THR:N	2.35	0.58
2:C:32:SER:C	2:C:34:THR:H	2.05	0.58
2:G:153:LYS:CD	2:G:153:LYS:CB	2.76	0.58
2:G:61:GLU:OE2	2:G:62:SER:N	2.37	0.58
3:H:20:ILE:HD11	3:H:80:TYR:HA	1.85	0.58
4:M:57:HIS:O	4:M:60:VAL:HG12	2.03	0.58
2:A:125:PRO:HD2	3:B:218:ARG:NH2	2.17	0.58
3:B:40:ALA:HB1	3:B:41:PRO:HD3	1.85	0.58
2:C:37:ASN:ND2	2:C:73:SER:HA	2.18	0.58
3:D:18:VAL:HG11	3:D:114:VAL:CG2	2.25	0.58
2:E:102:LEU:C	2:E:103:THR:CG2	2.66	0.58
3:H:182:LEU:CD1	3:H:183:SER:N	2.62	0.58
3:H:202:VAL:HG22	3:H:211:VAL:O	2.04	0.58
2:G:93:TYR:CE2	3:H:45:LEU:HD23	2.39	0.58
4:O:68:LEU:HB3	4:O:75:MET:HG3	1.85	0.58
2:A:118:ALA:N	2:A:118:ALA:CB	2.63	0.58
3:B:6:GLN:OE1	3:B:111:GLY:HA2	2.02	0.58
3:B:65:LYS:CA	3:B:65:LYS:NZ	2.63	0.58
2:C:62:SER:HA	1:Q:11:THR:O	2.02	0.58
2:E:24:LYS:HD2	2:E:76:ASP:HA	1.84	0.58
2:G:172:GLN:CG	2:G:179:TYR:CE2	2.85	0.58
2:G:93:TYR:CE1	3:H:45:LEU:CD2	2.87	0.58
2:A:141:PHE:C	2:A:142:LEU:HD23	2.23	0.58
2:C:82:SER:O	2:C:83:SER:CB	2.43	0.58
3:F:19:LYS:CE	3:F:19:LYS:CG	2.74	0.58
3:F:213:LYS:NZ	5:F:220:HOH:O	2.36	0.58
4:L:54:ALA:O	4:L:56:LEU:N	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:25:VAL:HG23	4:M:75:MET:HG2	1.85	0.58
4:N:42:THR:O	4:N:42:THR:HG23	2.04	0.58
4:O:53:TYR:HD1	4:O:56:LEU:HD23	1.66	0.58
2:A:162:GLN:NE2	2:A:162:GLN:CG	2.61	0.58
2:A:194:ARG:CG	2:A:195:HIS:H	2.11	0.58
3:D:155:VAL:CG1	3:D:156:THR:N	2.65	0.58
3:D:70:PHE:HE2	3:D:81:LEU:HD12	1.69	0.58
3:D:23:LYS:HA	3:D:78:THR:HA	1.85	0.58
3:F:129:LEU:HD12	3:F:144:GLY:C	2.24	0.58
3:F:73:GLU:O	3:F:75:SER:N	2.36	0.58
3:F:94:TYR:HD2	3:F:94:TYR:N	2.01	0.58
3:F:99:PHE:HD2	3:F:105:PHE:CD1	2.22	0.58
4:L:24:LYS:O	4:L:74:HIS:HA	2.04	0.58
2:A:55:TYR:C	2:A:57:ALA:N	2.54	0.58
3:B:150:TYR:N	3:B:179:LEU:HD23	2.19	0.58
2:C:166:LEU:CD2	3:D:174:VAL:HG11	2.34	0.58
3:F:129:LEU:HB2	3:F:144:GLY:C	2.23	0.58
3:F:174:VAL:O	3:F:180:TYR:HD1	1.87	0.58
3:F:199:THR:HG22	3:F:214:LYS:HB2	1.85	0.58
2:G:189:LYS:HG3	2:G:190:ASP:N	2.16	0.58
4:O:32:GLY:C	4:O:33:LYS:CG	2.72	0.58
4:O:55:ALA:O	4:O:56:LEU:C	2.37	0.58
2:A:13:VAL:HG21	2:A:84:VAL:HG21	1.86	0.58
2:C:62:SER:CB	1:Q:11:THR:O	2.51	0.58
2:E:42:TYR:HA	2:E:51:LYS:O	2.04	0.58
2:G:127:SER:C	2:G:129:GLU:H	2.04	0.58
2:G:128:SER:O	2:G:129:GLU:C	2.39	0.58
2:G:156:ILE:CG2	2:G:156:ILE:CA	2.75	0.58
4:L:57:HIS:HB3	4:L:61:ASN:ND2	2.07	0.58
2:A:118:ALA:C	2:A:118:ALA:CB	2.64	0.57
2:A:121:VAL:HG13	2:A:140:CYS:SG	2.44	0.57
3:D:152:PRO:O	3:D:154:PRO:N	2.37	0.57
3:D:165:SER:O	3:D:168:VAL:CG2	2.51	0.57
3:D:22:CYS:O	3:D:79:ALA:N	2.36	0.57
2:G:65:PRO:HB2	2:G:67:ARG:HG2	1.86	0.57
3:H:189:PRO:CD	3:H:192:THR:OG1	2.46	0.57
4:O:75:MET:O	4:O:77:ILE:HG13	2.04	0.57
2:C:29:LEU:HD12	2:C:39:LEU:HB2	1.84	0.57
3:D:176:GLN:O	3:D:176:GLN:OE1	2.22	0.57
3:F:56:GLY:O	3:F:58:PRO:HD3	2.04	0.57
4:N:68:LEU:CA	4:N:69:GLU:N	2.62	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:22:VAL:CA	1:Q:22:VAL:HB	2.17	0.57
3:D:103:GLN:NE2	3:D:103:GLN:CG	2.63	0.57
3:H:19:LYS:CA	3:H:19:LYS:CG	2.77	0.57
2:A:190:ASP:C	2:A:192:TYR:N	2.57	0.57
3:B:31:ASP:O	2:E:33:ARG:CZ	2.53	0.57
3:B:54:GLU:C	3:B:56:GLY:N	2.52	0.57
2:C:30:LEU:HG	2:C:30:LEU:CD1	2.18	0.57
2:E:125:PRO:HG3	2:E:215:PHE:CZ	2.39	0.57
3:F:78:THR:HG22	3:F:79:ALA:N	2.19	0.57
2:G:130:GLN:O	2:G:133:SER:CB	2.50	0.57
2:G:50:PRO:HD2	3:H:108:TRP:CD2	2.40	0.57
3:H:114:VAL:CG2	3:H:115:THR:N	2.67	0.57
3:H:164:LEU:CD1	3:H:164:LEU:CD2	2.79	0.57
4:M:28:ILE:CB	4:M:28:ILE:CD1	2.78	0.57
1:S:23:LYS:C	1:S:23:LYS:HD3	2.25	0.57
3:B:182:LEU:HD23	3:B:182:LEU:O	2.03	0.57
2:E:18:LYS:CG	2:E:19:VAL:N	2.67	0.57
3:B:54:GLU:O	3:B:56:GLY:N	2.38	0.57
2:C:4:MET:HG2	2:C:103:THR:HG22	1.85	0.57
2:E:7:SER:HA	2:E:8:PRO:C	2.20	0.57
3:F:11:LEU:HD22	3:F:11:LEU:C	2.25	0.57
3:F:148:LYS:HD2	3:F:181:THR:CG2	2.34	0.57
3:H:116:VAL:O	3:H:117:SER:HB2	2.05	0.57
4:M:29:PHE:HZ	4:M:57:HIS:NE2	2.02	0.57
3:B:169:HIS:O	3:B:171:PHE:CD1	2.57	0.57
2:C:144:ASN:HD22	2:C:144:ASN:H	1.52	0.57
2:C:130:GLN:HB2	3:D:127:TYR:CG	2.39	0.57
2:G:95:LYS:HE3	3:H:105:PHE:CE2	2.40	0.57
3:H:30:THR:HA	3:H:53:THR:CB	2.33	0.57
2:E:165:VAL:O	2:E:166:LEU:HG	2.05	0.57
3:F:10:GLU:O	3:F:114:VAL:HA	2.05	0.57
3:B:48:MET:HA	3:B:64:PHE:HD1	1.70	0.57
2:C:100:PRO:HB3	1:Q:31:VAL:CG1	2.33	0.57
3:D:36:TRP:CD1	3:D:70:PHE:CE2	2.92	0.57
2:E:201:GLU:HG2	2:E:212:VAL:HG21	1.86	0.57
2:E:85:GLN:O	2:E:87:GLU:N	2.38	0.57
3:F:100:LEU:CD2	3:F:101:LEU:H	2.02	0.57
2:G:89:GLN:C	2:G:89:GLN:CD	2.64	0.57
4:N:53:TYR:O	4:N:57:HIS:HB2	2.05	0.57
1:P:31:VAL:O	1:P:33:GLY:O	2.23	0.57
3:B:9:PRO:O	3:B:9:PRO:HG2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:8:PRO:HG2	2:C:108:THR:HG21	1.86	0.57
2:E:151:ASN:HD22	2:E:152:VAL:H	1.52	0.57
3:F:7:SER:HB2	3:F:21:SER:H	1.69	0.57
3:F:48:MET:HG2	3:F:64:PHE:HE1	1.70	0.57
2:G:194:ARG:NE	2:G:194:ARG:C	2.58	0.57
2:G:24:LYS:O	2:G:25:SER:O	2.23	0.57
2:G:53:LEU:O	2:G:54:ILE:HG23	2.03	0.57
1:S:29:GLN:NE2	3:H:52:ASN:CA	2.68	0.57
4:M:64:TRP:CE3	4:M:64:TRP:O	2.58	0.57
4:O:20:GLU:O	4:O:21:VAL:HG23	2.05	0.57
4:O:64:TRP:HE3	4:O:66:ALA:CB	2.15	0.57
2:A:75:THR:O	2:A:76:ASP:OD2	2.22	0.56
2:C:39:LEU:O	2:C:55:TYR:HA	2.04	0.56
3:D:197:THR:HA	3:D:214:LYS:HE2	1.87	0.56
3:F:41:PRO:O	3:F:42:GLY:C	2.43	0.56
2:G:53:LEU:HB3	2:G:54:ILE:HD13	1.86	0.56
3:H:129:LEU:CD1	3:H:145:CYS:N	2.68	0.56
3:H:211:VAL:HG23	3:H:212:ASP:N	2.20	0.56
2:A:126:PRO:CG	2:A:136:ALA:HB1	2.34	0.56
2:C:157:ASP:OD2	2:C:196:ASN:CB	2.52	0.56
2:C:205:LYS:HB2	2:C:205:LYS:NZ	2.20	0.56
3:D:39:GLN:HG3	3:D:44:GLY:O	2.06	0.56
2:E:196:ASN:OD1	2:E:196:ASN:O	2.22	0.56
2:G:20:THR:HG22	5:G:221:HOH:O	2.03	0.56
4:L:77:ILE:HD12	4:L:77:ILE:N	2.16	0.56
4:N:24:LYS:HG3	4:N:38:GLU:HG2	1.86	0.56
3:B:102:ARG:O	3:B:103:GLN:HG2	2.05	0.56
1:P:20:GLN:NE2	3:B:2:ILE:CD1	2.67	0.56
2:C:8:PRO:HG3	2:C:11:LEU:HG	1.86	0.56
3:D:174:VAL:O	3:D:175:LEU:O	2.24	0.56
3:F:20:ILE:HD12	3:F:112:THR:CB	2.34	0.56
2:G:126:PRO:HD3	2:G:138:VAL:HG22	1.87	0.56
3:H:129:LEU:HG	3:H:145:CYS:CA	2.35	0.56
3:H:173:ALA:HB1	3:H:180:TYR:CE1	2.40	0.56
3:H:29:PHE:HD2	3:H:74:THR:HG23	1.70	0.56
1:Q:11:THR:CG2	1:Q:11:THR:CA	2.75	0.56
2:A:126:PRO:HB2	2:A:131:LEU:HD21	1.87	0.56
2:A:89:GLN:NE2	2:A:173:ASP:O	2.38	0.56
3:D:15:GLY:N	3:D:86:LEU:O	2.37	0.56
2:E:156:ILE:O	2:E:157:ASP:C	2.42	0.56
2:G:169:TRP:CE3	2:G:169:TRP:N	2.73	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:26:ASN:CG	4:M:36:THR:HG23	2.25	0.56
1:S:40:ARG:HG2	1:S:41:GLY:H	1.69	0.56
3:B:36:TRP:CE3	3:B:81:LEU:HD12	2.40	0.56
2:C:144:ASN:ND2	2:C:144:ASN:H	2.03	0.56
2:C:155:LYS:NZ	2:C:158:GLY:HA2	2.21	0.56
3:D:102:ARG:CD	3:D:102:ARG:CB	2.77	0.56
3:D:20:ILE:CG2	3:D:112:THR:HG21	2.29	0.56
3:D:35:HIS:O	3:D:96:CYS:HA	2.04	0.56
3:F:11:LEU:O	3:F:11:LEU:CD1	2.46	0.56
3:H:65:LYS:O	3:H:67:ARG:N	2.35	0.56
2:C:130:GLN:O	2:C:133:SER:N	2.39	0.56
2:C:138:VAL:O	2:C:184:THR:HG23	2.04	0.56
2:E:123:ILE:C	2:E:124:PHE:CD1	2.79	0.56
2:G:131:LEU:O	2:G:134:GLY:N	2.28	0.56
3:H:1:GLN:HG2	3:H:2:ILE:N	2.20	0.56
2:A:141:PHE:CZ	3:B:185:SER:HB3	2.38	0.56
2:A:151:ASN:O	2:A:152:VAL:CG2	2.51	0.56
2:A:6:GLN:NE2	2:A:107:GLY:HA2	2.20	0.56
3:B:52:ASN:CB	3:B:55:THR:HB	2.36	0.56
3:D:52:ASN:C	3:D:54:GLU:N	2.57	0.56
2:E:8:PRO:HD3	4:N:53:TYR:CE1	2.41	0.56
3:H:160:ASN:O	3:H:161:SER:C	2.42	0.56
3:H:86:LEU:CB	3:H:86:LEU:CD1	2.79	0.56
2:C:11:LEU:CD2	4:M:37:ALA:HB2	2.35	0.56
2:A:220:CYS:HA	3:B:133:SER:CB	2.36	0.56
3:D:152:PRO:C	3:D:154:PRO:CD	2.68	0.56
3:F:159:TRP:CZ2	3:F:186:VAL:CG1	2.89	0.56
3:H:12:LYS:CE	3:H:12:LYS:HA	2.35	0.56
3:H:160:ASN:C	3:H:162:GLY:N	2.59	0.56
3:H:207:SER:CB	3:H:209:THR:HG23	2.35	0.56
2:C:62:SER:C	1:Q:11:THR:O	2.43	0.56
2:A:60:ARG:NH1	2:A:66:ASP:C	2.59	0.56
3:B:129:LEU:HB2	3:B:144:GLY:N	2.21	0.56
2:C:95:LYS:HZ3	3:D:104:TYR:HA	1.68	0.56
3:D:9:PRO:O	3:D:10:GLU:HG2	2.06	0.56
3:D:168:VAL:O	3:D:169:HIS:ND1	2.39	0.56
2:E:131:LEU:C	2:E:133:SER:H	2.09	0.56
2:E:55:TYR:HD1	3:F:104:TYR:CE2	2.23	0.56
3:H:20:ILE:HD11	3:H:80:TYR:CA	2.36	0.56
4:M:68:LEU:HD11	4:M:72:GLY:O	2.06	0.56
4:O:35:GLN:O	4:O:37:ALA:N	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:30:ILE:CG1	1:Q:30:ILE:O	2.52	0.56
2:C:61:GLU:HG3	2:C:62:SER:H	1.71	0.56
2:E:25:SER:OG	2:E:75:THR:HA	2.06	0.56
3:F:51:VAL:HG11	3:F:72:LEU:HD21	1.86	0.56
3:F:93:THR:C	3:F:94:TYR:CD2	2.79	0.56
2:G:102:LEU:HD22	3:H:47:TRP:HE1	1.70	0.56
2:G:152:VAL:HG13	2:G:201:GLU:C	2.26	0.56
4:L:75:MET:HE3	4:L:77:ILE:HD11	1.87	0.56
4:N:47:THR:O	4:N:51:TYR:CE1	2.59	0.56
2:A:118:ALA:HA	2:A:206:THR:HG21	1.87	0.56
3:D:17:THR:HG22	3:D:84:ASN:CA	2.35	0.56
3:F:199:THR:HG22	3:F:214:LYS:CA	2.36	0.56
3:H:161:SER:H	3:H:201:ASN:ND2	2.04	0.56
3:H:1:GLN:N	5:H:221:HOH:O	2.32	0.56
2:A:95:LYS:HD3	2:A:104:PHE:CE2	2.41	0.55
2:A:135:GLY:HA2	2:A:188:THR:HA	1.88	0.55
3:B:140:MET:O	3:B:141:VAL:HB	2.05	0.55
3:B:151:PHE:CG	3:B:152:PRO:HA	2.41	0.55
2:C:45:LYS:HG2	2:C:90:ALA:HB2	1.88	0.55
2:E:153:LYS:CE	2:E:160:GLU:OE2	2.52	0.55
2:E:188:THR:O	2:E:190:ASP:N	2.40	0.55
2:E:67:ARG:HH12	2:E:88:ASP:CG	2.09	0.55
3:F:14:PRO:O	3:F:16:GLU:N	2.38	0.55
2:G:194:ARG:O	2:G:194:ARG:NE	2.40	0.55
2:G:52:VAL:C	2:G:53:LEU:HD12	2.26	0.55
2:G:98:TYR:C	2:G:99:ILE:HG13	2.27	0.55
4:N:35:GLN:C	4:N:36:THR:OG1	2.37	0.55
4:O:58:ALA:CB	4:O:58:ALA:C	2.70	0.55
1:P:31:VAL:C	1:P:33:GLY:H	2.09	0.55
1:S:37:LEU:HD12	1:S:38:PRO:HD2	1.87	0.55
2:A:169:TRP:CE2	2:A:181:MET:HE3	2.42	0.55
2:E:145:PHE:C	2:E:145:PHE:CD1	2.79	0.55
2:G:19:VAL:O	2:G:80:THR:HA	2.06	0.55
3:H:214:LYS:CG	3:H:215:ILE:H	2.19	0.55
1:Q:23:LYS:CG	1:Q:23:LYS:CE	2.83	0.55
3:F:27:TYR:CZ	3:F:98:ARG:HD3	2.41	0.55
2:G:36:LYS:CB	2:G:36:LYS:CD	2.80	0.55
3:H:20:ILE:CD1	3:H:36:TRP:CH2	2.89	0.55
3:H:201:ASN:HB3	3:H:212:ASP:OD1	2.06	0.55
4:L:31:ASP:OD1	4:L:33:LYS:N	2.35	0.55
2:C:132:THR:O	2:C:133:SER:O	2.25	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:78:THR:CG2	3:D:79:ALA:H	2.19	0.55
2:E:18:LYS:HG2	2:E:19:VAL:H	1.70	0.55
2:G:128:SER:O	2:G:131:LEU:HB2	2.05	0.55
2:G:29:LEU:HD23	2:G:29:LEU:C	2.26	0.55
3:H:55:THR:N	3:H:55:THR:CB	2.62	0.55
3:H:67:ARG:HG3	3:H:68:PHE:CD2	2.41	0.55
3:B:218:ARG:C	3:B:218:ARG:CB	2.69	0.55
2:C:142:LEU:HD11	2:C:152:VAL:CG2	2.34	0.55
2:C:20:THR:HG23	2:C:20:THR:O	2.06	0.55
2:C:42:TYR:OH	3:D:105:PHE:N	2.31	0.55
2:E:31:ASN:CG	2:E:34:THR:HB	2.26	0.55
2:E:34:THR:O	2:E:35:ARG:HB2	2.06	0.55
2:E:37:ASN:HD21	2:E:74:GLY:H	1.53	0.55
3:F:40:ALA:HB3	3:F:43:LYS:HB2	1.88	0.55
2:G:112:LEU:HD23	2:G:177:SER:CB	2.36	0.55
2:G:157:ASP:HA	2:G:197:SER:HB2	1.89	0.55
2:G:7:SER:OG	2:G:24:LYS:HE3	2.06	0.55
4:M:34:ILE:HD13	4:M:34:ILE:C	2.26	0.55
4:O:79:PHE:N	4:O:79:PHE:CD1	2.73	0.55
2:A:205:LYS:CG	2:A:205:LYS:CA	2.81	0.55
3:B:120:LYS:CE	3:B:120:LYS:H	2.19	0.55
3:H:50:TRP:NE1	3:H:59:THR:CB	2.70	0.55
1:Q:40:ARG:CD	1:Q:45:GLY:O	2.55	0.55
2:A:189:LYS:O	2:A:192:TYR:HB3	2.06	0.55
3:B:170:THR:HA	3:B:184:SER:HB2	1.89	0.55
2:C:113:LYS:HD3	2:C:146:TYR:OH	2.07	0.55
3:D:1:GLN:HG2	3:D:2:ILE:H	1.72	0.55
2:G:196:ASN:ND2	2:G:216:ASN:C	2.60	0.55
2:G:36:LYS:HD3	2:G:56:TRP:CD2	2.42	0.55
3:H:103:GLN:CD	3:H:103:GLN:N	2.60	0.55
3:H:36:TRP:C	3:H:37:VAL:HG23	2.26	0.55
2:E:9:SER:N	4:N:38:GLU:O	2.37	0.55
2:A:171:ASP:O	2:A:172:GLN:C	2.34	0.55
2:A:27:GLN:O	2:A:28:SER:HB3	2.06	0.55
3:B:20:ILE:CG2	3:B:112:THR:HG21	2.37	0.55
2:C:50:PRO:O	2:C:51:LYS:NZ	2.32	0.55
3:D:111:GLY:C	3:D:112:THR:OG1	2.43	0.55
3:D:178:ASP:OD1	3:D:178:ASP:N	2.32	0.55
2:G:14:SER:O	2:G:17:GLU:HG3	2.07	0.55
2:G:29:LEU:HD23	2:G:29:LEU:O	2.04	0.55
3:H:129:LEU:HG	3:H:144:GLY:C	2.26	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:11:LEU:CD1	3:H:151:PHE:CE2	2.90	0.55
3:H:171:PHE:HB2	3:H:183:SER:O	2.07	0.55
3:H:17:THR:HG23	3:H:84:ASN:HA	1.89	0.55
4:M:49:GLU:HA	4:M:52:ARG:CB	2.28	0.55
3:B:160:ASN:HB2	3:B:163:SER:CB	2.34	0.55
3:B:204:HIS:CD2	3:B:204:HIS:C	2.80	0.55
2:E:31:ASN:HD22	2:E:34:THR:N	1.86	0.55
3:F:67:ARG:NH1	3:F:67:ARG:CG	2.61	0.55
3:F:99:PHE:CD2	3:F:105:PHE:CE1	2.94	0.55
2:G:61:GLU:O	2:G:62:SER:O	2.24	0.55
3:H:10:GLU:OE2	3:H:10:GLU:HA	2.07	0.55
3:H:188:VAL:CB	3:H:189:PRO:HD3	2.37	0.55
3:H:20:ILE:CD1	3:H:36:TRP:HH2	2.19	0.55
4:L:22:THR:OG1	4:L:40:LYS:HE2	2.07	0.55
1:P:36:LEU:O	1:P:37:LEU:CB	2.54	0.55
1:Q:32:GLY:O	1:Q:36:LEU:CB	2.55	0.55
2:A:112:LEU:HB3	2:A:172:GLN:NE2	2.22	0.55
2:A:167:ASN:HA	2:A:182:SER:O	2.06	0.55
2:A:144:ASN:OD1	3:B:169:HIS:CE1	2.60	0.55
3:B:182:LEU:HG	3:B:183:SER:H	1.71	0.55
3:B:33:SER:HA	3:B:53:THR:CG2	2.37	0.55
2:C:86:ALA:C	2:C:88:ASP:H	2.10	0.55
3:D:83:ILE:HG22	3:D:86:LEU:HD21	1.88	0.55
2:E:43:GLN:O	2:E:50:PRO:HA	2.07	0.55
3:F:82:GLN:CG	3:F:84:ASN:OD1	2.51	0.55
3:H:36:TRP:CZ2	3:H:80:TYR:O	2.59	0.55
3:B:33:SER:HA	3:B:53:THR:HG23	1.89	0.54
2:C:1:ASP:H2	2:C:27:GLN:NE2	2.02	0.54
3:D:11:LEU:HA	3:D:115:THR:O	2.07	0.54
2:E:144:ASN:HD21	3:F:169:HIS:CE1	2.25	0.54
2:E:36:LYS:HB3	2:E:56:TRP:CD1	2.43	0.54
3:F:120:LYS:CD	3:F:120:LYS:CB	2.77	0.54
2:G:167:ASN:ND2	2:G:167:ASN:O	2.35	0.54
3:H:188:VAL:HB	3:H:189:PRO:HD3	1.87	0.54
3:H:6:GLN:HA	3:H:21:SER:O	2.07	0.54
4:L:42:THR:O	4:L:43:PHE:C	2.45	0.54
4:O:34:ILE:O	4:O:35:GLN:CG	2.54	0.54
1:S:37:LEU:HG	1:S:37:LEU:CD2	2.21	0.54
2:A:198:TYR:O	2:A:215:PHE:N	2.40	0.54
3:D:27:TYR:CD2	3:D:28:THR:O	2.60	0.54
3:D:48:MET:HE1	3:D:94:TYR:CD1	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:176:ASP:CG	2:E:178:THR:HG23	2.28	0.54
2:G:171:ASP:OD1	2:G:172:GLN:N	2.41	0.54
3:H:210:LYS:O	3:H:210:LYS:HG2	2.06	0.54
4:N:42:THR:O	4:N:43:PHE:C	2.46	0.54
4:N:68:LEU:CD2	4:O:51:TYR:CZ	2.90	0.54
2:A:55:TYR:N	2:A:55:TYR:CD2	2.75	0.54
3:D:155:VAL:HG12	3:D:156:THR:N	2.20	0.54
3:F:130:ALA:HB2	3:F:215:ILE:HG22	1.88	0.54
2:G:123:ILE:HB	2:G:213:LYS:HB3	1.88	0.54
3:H:132:GLY:O	3:H:133:SER:C	2.45	0.54
3:H:1:GLN:CG	3:H:2:ILE:H	2.19	0.54
4:N:69:GLU:C	4:N:71:GLY:H	2.11	0.54
2:A:218:ASN:C	2:A:219:GLU:HG3	2.26	0.54
2:C:121:VAL:HB	2:C:213:LYS:HG3	1.89	0.54
3:D:10:GLU:HB3	3:D:114:VAL:HG23	1.89	0.54
3:D:215:ILE:N	3:D:215:ILE:HD12	2.17	0.54
3:F:194:PRO:HG3	3:F:217:PRO:HG2	1.90	0.54
2:G:126:PRO:HG3	2:G:137:SER:O	2.07	0.54
2:G:13:VAL:HG21	2:G:84:VAL:HG21	1.89	0.54
4:O:32:GLY:O	4:O:33:LYS:CG	2.54	0.54
4:O:67:ASP:OD1	4:O:76:ASN:O	2.24	0.54
3:B:60:TYR:HB2	3:B:65:LYS:NZ	2.21	0.54
2:E:146:TYR:CG	2:E:147:PRO:HA	2.43	0.54
3:H:174:VAL:HG23	3:H:181:THR:O	2.08	0.54
3:H:176:GLN:C	3:H:178:ASP:H	2.10	0.54
3:H:216:VAL:CB	3:H:216:VAL:C	2.73	0.54
2:C:176:ASP:C	2:C:178:THR:N	2.59	0.54
3:D:64:PHE:HD2	3:D:68:PHE:CZ	2.24	0.54
2:E:2:ILE:N	2:E:2:ILE:HD12	2.22	0.54
3:F:16:GLU:O	3:F:86:LEU:HB2	2.07	0.54
2:G:102:LEU:HB2	3:H:47:TRP:CG	2.43	0.54
2:G:156:ILE:HD12	2:G:161:ARG:HG3	1.89	0.54
4:O:57:HIS:C	4:O:60:VAL:HG12	2.27	0.54
4:O:29:PHE:HB3	4:O:61:ASN:ND2	2.23	0.54
2:A:46:PRO:O	2:A:46:PRO:HG2	2.08	0.54
2:A:95:LYS:HZ2	2:A:95:LYS:CB	2.18	0.54
2:C:55:TYR:C	2:C:57:ALA:N	2.57	0.54
2:C:62:SER:O	2:C:63:GLY:O	2.25	0.54
3:D:159:TRP:CE3	3:D:186:VAL:HG11	2.43	0.54
2:E:128:SER:C	2:E:130:GLN:N	2.58	0.54
2:E:125:PRO:HG3	2:E:215:PHE:CE2	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:29:LEU:HD12	2:E:39:LEU:HB2	1.88	0.54
2:E:39:LEU:HD22	2:E:39:LEU:C	2.27	0.54
3:F:73:GLU:O	3:F:74:THR:C	2.44	0.54
2:G:44:GLN:OE1	3:H:39:GLN:NE2	2.34	0.54
2:G:84:VAL:O	2:G:85:GLN:OE1	2.25	0.54
3:H:167:GLY:O	3:H:168:VAL:HG23	2.08	0.54
4:N:43:PHE:O	4:N:45:GLU:N	2.40	0.54
4:O:42:THR:HB	4:O:45:GLU:H	1.72	0.54
4:O:78:LYS:C	4:O:79:PHE:HD1	2.11	0.54
2:A:16:GLY:HA2	2:A:83:SER:HA	1.88	0.54
2:C:33:ARG:HD3	2:C:33:ARG:N	2.23	0.54
2:C:54:ILE:HG22	2:C:55:TYR:N	2.22	0.54
2:E:140:CYS:C	2:E:141:PHE:HD2	2.11	0.54
2:E:156:ILE:C	2:E:158:GLY:N	2.61	0.54
2:G:67:ARG:HB2	2:G:82:SER:OG	2.08	0.54
3:H:65:LYS:HD2	3:H:66:GLY:N	2.23	0.54
4:M:65:THR:H	4:M:65:THR:CG2	2.21	0.54
1:Q:15:THR:HA	1:Q:19:PRO:HG3	1.90	0.54
2:C:31:ASN:HB2	2:C:98:TYR:CZ	2.42	0.54
3:D:20:ILE:O	3:D:80:TYR:CD1	2.61	0.54
2:E:68:PHE:CE1	2:E:81:ILE:HG12	2.43	0.54
3:F:158:THR:HG23	3:F:201:ASN:CB	2.37	0.54
2:G:13:VAL:CG2	2:G:84:VAL:HG21	2.37	0.54
2:G:153:LYS:HD2	2:G:160:GLU:HG3	1.90	0.54
3:H:32:PHE:CE1	3:H:101:LEU:HG	2.43	0.54
4:L:65:THR:O	4:L:66:ALA:O	2.26	0.54
4:L:29:PHE:HA	4:L:79:PHE:HB2	1.88	0.54
1:S:3:THR:CG2	1:S:3:THR:CA	2.80	0.54
2:A:7:SER:OG	2:A:8:PRO:HA	2.07	0.54
2:C:131:LEU:HD12	2:C:136:ALA:HB2	1.89	0.54
2:E:24:LYS:NZ	2:E:24:LYS:CD	2.65	0.54
2:E:55:TYR:CD2	2:E:56:TRP:HB2	2.42	0.54
3:H:29:PHE:CD2	3:H:74:THR:HG23	2.42	0.54
4:M:21:VAL:O	4:M:41:GLY:CA	2.52	0.54
4:M:42:THR:HB	4:M:45:GLU:HB3	1.89	0.54
4:M:52:ARG:HH12	4:M:56:LEU:HD13	1.73	0.54
4:N:65:THR:CG2	4:N:65:THR:CA	2.80	0.54
4:O:27:LEU:CB	4:O:35:GLN:HB2	2.32	0.54
1:P:40:ARG:HG3	1:P:40:ARG:HH21	1.73	0.54
2:A:10:SER:HA	2:A:109:LYS:O	2.08	0.53
3:B:36:TRP:CE2	3:B:81:LEU:HB2	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:55:TYR:O	2:C:56:TRP:HB2	2.06	0.53
3:D:197:THR:HA	3:D:214:LYS:HE3	1.89	0.53
2:E:218:ASN:OD1	2:E:218:ASN:N	2.38	0.53
2:G:93:TYR:CZ	3:H:45:LEU:HD23	2.43	0.53
3:H:37:VAL:HG13	3:H:46:ASN:O	2.08	0.53
4:L:23:ILE:CG2	4:L:23:ILE:O	2.39	0.53
4:O:68:LEU:HD23	4:O:68:LEU:H	1.72	0.53
1:P:29:GLN:O	1:P:30:ILE:CB	2.55	0.53
3:D:43:LYS:HA	3:D:43:LYS:HE3	1.89	0.53
2:E:176:ASP:C	2:E:177:SER:OG	2.42	0.53
3:F:159:TRP:CH2	3:F:186:VAL:CG1	2.91	0.53
2:G:68:PHE:HD1	2:G:81:ILE:HD12	1.72	0.53
3:H:198:VAL:CA	3:H:198:VAL:CG2	2.79	0.53
3:H:78:THR:HG21	3:H:80:TYR:CZ	2.43	0.53
3:H:99:PHE:CG	3:H:99:PHE:CA	2.81	0.53
2:A:8:PRO:O	2:A:108:THR:HG23	2.07	0.53
2:A:196:ASN:C	2:A:196:ASN:OD1	2.47	0.53
2:A:23:CYS:O	2:A:77:PHE:HB2	2.08	0.53
2:A:98:TYR:CG	2:A:98:TYR:O	2.62	0.53
2:C:156:ILE:CD1	2:C:198:TYR:CD1	2.91	0.53
2:C:95:LYS:CE	3:D:104:TYR:HA	2.39	0.53
3:D:52:ASN:C	3:D:54:GLU:H	2.12	0.53
2:E:96:GLN:HE22	2:E:99:ILE:H	1.55	0.53
3:F:67:ARG:NH1	3:F:67:ARG:HG3	2.23	0.53
2:G:177:SER:C	2:G:178:THR:HG23	2.29	0.53
2:G:37:ASN:HB2	2:G:57:ALA:HB2	1.90	0.53
2:C:10:SER:O	4:M:37:ALA:HA	2.09	0.53
4:N:49:GLU:OE1	4:N:49:GLU:C	2.46	0.53
1:P:38:PRO:O	1:P:39:ARG:O	2.26	0.53
3:B:102:ARG:O	3:B:103:GLN:HB2	2.08	0.53
3:B:216:VAL:HG13	3:B:217:PRO:HD2	1.90	0.53
2:E:6:GLN:O	2:E:7:SER:HB3	2.07	0.53
2:G:173:ASP:HB3	2:G:177:SER:H	1.73	0.53
2:G:196:ASN:ND2	2:G:216:ASN:CB	2.71	0.53
3:H:20:ILE:HD11	3:H:81:LEU:N	2.24	0.53
4:N:56:LEU:HG	4:N:57:HIS:N	2.22	0.53
2:A:95:LYS:HD3	2:A:104:PHE:CZ	2.43	0.53
3:B:11:LEU:CD1	3:B:11:LEU:C	2.76	0.53
2:C:188:THR:HG23	2:C:191:GLU:HB2	1.90	0.53
3:D:161:SER:CA	3:D:201:ASN:HD21	2.22	0.53
2:E:215:PHE:O	2:E:215:PHE:CD1	2.61	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:30:LEU:HD23	2:E:31:ASN:N	2.23	0.53
3:F:175:LEU:HD13	3:F:180:TYR:CZ	2.43	0.53
2:G:205:LYS:O	2:G:207:SER:N	2.41	0.53
4:L:31:ASP:C	4:L:31:ASP:OD1	2.47	0.53
4:L:43:PHE:HA	4:L:46:ALA:HB3	1.91	0.53
2:A:110:LEU:O	2:A:110:LEU:HG	2.08	0.53
2:A:54:ILE:CD1	2:A:70:GLY:H	2.21	0.53
3:B:128:PRO:O	3:B:129:LEU:HD12	2.07	0.53
2:C:176:ASP:O	2:C:178:THR:N	2.41	0.53
2:C:182:SER:CB	3:D:171:PHE:CD2	2.92	0.53
2:C:19:VAL:HG13	2:C:81:ILE:HB	1.90	0.53
3:D:36:TRP:O	3:D:48:MET:HB2	2.09	0.53
2:E:175:LYS:O	2:E:175:LYS:CG	2.49	0.53
2:E:31:ASN:ND2	2:E:33:ARG:H	2.07	0.53
2:G:98:TYR:CD1	2:G:99:ILE:HG13	2.43	0.53
3:H:127:TYR:O	3:H:146:LEU:HB3	2.09	0.53
1:Q:12:LYS:O	1:Q:13:ARG:CG	2.54	0.53
2:A:68:PHE:CE1	2:A:81:ILE:HG12	2.44	0.53
3:B:86:LEU:HD23	3:B:116:VAL:HB	1.90	0.53
2:C:157:ASP:HA	2:C:197:SER:OG	2.08	0.53
2:E:135:GLY:HA2	2:E:188:THR:HA	1.91	0.53
2:E:144:ASN:ND2	3:F:169:HIS:CE1	2.77	0.53
2:E:49:SER:O	2:E:50:PRO:C	2.46	0.53
3:F:101:LEU:CD2	3:F:101:LEU:CD1	2.82	0.53
3:F:62:ASP:O	3:F:64:PHE:N	2.41	0.53
2:G:93:TYR:CD2	3:H:45:LEU:HD23	2.43	0.53
4:N:77:ILE:CG2	4:N:79:PHE:CZ	2.91	0.53
2:A:119:PRO:HG2	2:A:211:ILE:HD12	1.90	0.53
2:C:32:SER:C	2:C:34:THR:N	2.61	0.53
3:F:199:THR:HG22	3:F:214:LYS:HA	1.90	0.53
4:N:65:THR:CG2	4:N:65:THR:N	2.71	0.53
1:P:34:VAL:CB	2:A:38:TYR:OH	2.57	0.53
2:C:166:LEU:HD23	3:D:174:VAL:HG11	1.90	0.53
3:D:118:SER:C	3:D:119:ALA:O	2.39	0.53
2:E:127:SER:O	2:E:128:SER:C	2.45	0.53
3:F:1:GLN:CG	3:F:1:GLN:CA	2.83	0.53
4:L:57:HIS:O	4:L:61:ASN:OD1	2.26	0.53
4:L:68:LEU:N	4:L:68:LEU:HD12	2.23	0.53
2:A:60:ARG:CZ	2:A:66:ASP:HA	2.39	0.53
2:C:199:THR:HB	2:C:214:SER:HB2	1.89	0.53
2:G:130:GLN:O	2:G:131:LEU:O	2.26	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:137:SER:HG	2:G:186:THR:CA	2.17	0.53
2:G:6:GLN:NE2	2:G:108:THR:H	2.08	0.53
3:H:24:ALA:O	3:H:25:SER:HB3	2.09	0.53
2:A:196:ASN:HD21	2:A:218:ASN:H	1.55	0.52
3:F:48:MET:SD	3:F:48:MET:CB	2.90	0.52
4:M:75:MET:HG2	4:M:77:ILE:HD11	1.91	0.52
3:B:5:VAL:HG23	3:B:23:LYS:O	2.09	0.52
3:D:20:ILE:CG1	3:D:81:LEU:HB3	2.39	0.52
3:F:129:LEU:HB2	3:F:144:GLY:O	2.10	0.52
3:F:78:THR:CG2	3:F:79:ALA:N	2.71	0.52
4:M:52:ARG:HH12	4:M:56:LEU:CD1	2.22	0.52
2:A:118:ALA:HB2	2:A:206:THR:OG1	2.09	0.52
2:A:144:ASN:H	3:B:169:HIS:CE1	2.25	0.52
2:A:65:PRO:O	2:A:66:ASP:C	2.48	0.52
2:C:125:PRO:HB3	2:C:215:PHE:CE1	2.44	0.52
2:C:4:MET:CE	2:C:25:SER:HB3	2.37	0.52
3:D:186:VAL:O	3:D:186:VAL:HG22	2.08	0.52
3:F:20:ILE:HG23	3:F:81:LEU:HB3	1.92	0.52
4:N:53:TYR:CZ	4:N:57:HIS:ND1	2.77	0.52
3:B:67:ARG:NH2	3:B:68:PHE:HE2	2.08	0.52
3:B:36:TRP:CE3	3:B:95:PHE:O	2.63	0.52
2:C:156:ILE:HB	2:C:161:ARG:HG3	1.91	0.52
2:E:33:ARG:HH11	2:E:33:ARG:HG3	1.74	0.52
3:H:6:GLN:NE2	3:H:111:GLY:C	2.62	0.52
3:H:99:PHE:HB2	3:H:105:PHE:HE1	1.74	0.52
4:L:58:ALA:HA	4:L:62:GLY:O	2.10	0.52
4:O:27:LEU:O	4:O:34:ILE:CA	2.52	0.52
1:P:24:PHE:CB	1:P:25:PRO:CD	2.87	0.52
3:B:22:CYS:O	3:B:78:THR:HA	2.10	0.52
3:B:40:ALA:HB3	3:B:43:LYS:CB	2.39	0.52
2:C:108:THR:O	2:C:109:LYS:C	2.42	0.52
3:D:146:LEU:C	3:D:146:LEU:HD12	2.27	0.52
2:E:60:ARG:NH2	2:E:66:ASP:HA	2.24	0.52
3:F:17:THR:HG22	3:F:18:VAL:N	2.24	0.52
2:G:113:LYS:HG2	2:G:146:TYR:HH	1.69	0.52
2:G:20:THR:HB	2:G:80:THR:CG2	2.39	0.52
3:H:61:ALA:O	3:H:64:PHE:N	2.41	0.52
2:A:216:ASN:O	2:A:217:ARG:C	2.48	0.52
3:B:169:HIS:O	3:B:170:THR:C	2.43	0.52
3:B:67:ARG:HB3	3:B:67:ARG:NH1	2.24	0.52
2:C:144:ASN:N	2:C:144:ASN:HD22	2.05	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:130:GLN:HA	3:D:127:TYR:CE1	2.44	0.52
3:D:175:LEU:CD1	3:D:180:TYR:CE1	2.93	0.52
2:E:13:VAL:HG23	2:E:14:SER:O	2.10	0.52
2:E:96:GLN:CG	2:E:96:GLN:O	2.58	0.52
3:F:100:LEU:CD2	3:F:101:LEU:N	2.67	0.52
3:H:165:SER:O	3:H:167:GLY:N	2.43	0.52
3:H:29:PHE:CG	3:H:29:PHE:O	2.61	0.52
1:P:32:GLY:HA2	2:A:100:PRO:HD3	1.90	0.52
3:D:138:ASN:HD22	3:D:139:SER:N	1.99	0.52
3:D:201:ASN:HA	3:D:212:ASP:HA	1.91	0.52
1:P:40:ARG:HD3	3:F:100:LEU:HD11	1.91	0.52
3:F:41:PRO:O	3:F:43:LYS:HG3	2.09	0.52
3:F:91:THR:HG22	3:F:91:THR:O	2.05	0.52
1:Q:22:VAL:CB	1:Q:22:VAL:C	2.69	0.52
3:B:31:ASP:C	3:B:32:PHE:CG	2.83	0.52
3:B:73:GLU:OE2	3:B:75:SER:HB3	2.10	0.52
3:D:202:VAL:HG13	3:D:211:VAL:O	2.09	0.52
2:E:167:ASN:OD1	2:E:183:SER:CB	2.58	0.52
3:F:31:ASP:O	3:F:32:PHE:CD2	2.62	0.52
3:F:70:PHE:HE2	3:F:81:LEU:HD23	1.75	0.52
3:F:75:SER:C	3:F:77:SER:H	2.11	0.52
3:F:7:SER:HB3	3:F:20:ILE:CG1	2.32	0.52
2:G:127:SER:O	2:G:131:LEU:HD23	2.09	0.52
2:G:123:ILE:H	2:G:213:LYS:CE	2.23	0.52
3:H:164:LEU:HA	3:H:164:LEU:CD2	2.39	0.52
3:H:28:THR:HG22	3:H:31:ASP:H	1.74	0.52
3:H:52:ASN:CB	3:H:55:THR:HB	2.38	0.52
2:A:102:LEU:C	2:A:103:THR:CG2	2.78	0.52
2:A:20:THR:O	4:L:53:TYR:HE1	1.92	0.52
2:A:211:ILE:HG21	2:A:211:ILE:CD1	2.40	0.52
2:C:24:LYS:HD2	2:C:76:ASP:OD2	2.10	0.52
2:G:173:ASP:HB3	2:G:177:SER:N	2.25	0.52
3:H:194:PRO:O	3:H:195:SER:C	2.47	0.52
2:G:22:SER:HB3	4:O:56:LEU:HD21	1.92	0.52
1:S:19:PRO:HG2	1:S:20:GLN:HG2	1.92	0.52
2:A:130:GLN:C	2:A:132:THR:H	2.12	0.52
2:A:211:ILE:CD1	2:A:211:ILE:CG2	2.87	0.52
2:E:165:VAL:CG1	5:E:225:HOH:O	2.55	0.52
2:G:130:GLN:HG2	2:G:135:GLY:O	2.10	0.52
3:H:60:TYR:OH	3:H:69:ALA:CA	2.49	0.52
4:N:78:LYS:C	4:N:79:PHE:CD1	2.83	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:O:28:ILE:CD1	4:O:28:ILE:N	2.72	0.52
2:A:154:TRP:O	2:A:160:GLU:HA	2.10	0.51
2:A:167:ASN:HB3	2:A:181:MET:HE1	1.92	0.51
2:A:97:ALA:HA	2:A:102:LEU:CD2	2.40	0.51
3:B:151:PHE:CD1	3:B:152:PRO:CA	2.93	0.51
3:D:17:THR:CG2	3:D:84:ASN:HA	2.39	0.51
3:F:52:ASN:O	3:F:53:THR:C	2.47	0.51
2:G:53:LEU:O	2:G:54:ILE:CG2	2.58	0.51
3:H:2:ILE:HG21	3:H:27:TYR:CD1	2.45	0.51
3:H:72:LEU:HD23	3:H:74:THR:N	2.24	0.51
4:L:47:THR:HG22	4:L:48:ALA:N	2.25	0.51
4:M:20:GLU:HG2	4:M:20:GLU:O	2.09	0.51
4:O:58:ALA:O	4:O:61:ASN:N	2.28	0.51
1:S:22:VAL:CG1	1:S:22:VAL:O	2.52	0.51
2:A:151:ASN:C	2:A:152:VAL:HG23	2.31	0.51
2:C:130:GLN:HE22	2:C:137:SER:CB	2.22	0.51
2:E:11:LEU:HG	2:E:11:LEU:CD1	2.19	0.51
2:E:129:GLU:C	2:E:131:LEU:H	2.14	0.51
3:F:178:ASP:O	3:F:179:LEU:HD23	2.10	0.51
2:G:27:GLN:C	2:G:28:SER:O	2.48	0.51
3:H:150:TYR:O	3:H:180:TYR:HB2	2.11	0.51
4:O:58:ALA:C	4:O:60:VAL:N	2.64	0.51
3:D:1:GLN:HE22	1:Q:13:ARG:HD2	1.75	0.51
1:Q:42:PRO:O	1:Q:43:ARG:HB3	2.11	0.51
2:A:95:LYS:HA	2:A:103:THR:O	2.11	0.51
3:B:48:MET:SD	3:B:64:PHE:CE1	3.04	0.51
2:C:173:ASP:O	2:C:177:SER:N	2.43	0.51
2:C:56:TRP:O	2:C:57:ALA:CB	2.58	0.51
3:F:159:TRP:HE3	3:F:199:THR:O	1.92	0.51
3:F:58:PRO:CG	3:F:58:PRO:O	2.48	0.51
3:H:151:PHE:H	3:H:152:PRO:CD	2.23	0.51
3:H:65:LYS:C	3:H:67:ARG:N	2.64	0.51
3:H:87:LYS:HG3	5:H:227:HOH:O	2.09	0.51
4:M:55:ALA:HB2	5:M:83:HOH:O	2.10	0.51
3:B:52:ASN:OD1	3:B:55:THR:HB	2.11	0.51
2:E:154:TRP:CE2	2:E:185:LEU:HB3	2.45	0.51
2:E:43:GLN:HA	2:E:91:VAL:O	2.10	0.51
3:F:8:GLY:O	3:F:10:GLU:HG2	2.10	0.51
2:G:36:LYS:HD3	2:G:56:TRP:CE2	2.45	0.51
4:N:22:THR:CG2	4:N:23:ILE:N	2.68	0.51
2:A:86:ALA:O	2:A:89:GLN:HG3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:161:SER:H	3:B:201:ASN:HD21	1.56	0.51
2:C:169:TRP:NE1	2:C:181:MET:SD	2.83	0.51
3:D:2:ILE:HA	3:D:25:SER:O	2.11	0.51
3:F:143:LEU:HD12	3:F:198:VAL:HG11	1.92	0.51
3:F:75:SER:HG	3:F:76:ALA:H	1.55	0.51
3:H:182:LEU:CD1	3:H:182:LEU:C	2.62	0.51
2:C:145:PHE:C	2:C:145:PHE:HD1	2.14	0.51
2:C:137:SER:HA	2:C:186:THR:HA	1.92	0.51
3:D:40:ALA:HB3	3:D:43:LYS:HG3	1.93	0.51
2:E:194:ARG:CZ	2:E:195:HIS:NE2	2.74	0.51
2:E:88:ASP:C	2:E:90:ALA:N	2.64	0.51
3:F:93:THR:HG23	3:F:113:THR:HG23	1.93	0.51
3:H:17:THR:HA	3:H:86:LEU:HD13	1.93	0.51
4:L:53:TYR:CZ	4:L:57:HIS:NE2	2.79	0.51
4:L:53:TYR:O	4:L:56:LEU:HB3	2.11	0.51
4:N:44:GLU:OE2	4:O:52:ARG:NH1	2.42	0.51
4:O:26:ASN:O	4:O:27:LEU:HD23	2.10	0.51
4:O:67:ASP:OD1	4:O:67:ASP:N	2.43	0.51
1:Q:22:VAL:CG2	1:Q:22:VAL:CA	2.82	0.51
2:A:88:ASP:C	2:A:90:ALA:N	2.62	0.51
2:C:3:VAL:HG12	2:C:4:MET:N	2.25	0.51
2:C:52:VAL:HG21	3:D:104:TYR:HD1	1.75	0.51
3:D:158:THR:HG1	3:D:201:ASN:ND2	2.09	0.51
3:D:3:GLN:HG2	3:D:4:LEU:N	2.21	0.51
3:D:74:THR:O	3:D:76:ALA:N	2.44	0.51
2:A:12:ALA:N	4:L:36:THR:O	2.42	0.51
3:B:159:TRP:O	3:B:160:ASN:HB2	2.09	0.51
3:B:193:TRP:CG	3:B:194:PRO:CA	2.90	0.51
3:B:62:ASP:C	3:B:64:PHE:H	2.14	0.51
3:B:9:PRO:CG	3:B:9:PRO:O	2.55	0.51
2:E:148:LYS:NZ	2:E:148:LYS:CB	2.74	0.51
2:E:65:PRO:O	2:E:67:ARG:N	2.44	0.51
3:F:174:VAL:HG12	3:F:175:LEU:N	2.26	0.51
2:G:198:TYR:O	2:G:215:PHE:N	2.44	0.51
2:G:55:TYR:CE1	2:G:59:THR:HG22	2.46	0.51
2:G:86:ALA:C	2:G:88:ASP:N	2.63	0.51
3:H:18:VAL:HG13	3:H:18:VAL:O	2.11	0.51
4:M:65:THR:H	4:M:65:THR:HG22	1.76	0.51
3:D:54:GLU:OE1	1:Q:27:GLY:CA	2.58	0.51
2:C:36:LYS:HA	2:C:36:LYS:HE2	1.93	0.51
3:D:86:LEU:HD13	3:D:116:VAL:HG22	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:217:ARG:O	2:E:218:ASN:C	2.49	0.51
2:E:21:MET:O	2:E:78:THR:HG22	2.11	0.51
2:G:186:THR:C	2:G:187:LEU:HG	2.30	0.51
2:G:203:THR:HA	2:G:210:PRO:CG	2.40	0.51
2:G:55:TYR:CE1	2:G:59:THR:CG2	2.94	0.51
3:H:20:ILE:HD11	3:H:80:TYR:C	2.30	0.51
2:C:218:ASN:N	2:C:218:ASN:OD1	2.43	0.51
3:F:158:THR:HG23	3:F:201:ASN:O	2.11	0.51
2:G:130:GLN:O	2:G:133:SER:N	2.43	0.51
2:G:137:SER:OG	2:G:186:THR:CA	2.51	0.51
2:G:175:LYS:CE	2:G:175:LYS:CG	2.82	0.51
3:H:197:THR:HG22	3:H:214:LYS:HE3	1.92	0.51
4:O:58:ALA:HA	4:O:62:GLY:O	2.11	0.51
2:A:176:ASP:CG	2:A:178:THR:CG2	2.74	0.50
2:A:50:PRO:HB2	3:B:108:TRP:CZ2	2.46	0.50
3:B:131:PRO:O	3:B:218:ARG:HG3	2.11	0.50
2:C:160:GLU:C	2:C:161:ARG:HG2	2.30	0.50
2:G:68:PHE:CE1	2:G:81:ILE:HD12	2.46	0.50
3:H:149:GLY:O	3:H:150:TYR:C	2.48	0.50
3:H:217:PRO:O	3:H:218:ARG:O	2.29	0.50
3:H:18:VAL:HG12	3:H:86:LEU:HD21	1.93	0.50
4:O:51:TYR:O	4:O:52:ARG:C	2.43	0.50
2:A:188:THR:HG21	2:A:191:GLU:OE2	2.11	0.50
2:A:138:VAL:HG21	2:A:198:TYR:CD1	2.46	0.50
3:B:120:LYS:O	3:B:121:THR:C	2.49	0.50
2:C:198:TYR:O	2:C:214:SER:HB2	2.11	0.50
3:D:65:LYS:O	3:D:65:LYS:HG2	2.11	0.50
2:E:146:TYR:CD2	2:E:147:PRO:HA	2.47	0.50
3:F:156:THR:CG2	3:F:156:THR:CA	2.83	0.50
3:F:174:VAL:O	3:F:180:TYR:HA	2.12	0.50
2:G:152:VAL:HG22	2:G:202:ALA:HA	1.94	0.50
3:H:6:GLN:CD	3:H:111:GLY:N	2.63	0.50
4:O:35:GLN:O	4:O:36:THR:C	2.45	0.50
2:A:187:LEU:HD12	2:A:192:TYR:HB2	1.93	0.50
2:A:196:ASN:OD1	2:A:216:ASN:HB3	2.11	0.50
2:C:130:GLN:O	2:C:131:LEU:C	2.50	0.50
3:D:35:HIS:NE2	3:D:99:PHE:CB	2.74	0.50
3:F:159:TRP:CE3	3:F:199:THR:O	2.65	0.50
2:G:130:GLN:O	2:G:131:LEU:C	2.47	0.50
3:H:1:GLN:O	3:H:2:ILE:C	2.49	0.50
2:A:198:TYR:HB3	2:A:215:PHE:HD2	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:29:LEU:HD12	2:A:77:PHE:CE2	2.45	0.50
2:C:211:ILE:O	2:C:211:ILE:HG22	2.10	0.50
2:C:54:ILE:HG21	2:C:70:GLY:HA3	1.92	0.50
3:D:7:SER:O	3:D:112:THR:HG23	2.12	0.50
3:D:146:LEU:HD12	3:D:147:VAL:H	1.77	0.50
2:E:2:ILE:N	2:E:2:ILE:CD1	2.75	0.50
2:E:141:PHE:HZ	3:F:183:SER:HB2	1.75	0.50
2:G:203:THR:HA	2:G:210:PRO:CB	2.41	0.50
2:G:87:GLU:CD	2:G:87:GLU:H	2.14	0.50
1:P:24:PHE:CB	1:P:25:PRO:HD2	2.35	0.50
1:P:40:ARG:NE	3:F:98:ARG:NH1	2.54	0.50
3:B:176:GLN:O	3:B:177:SER:CB	2.59	0.50
2:G:54:ILE:CD1	2:G:54:ILE:CG2	2.89	0.50
4:N:46:ALA:C	4:N:48:ALA:N	2.59	0.50
4:N:64:TRP:HA	4:N:78:LYS:O	2.11	0.50
1:S:11:THR:CG2	1:S:12:LYS:HZ2	2.24	0.50
1:S:23:LYS:CD	1:S:23:LYS:C	2.79	0.50
2:A:25:SER:HB3	2:A:29:LEU:HD11	1.92	0.50
3:D:151:PHE:O	3:D:152:PRO:C	2.50	0.50
2:E:189:LYS:O	2:E:189:LYS:HD3	2.12	0.50
2:E:31:ASN:C	2:E:31:ASN:ND2	2.65	0.50
3:F:52:ASN:ND2	3:F:57:GLU:HB2	2.21	0.50
2:G:125:PRO:CB	2:G:215:PHE:CZ	2.92	0.50
2:G:52:VAL:HG22	2:G:53:LEU:H	1.77	0.50
2:G:54:ILE:CD1	2:G:54:ILE:CB	2.81	0.50
2:G:81:ILE:CG2	2:G:84:VAL:HG12	2.41	0.50
2:G:95:LYS:HE3	2:G:102:LEU:HD23	1.93	0.50
3:H:132:GLY:O	3:H:135:ALA:N	2.44	0.50
3:H:35:HIS:HA	3:H:49:GLY:O	2.11	0.50
4:L:58:ALA:C	4:L:60:VAL:H	2.15	0.50
4:M:64:TRP:CD2	4:M:64:TRP:O	2.64	0.50
4:N:52:ARG:NH1	4:O:43:PHE:CD2	2.80	0.50
2:A:6:GLN:HG2	2:A:94:CYS:SG	2.51	0.50
2:A:6:GLN:OE1	2:A:93:TYR:HA	2.12	0.50
3:B:55:THR:HG22	3:B:57:GLU:CB	2.41	0.50
2:E:151:ASN:ND2	2:E:152:VAL:H	2.10	0.50
2:E:9:SER:HB3	4:N:38:GLU:O	2.12	0.50
2:G:156:ILE:CG2	2:G:156:ILE:C	2.80	0.50
2:G:55:TYR:CZ	2:G:59:THR:CG2	2.94	0.50
3:H:4:LEU:CD2	3:H:24:ALA:HA	2.38	0.50
3:H:1:GLN:CG	3:H:2:ILE:N	2.74	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:126:PRO:HB2	2:A:131:LEU:CD2	2.42	0.50
2:C:16:GLY:HA2	2:C:84:VAL:O	2.11	0.50
2:C:67:ARG:HG3	2:C:68:PHE:N	2.26	0.50
2:E:12:ALA:CB	2:E:113:LYS:NZ	2.75	0.50
2:E:31:ASN:HD21	2:E:34:THR:N	2.05	0.50
3:F:188:VAL:HG11	5:F:221:HOH:O	2.10	0.50
2:G:112:LEU:HG	2:G:113:LYS:H	1.77	0.50
2:G:205:LYS:CD	2:G:205:LYS:NZ	2.67	0.50
3:H:214:LYS:CG	3:H:215:ILE:N	2.70	0.50
1:Q:31:VAL:CG2	1:Q:31:VAL:CA	2.79	0.50
2:A:165:VAL:C	2:A:166:LEU:HD12	2.32	0.50
2:A:67:ARG:NH2	2:A:88:ASP:OD1	2.45	0.50
3:B:120:LYS:HD3	3:B:120:LYS:N	2.10	0.50
3:B:136:GLN:CD	3:B:136:GLN:H	2.16	0.50
3:B:181:THR:HG22	3:B:182:LEU:N	2.27	0.50
3:B:48:MET:HA	3:B:64:PHE:HE1	1.75	0.50
2:C:194:ARG:O	2:C:195:HIS:O	2.30	0.50
3:D:125:SER:C	3:D:126:VAL:HG23	2.31	0.50
2:E:204:HIS:CE1	2:E:205:LYS:HG3	2.46	0.50
2:E:85:GLN:C	2:E:87:GLU:N	2.65	0.50
3:F:50:TRP:N	3:F:50:TRP:CD1	2.77	0.50
3:F:7:SER:N	3:F:21:SER:OG	2.44	0.50
2:G:122:SER:CA	2:G:213:LYS:HE3	2.33	0.50
2:G:93:TYR:CD1	3:H:45:LEU:HD23	2.47	0.50
2:G:56:TRP:CZ2	3:H:102:ARG:HD3	2.46	0.50
3:H:181:THR:OG1	3:H:182:LEU:N	2.43	0.50
3:H:36:TRP:CA	3:H:95:PHE:O	2.55	0.50
2:A:34:THR:O	2:A:35:ARG:HB2	2.12	0.49
3:B:170:THR:HA	3:B:184:SER:HA	1.93	0.49
2:A:168:SER:OG	3:B:172:PRO:O	2.20	0.49
3:B:177:SER:O	3:B:178:ASP:C	2.50	0.49
2:C:124:PHE:HB2	2:C:139:VAL:HB	1.94	0.49
3:D:162:GLY:O	3:D:164:LEU:N	2.45	0.49
3:D:161:SER:HA	3:D:201:ASN:HD21	1.77	0.49
2:E:55:TYR:C	2:E:57:ALA:N	2.64	0.49
2:E:88:ASP:HB3	2:E:92:TYR:OH	2.11	0.49
3:H:133:SER:N	3:H:218:ARG:HD3	2.21	0.49
4:L:68:LEU:HG	4:L:75:MET:HG3	1.94	0.49
2:A:117:ALA:O	2:A:118:ALA:C	2.48	0.49
3:B:36:TRP:HB2	3:B:48:MET:HB2	1.93	0.49
3:B:67:ARG:NH1	3:B:84:ASN:O	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:139:VAL:HG12	2:C:140:CYS:N	2.27	0.49
2:C:172:GLN:HG3	2:C:179:TYR:CE1	2.47	0.49
3:D:132:GLY:O	3:D:133:SER:C	2.50	0.49
3:F:165:SER:O	3:F:168:VAL:CG2	2.52	0.49
2:G:208:THR:C	2:G:210:PRO:HD3	2.33	0.49
2:G:29:LEU:O	2:G:30:LEU:HB3	2.12	0.49
3:H:132:GLY:O	3:H:135:ALA:CB	2.60	0.49
3:H:167:GLY:C	3:H:168:VAL:HG23	2.32	0.49
4:N:34:ILE:CG2	4:N:35:GLN:N	2.75	0.49
4:N:66:ALA:N	4:O:68:LEU:O	2.45	0.49
1:Q:16:ASN:HD21	1:Q:17:ARG:HG3	1.71	0.49
2:A:191:GLU:N	2:A:192:TYR:N	2.59	0.49
2:A:121:VAL:O	2:A:213:LYS:HE2	2.12	0.49
2:C:214:SER:OG	2:C:215:PHE:N	2.28	0.49
2:G:97:ALA:O	2:G:99:ILE:N	2.44	0.49
3:H:6:GLN:OE1	3:H:111:GLY:N	2.46	0.49
3:H:199:THR:HA	3:H:214:LYS:HA	1.94	0.49
3:H:1:GLN:O	3:H:2:ILE:O	2.31	0.49
4:L:64:TRP:HZ3	4:L:66:ALA:HB3	1.77	0.49
4:M:27:LEU:HB3	4:M:29:PHE:HE1	1.76	0.49
4:M:47:THR:C	4:M:49:GLU:H	2.16	0.49
4:N:31:ASP:OD2	4:N:33:LYS:CG	2.50	0.49
4:N:58:ALA:C	4:N:60:VAL:N	2.66	0.49
3:B:159:TRP:CE2	3:B:186:VAL:HG13	2.47	0.49
2:C:155:LYS:CE	2:C:158:GLY:HA2	2.42	0.49
2:C:61:GLU:O	2:C:64:VAL:HG23	2.12	0.49
3:D:97:ALA:HB2	3:D:108:TRP:CB	2.42	0.49
3:D:11:LEU:HG	3:D:152:PRO:HG3	1.93	0.49
3:D:159:TRP:CZ3	3:D:186:VAL:HG11	2.46	0.49
2:C:170:THR:HG23	3:D:171:PHE:CD1	2.47	0.49
3:D:30:THR:CG2	3:D:31:ASP:OD1	2.57	0.49
3:D:96:CYS:SG	3:D:96:CYS:O	2.70	0.49
2:E:41:TRP:CD2	2:E:79:LEU:HB2	2.47	0.49
3:F:29:PHE:CG	3:F:29:PHE:O	2.65	0.49
3:F:93:THR:C	3:F:94:TYR:HD2	2.16	0.49
2:G:121:VAL:HG13	2:G:140:CYS:SG	2.53	0.49
1:S:29:GLN:HA	3:H:101:LEU:HD22	1.93	0.49
4:N:62:GLY:HA3	4:N:79:PHE:HB3	1.93	0.49
4:O:54:ALA:O	4:O:57:HIS:N	2.40	0.49
1:P:23:LYS:O	1:P:24:PHE:C	2.50	0.49
1:Q:15:THR:HA	1:Q:19:PRO:CG	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:40:ARG:HB3	1:Q:40:ARG:HH11	1.76	0.49
1:S:29:GLN:NE2	3:H:53:THR:OG1	2.45	0.49
2:E:36:LYS:HE2	2:E:37:ASN:N	2.22	0.49
3:F:121:THR:HG23	3:F:152:PRO:HD3	1.94	0.49
3:F:4:LEU:N	3:F:4:LEU:HD12	2.27	0.49
2:G:151:ASN:C	2:G:152:VAL:CG2	2.81	0.49
3:H:148:LYS:HA	3:H:181:THR:HA	1.94	0.49
3:H:93:THR:HG23	3:H:113:THR:HA	1.95	0.49
4:L:55:ALA:CB	4:L:55:ALA:C	2.69	0.49
4:L:56:LEU:C	4:L:58:ALA:N	2.66	0.49
4:M:26:ASN:OD1	4:M:34:ILE:HD11	2.12	0.49
4:M:65:THR:OG1	4:M:66:ALA:N	2.43	0.49
4:O:26:ASN:CB	4:O:76:ASN:ND2	2.76	0.49
1:Q:23:LYS:CB	1:Q:23:LYS:CD	2.83	0.49
1:Q:33:GLY:HA2	1:Q:36:LEU:CB	2.20	0.49
2:A:151:ASN:OD1	2:A:152:VAL:O	2.30	0.49
3:B:101:LEU:O	3:B:103:GLN:OE1	2.30	0.49
2:C:17:GLU:O	2:C:19:VAL:HG12	2.13	0.49
2:C:54:ILE:HG21	2:C:57:ALA:O	2.12	0.49
3:D:123:PRO:O	3:D:123:PRO:HG2	2.12	0.49
3:D:150:TYR:OH	3:D:182:LEU:HD22	2.12	0.49
2:E:11:LEU:HD13	2:E:19:VAL:CG2	2.42	0.49
2:G:112:LEU:CD2	2:G:112:LEU:CD1	2.77	0.49
3:H:170:THR:O	3:H:171:PHE:HB2	2.11	0.49
3:H:52:ASN:CG	3:H:55:THR:HB	2.33	0.49
3:H:81:LEU:HD22	3:H:82:GLN:N	2.28	0.49
3:H:99:PHE:CB	3:H:99:PHE:C	2.75	0.49
4:O:25:VAL:CG1	4:O:39:PHE:HE1	2.23	0.49
3:B:146:LEU:HD12	3:B:147:VAL:N	2.27	0.49
3:B:69:ALA:C	3:B:70:PHE:HD2	2.16	0.49
3:D:118:SER:O	3:D:119:ALA:C	2.35	0.49
3:F:3:GLN:C	3:F:4:LEU:HD12	2.33	0.49
2:G:162:GLN:O	2:G:163:ASN:CG	2.50	0.49
2:G:42:TYR:HA	2:G:51:LYS:O	2.12	0.49
3:H:123:PRO:HA	3:H:124:PRO:HD2	1.53	0.49
3:H:125:SER:OG	3:H:127:TYR:OH	2.19	0.49
3:H:214:LYS:C	3:H:215:ILE:CG1	2.79	0.49
1:Q:31:VAL:C	1:Q:31:VAL:CB	2.74	0.49
3:B:182:LEU:HD23	3:B:183:SER:N	2.26	0.49
2:C:41:TRP:HD1	2:C:54:ILE:HB	1.78	0.49
2:E:155:LYS:HB2	2:E:199:THR:OG1	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:139:VAL:HA	2:G:154:TRP:HH2	1.77	0.49
2:G:7:SER:O	2:G:22:SER:N	2.40	0.49
3:H:83:ILE:O	3:H:86:LEU:CD1	2.60	0.49
3:H:88:ASN:C	3:H:90:ASP:N	2.61	0.49
4:L:51:TYR:CD1	4:L:64:TRP:CH2	3.01	0.49
2:A:204:HIS:CE1	2:A:206:THR:HG23	2.47	0.49
3:B:141:VAL:HG13	3:B:142:THR:N	2.27	0.49
3:B:177:SER:O	3:B:179:LEU:N	2.46	0.49
2:C:29:LEU:CD1	2:C:39:LEU:HB2	2.43	0.49
3:D:36:TRP:C	3:D:37:VAL:CG2	2.81	0.49
3:D:60:TYR:CZ	3:D:68:PHE:O	2.66	0.49
2:E:148:LYS:HD3	2:E:179:TYR:HE2	1.78	0.49
2:E:156:ILE:O	2:E:158:GLY:N	2.45	0.49
2:E:179:TYR:C	2:E:180:SER:OG	2.51	0.49
3:F:73:GLU:CG	3:F:76:ALA:HB3	2.43	0.49
2:G:29:LEU:CD2	2:G:29:LEU:C	2.81	0.49
3:H:27:TYR:H	3:H:27:TYR:HD1	1.57	0.49
4:N:27:LEU:HA	4:N:77:ILE:O	2.13	0.49
4:N:65:THR:CG2	4:N:65:THR:OG1	2.54	0.49
2:A:7:SER:OG	2:A:8:PRO:CA	2.61	0.49
3:B:52:ASN:HB3	3:B:55:THR:HB	1.95	0.49
3:B:6:GLN:O	3:B:7:SER:C	2.51	0.49
3:D:189:PRO:C	3:D:191:SER:N	2.66	0.49
3:F:131:PRO:O	3:F:132:GLY:C	2.48	0.49
4:N:51:TYR:H	4:N:51:TYR:HD1	1.59	0.49
3:B:20:ILE:HD11	3:B:81:LEU:HD13	1.94	0.48
3:D:1:GLN:OE1	1:Q:13:ARG:CD	2.52	0.48
2:E:211:ILE:O	2:E:211:ILE:HG22	2.12	0.48
2:E:1:ASP:O	2:E:2:ILE:HD12	2.13	0.48
2:E:83:SER:O	2:E:84:VAL:O	2.30	0.48
3:F:38:ASN:OD1	3:F:39:GLN:N	2.46	0.48
2:G:95:LYS:HE2	2:G:102:LEU:HG	1.94	0.48
2:G:141:PHE:O	2:G:142:LEU:HD23	2.12	0.48
3:H:176:GLN:O	3:H:178:ASP:N	2.46	0.48
2:A:128:SER:O	2:A:131:LEU:HB2	2.13	0.48
2:A:16:GLY:C	2:A:83:SER:HA	2.34	0.48
2:C:41:TRP:CE3	2:C:94:CYS:HB3	2.48	0.48
2:E:131:LEU:C	2:E:133:SER:N	2.66	0.48
4:N:60:VAL:CG2	4:N:60:VAL:O	2.60	0.48
2:A:42:TYR:HE2	3:B:105:PHE:HB2	1.79	0.48
3:B:13:LYS:O	3:B:16:GLU:HG3	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:54:GLU:C	3:B:56:GLY:H	2.15	0.48
3:D:97:ALA:HB1	3:D:107:VAL:O	2.14	0.48
3:D:33:SER:HB2	3:D:99:PHE:HB3	1.95	0.48
2:E:31:ASN:HD22	2:E:33:ARG:N	2.10	0.48
3:F:159:TRP:CH2	3:F:186:VAL:HG11	2.48	0.48
3:F:159:TRP:CH2	3:F:186:VAL:HG12	2.47	0.48
3:F:70:PHE:CE2	3:F:81:LEU:HD23	2.47	0.48
2:G:11:LEU:O	2:G:110:LEU:HD12	2.13	0.48
2:G:125:PRO:O	2:G:126:PRO:C	2.51	0.48
2:G:19:VAL:CG2	2:G:20:THR:N	2.76	0.48
2:G:38:TYR:HD1	2:G:98:TYR:HB2	1.78	0.48
3:H:164:LEU:CA	3:H:164:LEU:CD2	2.91	0.48
3:H:216:VAL:N	3:H:216:VAL:CB	2.70	0.48
3:H:217:PRO:O	3:H:217:PRO:CG	2.58	0.48
3:H:99:PHE:HB2	3:H:105:PHE:CE1	2.49	0.48
2:G:10:SER:HB3	4:O:38:GLU:HB2	1.94	0.48
2:A:196:ASN:O	2:A:196:ASN:OD1	2.32	0.48
2:A:16:GLY:CA	2:A:83:SER:HA	2.44	0.48
1:P:36:LEU:HD22	3:B:102:ARG:HH22	1.77	0.48
3:B:120:LYS:HE2	3:B:120:LYS:N	2.28	0.48
3:D:53:THR:HG22	3:D:72:LEU:CD2	2.37	0.48
2:E:157:ASP:OD2	2:E:195:HIS:HB3	2.12	0.48
3:F:31:ASP:O	3:F:32:PHE:CD1	2.66	0.48
2:G:113:LYS:HA	2:G:146:TYR:CZ	2.48	0.48
2:G:30:LEU:CA	2:G:38:TYR:CE1	2.80	0.48
3:H:6:GLN:CD	3:H:111:GLY:CA	2.81	0.48
4:M:60:VAL:HG22	4:M:60:VAL:O	2.13	0.48
2:A:88:ASP:O	2:A:110:LEU:HD23	2.14	0.48
3:B:126:VAL:HG22	3:B:202:VAL:HG11	1.96	0.48
2:C:87:GLU:O	2:C:87:GLU:HG3	2.13	0.48
3:D:153:GLU:HG2	3:D:180:TYR:CZ	2.49	0.48
3:H:72:LEU:CD2	3:H:74:THR:N	2.74	0.48
4:N:77:ILE:CG2	4:N:79:PHE:CE1	2.92	0.48
1:S:12:LYS:HD2	1:S:12:LYS:N	2.28	0.48
2:C:124:PHE:HA	2:C:125:PRO:HD3	1.71	0.48
2:C:185:LEU:HD11	2:C:187:LEU:HG	1.96	0.48
3:D:92:ALA:HB3	3:D:94:TYR:CE2	2.48	0.48
2:E:102:LEU:HB2	3:F:47:TRP:CG	2.47	0.48
2:G:19:VAL:HG11	2:G:110:LEU:HD21	1.96	0.48
2:G:219:GLU:OE2	3:H:134:ALA:HB2	2.13	0.48
2:G:53:LEU:HB2	2:G:54:ILE:CD1	2.31	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:93:TYR:CE1	3:H:45:LEU:HD21	2.48	0.48
1:S:24:PHE:CZ	3:H:32:PHE:HZ	2.31	0.48
3:H:8:GLY:O	3:H:112:THR:CG2	2.62	0.48
4:M:43:PHE:O	4:M:44:GLU:C	2.52	0.48
1:Q:40:ARG:NE	1:Q:45:GLY:C	2.67	0.48
2:A:2:ILE:HG22	2:A:4:MET:SD	2.54	0.48
3:B:141:VAL:O	3:B:187:THR:HG23	2.13	0.48
3:B:153:GLU:HB3	3:B:154:PRO:CA	2.43	0.48
3:B:97:ALA:CB	3:B:108:TRP:HA	2.43	0.48
3:D:207:SER:O	3:D:208:SER:HB2	2.13	0.48
3:F:166:SER:HB2	5:F:239:HOH:O	2.13	0.48
2:G:161:ARG:O	2:G:162:GLN:HB2	2.13	0.48
3:H:188:VAL:CG2	3:H:188:VAL:CA	2.83	0.48
4:M:57:HIS:O	4:M:58:ALA:C	2.50	0.48
4:M:65:THR:N	4:M:65:THR:CG2	2.76	0.48
1:Q:12:LYS:C	1:Q:13:ARG:HG2	2.32	0.48
2:A:188:THR:OG1	2:A:191:GLU:CB	2.61	0.48
2:A:72:GLY:HA3	2:A:77:PHE:HA	1.96	0.48
2:A:130:GLN:NE2	3:B:148:LYS:HD3	2.28	0.48
2:C:99:ILE:HA	2:C:100:PRO:HD2	1.63	0.48
2:C:34:THR:C	2:C:36:LYS:H	2.17	0.48
3:D:133:SER:C	3:D:135:ALA:H	2.16	0.48
2:E:188:THR:OG1	2:E:189:LYS:N	2.39	0.48
3:H:10:GLU:OE2	3:H:10:GLU:CA	2.54	0.48
3:H:20:ILE:HD13	3:H:36:TRP:HH2	1.79	0.48
4:O:42:THR:C	4:O:44:GLU:N	2.61	0.48
1:Q:9:ARG:O	1:Q:10:LYS:C	2.52	0.48
1:Q:25:PRO:HG3	1:Q:39:ARG:CD	2.44	0.48
2:A:7:SER:HA	2:A:8:PRO:C	2.34	0.48
3:B:147:VAL:HB	3:B:182:LEU:O	2.14	0.48
2:C:144:ASN:HA	2:C:178:THR:CG2	2.44	0.48
2:G:202:ALA:N	2:G:211:ILE:O	2.46	0.48
4:L:55:ALA:HA	4:L:64:TRP:NE1	2.29	0.48
2:A:10:SER:HA	2:A:109:LYS:HB3	1.96	0.48
2:A:34:THR:HG21	2:A:36:LYS:HB2	1.96	0.48
2:C:42:TYR:HA	2:C:51:LYS:O	2.13	0.48
3:D:1:GLN:HE22	1:Q:13:ARG:CD	2.27	0.48
3:D:35:HIS:CD2	3:D:50:TRP:HB2	2.49	0.48
3:D:35:HIS:ND1	3:D:50:TRP:HB3	2.29	0.48
2:E:65:PRO:C	2:E:67:ARG:N	2.67	0.48
3:F:101:LEU:CD2	3:F:101:LEU:HG	2.19	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:76:ALA:O	3:F:77:SER:C	2.52	0.48
2:G:84:VAL:HG11	2:G:110:LEU:HD21	1.96	0.48
2:G:201:GLU:HG2	2:G:212:VAL:HG12	1.92	0.48
2:G:6:GLN:HE22	2:G:108:THR:H	1.62	0.48
3:H:169:HIS:CB	3:H:171:PHE:CE1	2.97	0.48
3:H:156:THR:HG1	3:H:203:ALA:HB3	1.74	0.48
4:N:19:GLU:O	4:N:20:GLU:O	2.32	0.48
1:S:14:ASN:N	2:G:62:SER:CB	2.72	0.48
2:A:185:LEU:HD12	2:A:186:THR:H	1.78	0.47
2:A:190:ASP:HA	2:A:193:GLU:HB2	1.95	0.47
3:B:126:VAL:HG21	3:B:211:VAL:CG2	2.44	0.47
3:B:41:PRO:O	3:B:43:LYS:N	2.47	0.47
2:C:70:GLY:O	2:C:71:ARG:HG3	2.14	0.47
1:S:23:LYS:HD3	1:S:24:PHE:HB2	1.95	0.47
2:A:200:CYS:N	2:A:213:LYS:O	2.46	0.47
2:A:196:ASN:HD21	2:A:218:ASN:N	2.12	0.47
2:A:6:GLN:HE21	2:A:105:GLY:HA3	1.79	0.47
3:B:159:TRP:HB2	3:B:164:LEU:HB2	1.97	0.47
3:D:180:TYR:C	3:D:181:THR:CG2	2.80	0.47
3:D:52:ASN:ND2	3:D:54:GLU:H	2.11	0.47
3:D:97:ALA:HB2	3:D:108:TRP:CA	2.44	0.47
2:E:6:GLN:NE2	2:E:41:TRP:CZ3	2.79	0.47
2:G:152:VAL:CG1	2:G:153:LYS:H	2.24	0.47
2:G:190:ASP:O	2:G:194:ARG:HB2	2.14	0.47
4:L:58:ALA:O	4:L:60:VAL:N	2.47	0.47
4:L:69:GLU:HG2	4:L:70:ASP:H	1.78	0.47
1:S:9:ARG:O	1:S:10:LYS:O	2.32	0.47
1:S:35:TYR:O	1:S:36:LEU:CB	2.58	0.47
3:B:129:LEU:O	3:B:144:GLY:N	2.26	0.47
2:C:96:GLN:O	2:C:102:LEU:HA	2.14	0.47
2:E:167:ASN:OD1	2:E:183:SER:HA	2.14	0.47
2:G:166:LEU:CD1	2:G:166:LEU:CD2	2.84	0.47
2:G:19:VAL:HG13	2:G:81:ILE:CB	2.42	0.47
2:G:50:PRO:HG2	3:H:108:TRP:CH2	2.49	0.47
3:H:94:TYR:HE2	3:H:114:VAL:HG11	1.79	0.47
3:H:153:GLU:N	3:H:154:PRO:CD	2.76	0.47
3:H:2:ILE:HG12	3:H:98:ARG:NH1	2.28	0.47
4:N:40:LYS:CG	4:N:41:GLY:N	2.77	0.47
4:O:27:LEU:O	4:O:34:ILE:C	2.52	0.47
1:Q:18:ARG:N	1:Q:19:PRO:HD2	2.29	0.47
1:Q:33:GLY:CA	1:Q:36:LEU:HD22	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:149:GLY:C	3:B:179:LEU:HD23	2.34	0.47
2:E:12:ALA:HB3	4:N:36:THR:HB	1.96	0.47
3:F:136:GLN:C	3:F:138:ASN:H	2.16	0.47
2:G:186:THR:O	2:G:187:LEU:HG	2.14	0.47
2:G:43:GLN:HB2	2:G:92:TYR:CE2	2.50	0.47
3:H:150:TYR:CD2	3:H:180:TYR:HB3	2.49	0.47
3:H:150:TYR:OH	3:H:182:LEU:HD23	2.14	0.47
4:L:23:ILE:N	4:L:39:PHE:O	2.47	0.47
2:G:10:SER:HB3	4:O:38:GLU:OE2	2.14	0.47
2:A:6:GLN:HG3	2:A:105:GLY:HA3	1.96	0.47
2:A:113:LYS:O	2:A:114:ARG:CB	2.60	0.47
3:B:102:ARG:O	3:B:103:GLN:CB	2.61	0.47
3:B:194:PRO:C	3:B:196:GLU:H	2.17	0.47
2:C:205:LYS:C	2:C:207:SER:H	2.17	0.47
3:D:125:SER:O	3:D:126:VAL:CG2	2.63	0.47
2:E:130:GLN:HE21	2:E:136:ALA:CA	2.26	0.47
2:E:87:GLU:O	2:E:87:GLU:HG2	2.14	0.47
3:F:73:GLU:HG2	3:F:76:ALA:HB3	1.96	0.47
2:G:121:VAL:HA	2:G:141:PHE:O	2.15	0.47
2:G:202:ALA:HB3	2:G:211:ILE:HG23	1.96	0.47
2:G:52:VAL:CG2	2:G:53:LEU:H	2.26	0.47
3:H:46:ASN:O	3:H:48:MET:N	2.48	0.47
4:O:31:ASP:OD2	4:O:33:LYS:CG	2.62	0.47
2:A:128:SER:O	2:A:129:GLU:O	2.32	0.47
3:B:216:VAL:CG1	3:B:217:PRO:HD2	2.44	0.47
2:C:192:TYR:CD1	2:C:198:TYR:CZ	3.03	0.47
3:D:93:THR:HG22	3:D:94:TYR:N	2.27	0.47
2:E:137:SER:HA	2:E:186:THR:HA	1.96	0.47
2:E:172:GLN:O	2:E:173:ASP:C	2.52	0.47
2:E:36:LYS:HA	2:E:36:LYS:CE	2.45	0.47
2:E:85:GLN:OE1	5:E:226:HOH:O	2.20	0.47
3:F:149:GLY:HA2	3:F:180:TYR:O	2.15	0.47
2:G:189:LYS:HE3	2:G:193:GLU:HG3	1.96	0.47
3:H:36:TRP:C	3:H:37:VAL:CG2	2.83	0.47
3:B:143:LEU:HB2	3:B:186:VAL:HG23	1.96	0.47
3:B:182:LEU:CD2	3:B:183:SER:N	2.78	0.47
3:D:150:TYR:CE2	3:D:155:VAL:HG21	2.49	0.47
2:E:77:PHE:N	2:E:77:PHE:CD2	2.82	0.47
2:E:16:GLY:CA	2:E:83:SER:HA	2.45	0.47
3:F:198:VAL:O	3:F:215:ILE:HG12	2.14	0.47
2:G:53:LEU:CB	2:G:54:ILE:CD1	2.82	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:149:GLY:O	3:H:179:LEU:HG	2.14	0.47
5:G:224:HOH:O	3:H:167:GLY:CA	2.57	0.47
3:H:72:LEU:HD21	3:H:74:THR:HG1	1.78	0.47
1:P:40:ARG:HH11	3:F:98:ARG:NH1	2.13	0.47
2:A:127:SER:CB	3:B:128:PRO:HD2	2.44	0.47
3:B:33:SER:HA	3:B:53:THR:OG1	2.15	0.47
3:B:8:GLY:C	3:B:9:PRO:O	2.48	0.47
2:C:125:PRO:O	2:C:125:PRO:HD2	2.14	0.47
2:C:1:ASP:O	2:C:2:ILE:C	2.53	0.47
2:C:37:ASN:O	2:C:56:TRP:C	2.53	0.47
3:D:124:PRO:HB3	3:D:150:TYR:HB3	1.97	0.47
2:E:113:LYS:HA	2:E:146:TYR:OH	2.15	0.47
2:E:111:GLU:HG2	2:E:179:TYR:OH	2.14	0.47
2:E:68:PHE:CD1	2:E:81:ILE:CG1	2.97	0.47
2:E:18:LYS:CA	2:E:82:SER:HA	2.32	0.47
3:F:190:SER:O	3:F:191:SER:C	2.50	0.47
2:G:126:PRO:HB3	2:G:136:ALA:HB1	1.97	0.47
1:S:31:VAL:HB	3:H:50:TRP:CE3	2.50	0.47
4:M:29:PHE:HZ	4:M:57:HIS:CE1	2.32	0.47
4:O:51:TYR:O	4:O:54:ALA:HB3	2.14	0.47
1:S:11:THR:HG22	1:S:12:LYS:HZ2	1.80	0.47
1:S:40:ARG:CG	1:S:41:GLY:H	2.27	0.47
2:A:36:LYS:HE3	2:A:56:TRP:CE3	2.50	0.47
3:D:64:PHE:C	3:D:66:GLY:H	2.18	0.47
2:E:58:SER:HB2	2:E:70:GLY:O	2.14	0.47
2:G:167:ASN:N	2:G:167:ASN:HD22	1.97	0.47
2:G:149:ASP:O	2:G:204:HIS:CD2	2.68	0.47
2:G:2:ILE:O	2:G:3:VAL:C	2.52	0.47
4:O:23:ILE:O	4:O:23:ILE:HG22	2.06	0.47
4:O:32:GLY:O	4:O:33:LYS:O	2.33	0.47
4:O:69:GLU:HG3	4:O:70:ASP:OD1	2.14	0.47
1:S:42:PRO:O	1:S:43:ARG:O	2.33	0.47
3:B:143:LEU:HD13	3:B:215:ILE:HG21	1.97	0.47
2:C:42:TYR:HH	2:C:95:LYS:HE2	1.79	0.47
3:D:10:GLU:HA	3:D:10:GLU:OE2	2.14	0.47
3:D:170:THR:CG2	3:D:170:THR:HB	2.21	0.47
2:E:140:CYS:C	2:E:141:PHE:CD2	2.88	0.47
2:E:55:TYR:C	2:E:55:TYR:CD2	2.87	0.47
2:G:124:PHE:HB3	2:G:125:PRO:HD2	1.96	0.47
2:G:19:VAL:HG21	2:G:110:LEU:HD13	1.96	0.47
1:S:34:VAL:CG2	2:G:31:ASN:HB2	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:176:GLN:O	3:H:177:SER:C	2.49	0.47
3:H:173:ALA:CB	3:H:180:TYR:CE1	2.98	0.47
4:O:28:ILE:HD12	4:O:28:ILE:N	2.30	0.47
1:Q:33:GLY:HA2	1:Q:36:LEU:HD22	1.97	0.47
1:S:13:ARG:O	1:S:14:ASN:CG	2.54	0.47
3:B:127:TYR:O	3:B:145:CYS:HA	2.15	0.47
2:A:180:SER:OG	3:B:169:HIS:CE1	2.68	0.47
3:D:141:VAL:HG13	3:D:142:THR:N	2.30	0.47
3:D:156:THR:HG23	3:D:203:ALA:CB	2.42	0.47
2:E:89:GLN:OE1	2:E:112:LEU:HB2	2.15	0.47
2:E:127:SER:O	2:E:131:LEU:HG	2.15	0.47
2:E:96:GLN:OE1	2:E:99:ILE:O	2.33	0.47
3:F:189:PRO:HB2	3:F:192:THR:HG23	1.97	0.47
2:A:155:LYS:HA	2:A:159:SER:O	2.15	0.46
2:A:17:GLU:OE1	4:L:35:GLN:CG	2.63	0.46
2:A:68:PHE:CD1	2:A:81:ILE:HG12	2.51	0.46
3:B:124:PRO:HB3	3:B:150:TYR:HB3	1.97	0.46
3:B:177:SER:O	3:B:179:LEU:HB2	2.15	0.46
2:C:187:LEU:HB3	2:C:188:THR:H	1.26	0.46
2:C:31:ASN:HB2	2:C:98:TYR:OH	2.15	0.46
2:C:67:ARG:HG3	2:C:68:PHE:CD2	2.50	0.46
3:D:218:ARG:HH21	3:D:218:ARG:HG2	1.81	0.46
3:D:55:THR:HG23	3:D:56:GLY:H	1.80	0.46
2:E:18:LYS:CG	2:E:19:VAL:H	2.25	0.46
2:E:204:HIS:C	2:E:206:THR:H	2.18	0.46
2:E:91:VAL:HG13	2:E:108:THR:O	2.15	0.46
3:F:102:ARG:NH2	3:F:102:ARG:HG2	2.29	0.46
3:F:101:LEU:O	3:F:103:GLN:OE1	2.33	0.46
3:H:130:ALA:HB1	3:H:131:PRO:HD2	1.96	0.46
3:H:186:VAL:HG22	3:H:187:THR:H	1.79	0.46
3:H:30:THR:OG1	3:H:31:ASP:N	2.48	0.46
3:H:34:MET:HB3	3:H:51:VAL:HG21	1.97	0.46
4:M:21:VAL:HG12	4:M:22:THR:N	2.28	0.46
4:M:53:TYR:O	4:M:54:ALA:C	2.50	0.46
4:M:74:HIS:O	4:M:75:MET:HB2	2.15	0.46
2:A:102:LEU:HB2	3:B:47:TRP:CG	2.49	0.46
2:A:89:GLN:CD	2:A:172:GLN:HG2	2.34	0.46
3:B:130:ALA:HB1	3:B:131:PRO:HD2	1.96	0.46
3:B:136:GLN:NE2	3:B:136:GLN:N	2.64	0.46
2:C:144:ASN:HA	2:C:178:THR:HG22	1.97	0.46
2:E:45:LYS:CG	2:E:90:ALA:HB2	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:175:LEU:HB2	3:F:180:TYR:HE1	1.79	0.46
3:F:143:LEU:N	3:F:186:VAL:O	2.47	0.46
3:F:86:LEU:HD13	3:F:116:VAL:CG2	2.45	0.46
2:G:89:GLN:NE2	2:G:90:ALA:N	2.63	0.46
3:H:20:ILE:HD11	3:H:36:TRP:CH2	2.49	0.46
4:L:43:PHE:O	4:L:44:GLU:O	2.34	0.46
1:Q:43:ARG:HG2	1:Q:44:LEU:HD12	1.97	0.46
1:S:12:LYS:H	1:S:12:LYS:HD2	1.80	0.46
2:A:21:MET:CB	2:A:108:THR:HG21	2.45	0.46
2:A:139:VAL:HB	3:B:129:LEU:HD21	1.96	0.46
2:A:114:ARG:NE	2:A:146:TYR:CB	2.78	0.46
3:B:36:TRP:CD2	3:B:81:LEU:HD12	2.50	0.46
3:B:93:THR:HG23	3:B:113:THR:HA	1.97	0.46
2:C:61:GLU:OE2	3:D:104:TYR:OH	2.27	0.46
3:D:189:PRO:HB2	3:D:192:THR:CG2	2.38	0.46
3:B:31:ASP:HA	2:E:33:ARG:HD2	1.97	0.46
2:G:112:LEU:HA	2:G:112:LEU:HD12	1.28	0.46
2:G:68:PHE:O	2:G:69:THR:C	2.52	0.46
3:H:201:ASN:CB	3:H:212:ASP:OD1	2.63	0.46
4:L:55:ALA:HA	4:L:64:TRP:HE1	1.80	0.46
2:G:113:LYS:NZ	4:O:34:ILE:HG13	2.31	0.46
2:A:136:ALA:N	2:A:187:LEU:O	2.44	0.46
2:A:2:ILE:HG21	2:A:96:GLN:HG2	1.98	0.46
3:B:12:LYS:O	3:B:116:VAL:HA	2.16	0.46
3:B:175:LEU:HB2	3:B:180:TYR:HE1	1.65	0.46
3:D:182:LEU:N	3:D:182:LEU:HD23	2.31	0.46
3:D:161:SER:N	3:D:201:ASN:HD21	2.14	0.46
3:D:31:ASP:C	3:D:32:PHE:CD2	2.87	0.46
2:E:101:PRO:O	2:E:102:LEU:C	2.53	0.46
2:E:128:SER:O	2:E:131:LEU:HG	2.16	0.46
2:E:151:ASN:ND2	2:E:152:VAL:N	2.63	0.46
2:E:161:ARG:HG3	2:E:161:ARG:HH21	1.80	0.46
2:E:42:TYR:OH	2:E:95:LYS:CE	2.63	0.46
2:E:95:LYS:HD3	2:E:104:PHE:CE2	2.46	0.46
2:E:96:GLN:O	2:E:96:GLN:HG3	2.15	0.46
3:F:12:LYS:O	3:F:116:VAL:HA	2.16	0.46
2:G:195:HIS:HB2	2:G:198:TYR:OH	2.15	0.46
4:N:31:ASP:OD1	4:N:33:LYS:HD3	2.14	0.46
1:S:44:LEU:O	1:S:45:GLY:C	2.52	0.46
3:B:179:LEU:CD2	3:B:179:LEU:CD1	2.88	0.46
3:F:71:SER:HB2	3:F:80:TYR:HD2	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:173:ASP:OD2	2:G:175:LYS:N	2.32	0.46
2:G:93:TYR:CE1	3:H:45:LEU:HD23	2.50	0.46
2:G:93:TYR:CG	3:H:45:LEU:HD23	2.50	0.46
3:H:152:PRO:O	3:H:154:PRO:N	2.48	0.46
3:H:37:VAL:HG13	3:H:46:ASN:C	2.36	0.46
2:A:34:THR:O	2:A:35:ARG:CB	2.60	0.46
3:B:174:VAL:O	3:B:180:TYR:HD1	1.99	0.46
2:C:125:PRO:CD	2:C:125:PRO:O	2.60	0.46
2:C:2:ILE:HG12	2:C:96:GLN:NE2	2.31	0.46
2:E:130:GLN:HE22	2:E:137:SER:H	1.55	0.46
3:F:103:GLN:N	3:F:103:GLN:CD	2.69	0.46
3:F:74:THR:CA	3:F:74:THR:CG2	2.86	0.46
2:G:124:PHE:CE1	2:G:141:PHE:CD2	2.96	0.46
3:H:119:ALA:HB3	3:H:151:PHE:CE2	2.50	0.46
4:M:28:ILE:CD1	4:M:76:ASN:HB3	2.46	0.46
1:Q:30:ILE:CD1	1:Q:36:LEU:HB2	2.40	0.46
1:S:37:LEU:HD13	1:S:37:LEU:HA	1.64	0.46
2:A:59:THR:HG22	2:A:60:ARG:N	2.24	0.46
2:C:176:ASP:O	2:C:177:SER:C	2.54	0.46
3:D:151:PHE:CB	3:D:152:PRO:CD	2.92	0.46
3:D:150:TYR:HD2	3:D:204:HIS:CD2	2.34	0.46
3:F:93:THR:CG2	3:F:113:THR:HG23	2.45	0.46
2:E:144:ASN:HD21	3:F:169:HIS:HE1	1.60	0.46
3:F:20:ILE:CG1	3:F:21:SER:N	2.78	0.46
2:G:146:TYR:HA	2:G:147:PRO:C	2.33	0.46
2:G:39:LEU:O	2:G:40:ALA:HB2	2.15	0.46
2:G:54:ILE:CD1	2:G:54:ILE:HG23	2.46	0.46
4:L:51:TYR:CE1	4:L:64:TRP:CH2	3.03	0.46
4:N:68:LEU:O	4:N:69:GLU:C	2.51	0.46
4:O:25:VAL:HG23	4:O:77:ILE:HG13	1.98	0.46
2:A:92:TYR:CD1	2:A:92:TYR:N	2.83	0.46
3:B:120:LYS:CE	3:B:120:LYS:N	2.79	0.46
3:B:31:ASP:O	3:B:32:PHE:CD2	2.67	0.46
2:C:37:ASN:CG	2:C:73:SER:HA	2.36	0.46
3:D:14:PRO:HG2	3:D:14:PRO:O	2.15	0.46
2:E:188:THR:HG23	2:E:191:GLU:HB3	1.93	0.46
3:F:64:PHE:HE2	5:F:228:HOH:O	1.98	0.46
2:G:61:GLU:O	2:G:62:SER:C	2.54	0.46
2:G:84:VAL:CA	2:G:88:ASP:OD1	2.57	0.46
4:O:42:THR:O	4:O:46:ALA:N	2.48	0.46
2:A:7:SER:OG	2:A:8:PRO:N	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:49:SER:O	2:C:50:PRO:O	2.33	0.46
2:C:17:GLU:N	2:C:83:SER:HA	2.31	0.46
3:D:162:GLY:C	3:D:164:LEU:N	2.69	0.46
2:E:55:TYR:CE2	2:E:59:THR:CG2	2.99	0.46
2:G:43:GLN:NE2	2:G:45:LYS:HE3	2.31	0.46
3:H:156:THR:O	3:H:202:VAL:HA	2.15	0.46
3:H:20:ILE:CD1	3:H:80:TYR:HA	2.46	0.46
2:A:17:GLU:OE1	4:L:35:GLN:HG2	2.16	0.46
4:L:67:ASP:OD1	4:L:67:ASP:O	2.34	0.46
2:A:156:ILE:O	2:A:159:SER:HB2	2.16	0.46
2:A:199:THR:CA	2:A:199:THR:CG2	2.85	0.46
3:B:126:VAL:CG2	3:B:202:VAL:HG11	2.46	0.46
2:C:56:TRP:CG	2:C:56:TRP:CA	2.91	0.46
3:D:133:SER:O	3:D:135:ALA:N	2.40	0.46
3:D:159:TRP:CZ3	3:D:215:ILE:HD11	2.43	0.46
2:G:194:ARG:O	2:G:194:ARG:HD3	2.16	0.46
2:G:89:GLN:O	2:G:90:ALA:HB2	2.16	0.46
3:H:11:LEU:HD12	3:H:152:PRO:HG3	1.98	0.46
3:H:76:ALA:O	3:H:77:SER:C	2.53	0.46
4:O:61:ASN:HB3	4:O:79:PHE:CE2	2.51	0.46
2:A:60:ARG:HH12	2:A:68:PHE:N	2.12	0.45
3:B:52:ASN:CG	3:B:55:THR:CB	2.77	0.45
2:C:76:ASP:C	2:C:77:PHE:CD2	2.89	0.45
3:D:158:THR:HG1	3:D:201:ASN:HD22	1.56	0.45
2:E:179:TYR:C	2:E:180:SER:HG	2.19	0.45
3:F:68:PHE:N	3:F:68:PHE:CD2	2.76	0.45
2:G:52:VAL:HG22	2:G:54:ILE:N	2.31	0.45
2:G:56:TRP:C	2:G:58:SER:H	2.20	0.45
3:H:27:TYR:CD2	3:H:28:THR:O	2.69	0.45
3:H:55:THR:CG2	3:H:55:THR:CA	2.88	0.45
4:M:25:VAL:C	4:M:75:MET:O	2.53	0.45
4:N:49:GLU:OE1	4:N:49:GLU:CA	2.60	0.45
4:O:52:ARG:CD	4:O:52:ARG:CB	2.86	0.45
4:O:73:ASN:OD1	4:O:73:ASN:C	2.55	0.45
1:S:17:ARG:O	1:S:17:ARG:CG	2.64	0.45
2:A:60:ARG:NH2	2:A:66:ASP:O	2.49	0.45
2:A:97:ALA:C	2:A:99:ILE:N	2.68	0.45
3:B:4:LEU:CD2	3:B:34:MET:HE3	2.45	0.45
2:C:127:SER:O	2:C:128:SER:C	2.53	0.45
2:C:150:ILE:HG12	2:C:151:ASN:N	2.31	0.45
2:C:125:PRO:HG3	2:C:215:PHE:CE1	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:170:THR:HA	3:D:184:SER:OG	2.16	0.45
3:D:201:ASN:HB3	3:D:212:ASP:OD1	2.16	0.45
2:E:189:LYS:HB3	2:E:190:ASP:OD2	2.16	0.45
2:E:98:TYR:CD2	2:E:99:ILE:HG12	2.50	0.45
3:F:175:LEU:HD23	5:F:224:HOH:O	2.15	0.45
2:G:132:THR:HG23	2:G:132:THR:H	1.48	0.45
2:G:190:ASP:HA	2:G:193:GLU:HB2	1.97	0.45
3:H:142:THR:HG23	3:H:186:VAL:O	2.15	0.45
4:M:77:ILE:HG23	4:M:77:ILE:HD12	1.74	0.45
3:B:20:ILE:HG21	3:B:112:THR:HG21	1.99	0.45
3:D:108:TRP:HD1	3:D:108:TRP:N	2.10	0.45
3:D:153:GLU:N	3:D:154:PRO:CD	2.78	0.45
2:E:11:LEU:CB	2:E:11:LEU:CD1	2.84	0.45
4:O:48:ALA:HB1	4:O:52:ARG:HD3	1.99	0.45
1:P:29:GLN:C	1:P:30:ILE:HG12	2.37	0.45
1:S:13:ARG:C	2:G:62:SER:CB	2.69	0.45
1:S:40:ARG:HG2	1:S:41:GLY:N	2.30	0.45
2:A:33:ARG:CG	2:A:33:ARG:CA	2.87	0.45
3:B:150:TYR:CZ	3:B:180:TYR:HB3	2.52	0.45
2:C:152:VAL:HG13	2:C:153:LYS:H	1.81	0.45
2:C:161:ARG:HH12	2:C:187:LEU:HD21	1.82	0.45
3:D:48:MET:HE1	3:D:94:TYR:HD1	1.82	0.45
3:F:34:MET:HG3	3:F:35:HIS:H	1.79	0.45
2:G:196:ASN:HA	2:G:217:ARG:HB2	1.97	0.45
2:G:61:GLU:O	2:G:64:VAL:HG12	2.16	0.45
3:H:73:GLU:O	3:H:75:SER:N	2.50	0.45
4:O:60:VAL:HG13	4:O:61:ASN:N	2.31	0.45
3:B:199:THR:HG22	3:B:214:LYS:HB2	1.99	0.45
3:D:193:TRP:HA	3:D:195:SER:H	1.81	0.45
2:E:54:ILE:HG21	2:E:58:SER:HA	1.98	0.45
2:E:54:ILE:HG21	2:E:70:GLY:HA3	1.98	0.45
3:F:202:VAL:H	3:F:202:VAL:HG13	1.46	0.45
3:F:35:HIS:CD2	3:F:50:TRP:HB2	2.52	0.45
4:M:27:LEU:HB3	4:M:29:PHE:CE1	2.51	0.45
4:O:27:LEU:C	4:O:28:ILE:HD12	2.37	0.45
4:O:47:THR:O	4:O:51:TYR:CD2	2.69	0.45
1:S:32:GLY:O	2:G:97:ALA:HB1	2.16	0.45
2:A:6:GLN:CD	2:A:93:TYR:HA	2.37	0.45
3:B:146:LEU:HD21	3:B:148:LYS:HG3	1.99	0.45
3:B:20:ILE:HD13	3:B:20:ILE:HG21	1.37	0.45
3:B:211:VAL:HG22	3:B:211:VAL:O	2.11	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:18:LYS:HE3	4:M:57:HIS:HD2	1.82	0.45
2:C:42:TYR:CE2	3:D:108:TRP:HZ2	2.33	0.45
2:E:24:LYS:CG	2:E:24:LYS:CE	2.83	0.45
2:E:55:TYR:C	2:E:57:ALA:H	2.20	0.45
3:F:139:SER:O	3:F:190:SER:HB3	2.16	0.45
3:F:31:ASP:C	3:F:32:PHE:CG	2.89	0.45
2:G:145:PHE:N	2:G:178:THR:HB	2.31	0.45
3:H:92:ALA:O	3:H:114:VAL:HG12	2.17	0.45
3:H:99:PHE:CZ	3:H:103:GLN:HA	2.52	0.45
2:A:11:LEU:HD23	2:A:11:LEU:HA	1.68	0.45
2:A:188:THR:OG1	2:A:191:GLU:CG	2.64	0.45
3:B:149:GLY:HA2	3:B:179:LEU:HD22	1.98	0.45
2:C:84:VAL:O	2:C:85:GLN:HG2	2.17	0.45
3:D:176:GLN:O	3:D:177:SER:C	2.55	0.45
2:E:53:LEU:O	2:E:60:ARG:HA	2.17	0.45
2:E:56:TRP:O	2:E:57:ALA:CB	2.64	0.45
2:G:8:PRO:HG2	2:G:11:LEU:HG	1.99	0.45
3:H:36:TRP:CZ2	3:H:80:TYR:C	2.90	0.45
1:Q:25:PRO:HG3	1:Q:39:ARG:CZ	2.46	0.45
2:A:187:LEU:HD11	2:A:192:TYR:HD1	1.80	0.45
3:B:20:ILE:HG22	3:B:112:THR:HG21	1.99	0.45
3:B:170:THR:HA	3:B:184:SER:CB	2.46	0.45
2:C:105:GLY:O	2:C:106:ALA:C	2.43	0.45
2:C:146:TYR:CG	2:C:147:PRO:CA	2.97	0.45
2:C:192:TYR:HA	2:C:198:TYR:OH	2.17	0.45
2:C:204:HIS:CE1	2:C:206:THR:CG2	2.99	0.45
2:C:19:VAL:HG11	2:C:84:VAL:CG1	2.47	0.45
3:F:7:SER:CA	3:F:21:SER:OG	2.65	0.45
2:G:21:MET:HG2	2:G:108:THR:HG21	1.98	0.45
2:A:48:GLN:H	2:A:48:GLN:CD	2.20	0.45
2:C:9:SER:C	2:C:108:THR:HA	2.37	0.45
2:C:52:VAL:HG11	3:D:104:TYR:HE1	1.81	0.45
3:D:29:PHE:CG	3:D:29:PHE:O	2.70	0.45
3:D:35:HIS:CG	3:D:50:TRP:HB3	2.52	0.45
2:E:115:ALA:O	2:E:116:ASP:O	2.35	0.45
2:G:21:MET:HG2	2:G:108:THR:CB	2.46	0.45
3:H:151:PHE:CB	3:H:152:PRO:HD3	2.38	0.45
3:H:40:ALA:O	3:H:43:LYS:CB	2.63	0.45
2:E:11:LEU:HA	4:N:36:THR:O	2.16	0.45
4:O:25:VAL:HG11	4:O:39:PHE:CE1	2.45	0.45
3:B:122:THR:O	3:B:150:TYR:HA	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:70:PHE:CD2	3:B:70:PHE:N	2.83	0.45
3:D:152:PRO:O	3:D:154:PRO:HG2	2.17	0.45
3:D:6:GLN:OE1	3:D:96:CYS:SG	2.75	0.45
2:E:45:LYS:O	2:E:46:PRO:O	2.35	0.45
2:E:68:PHE:CE1	2:E:81:ILE:CG1	3.00	0.45
2:G:173:ASP:HB3	2:G:176:ASP:HB3	1.99	0.45
2:A:39:LEU:HB3	2:A:57:ALA:HB2	1.99	0.44
2:A:61:GLU:HB3	2:A:64:VAL:CG2	2.47	0.44
3:D:160:ASN:C	3:D:162:GLY:H	2.20	0.44
3:D:43:LYS:CA	3:D:43:LYS:HE3	2.47	0.44
2:E:148:LYS:HA	2:E:179:TYR:CD2	2.52	0.44
2:E:194:ARG:NH2	2:E:195:HIS:NE2	2.64	0.44
2:E:3:VAL:HG12	2:E:4:MET:N	2.32	0.44
2:G:190:ASP:O	2:G:194:ARG:N	2.49	0.44
4:M:25:VAL:HA	4:M:75:MET:CB	2.32	0.44
4:N:67:ASP:OD2	4:N:76:ASN:ND2	2.49	0.44
4:O:79:PHE:N	4:O:79:PHE:HD1	2.15	0.44
1:P:38:PRO:HG2	1:P:38:PRO:O	2.17	0.44
1:S:11:THR:CG2	1:S:12:LYS:HD2	2.47	0.44
2:A:11:LEU:O	2:A:111:GLU:N	2.50	0.44
2:A:156:ILE:CG2	2:A:195:HIS:CD2	2.78	0.44
2:A:205:LYS:CB	2:A:205:LYS:CD	2.83	0.44
2:C:14:SER:CA	2:C:113:LYS:HB2	2.35	0.44
2:C:13:VAL:CG2	2:C:14:SER:N	2.80	0.44
2:C:209:SER:O	2:C:210:PRO:C	2.56	0.44
3:D:97:ALA:HB2	3:D:108:TRP:CG	2.52	0.44
3:D:150:TYR:N	3:D:150:TYR:CD1	2.85	0.44
2:E:95:LYS:HE2	3:F:105:PHE:CE2	2.51	0.44
3:F:40:ALA:CB	3:F:41:PRO:CD	2.80	0.44
3:H:129:LEU:CG	3:H:145:CYS:N	2.80	0.44
3:H:40:ALA:CB	3:H:43:LYS:HG3	2.44	0.44
4:N:27:LEU:HB3	4:N:77:ILE:HB	2.00	0.44
1:Q:37:LEU:HB3	1:Q:38:PRO:CD	2.45	0.44
1:Q:40:ARG:HD3	1:Q:45:GLY:O	2.17	0.44
2:A:96:GLN:CG	2:A:103:THR:OG1	2.63	0.44
2:A:165:VAL:HG22	2:A:166:LEU:N	2.32	0.44
2:A:34:THR:HG22	2:A:36:LYS:N	2.32	0.44
2:A:82:SER:O	2:A:83:SER:O	2.31	0.44
2:C:138:VAL:HG12	2:C:139:VAL:N	2.32	0.44
3:D:171:PHE:HA	3:D:172:PRO:HD3	1.78	0.44
3:D:3:GLN:CG	3:D:4:LEU:H	2.24	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:154:TRP:HZ2	2:E:183:SER:O	2.00	0.44
2:E:114:ARG:CD	2:E:178:THR:HG22	2.46	0.44
2:G:67:ARG:O	2:G:69:THR:N	2.51	0.44
3:H:129:LEU:HD12	3:H:144:GLY:CA	2.40	0.44
3:H:6:GLN:CD	3:H:111:GLY:HA2	2.38	0.44
4:N:43:PHE:CE2	4:N:47:THR:HB	2.52	0.44
4:O:53:TYR:CD1	4:O:56:LEU:HD23	2.51	0.44
1:Q:22:VAL:CG1	1:Q:22:VAL:CA	2.84	0.44
2:A:39:LEU:HD13	2:A:40:ALA:N	2.32	0.44
2:A:124:PHE:CE2	3:B:131:PRO:HA	2.53	0.44
2:C:205:LYS:C	2:C:207:SER:N	2.71	0.44
2:C:65:PRO:HB3	2:C:67:ARG:HH21	1.82	0.44
2:C:2:ILE:CD1	2:C:96:GLN:OE1	2.56	0.44
2:C:42:TYR:CD2	3:D:108:TRP:HZ2	2.36	0.44
2:E:113:LYS:HE2	4:N:36:THR:OG1	2.17	0.44
3:F:39:GLN:C	3:F:92:ALA:HB1	2.38	0.44
2:G:201:GLU:CA	2:G:212:VAL:HG12	2.42	0.44
2:G:73:SER:O	2:G:76:ASP:O	2.36	0.44
4:M:27:LEU:O	4:M:34:ILE:CD1	2.63	0.44
4:O:73:ASN:CG	4:O:73:ASN:C	2.76	0.44
3:B:151:PHE:CD1	3:B:152:PRO:HA	2.52	0.44
3:B:149:GLY:CA	3:B:179:LEU:CD2	2.95	0.44
3:B:196:GLU:OE1	3:B:196:GLU:CA	2.63	0.44
2:C:108:THR:CG2	2:C:108:THR:CA	2.85	0.44
2:C:114:ARG:NE	2:C:115:ALA:O	2.49	0.44
2:C:125:PRO:HB3	2:C:215:PHE:HE1	1.82	0.44
2:C:166:LEU:HD21	3:D:174:VAL:CG1	2.47	0.44
2:C:2:ILE:HB	2:C:96:GLN:CD	2.38	0.44
3:D:106:ASP:OD2	3:D:107:VAL:N	2.51	0.44
3:F:14:PRO:C	3:F:16:GLU:H	2.20	0.44
4:N:23:ILE:HG23	4:N:72:GLY:O	2.17	0.44
4:O:33:LYS:CD	4:O:33:LYS:CB	2.89	0.44
2:A:13:VAL:HG23	2:A:14:SER:N	2.30	0.44
2:A:204:HIS:CG	2:A:205:LYS:H	2.31	0.44
2:A:65:PRO:C	2:A:67:ARG:N	2.61	0.44
3:B:4:LEU:HD13	3:B:107:VAL:HG22	1.98	0.44
3:D:207:SER:C	3:D:209:THR:N	2.65	0.44
2:E:164:GLY:O	2:E:166:LEU:HD12	2.18	0.44
2:E:61:GLU:O	2:E:64:VAL:HB	2.17	0.44
2:G:182:SER:HB3	3:H:171:PHE:CZ	2.49	0.44
2:G:55:TYR:CE2	2:G:59:THR:HG21	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:25:VAL:CG2	4:M:26:ASN:H	2.06	0.44
1:Q:22:VAL:CB	1:Q:22:VAL:N	2.72	0.44
1:S:30:ILE:O	1:S:30:ILE:CG1	2.64	0.44
1:S:31:VAL:CG2	1:S:31:VAL:CG1	2.84	0.44
2:A:124:PHE:HE2	3:B:130:ALA:C	2.20	0.44
2:A:196:ASN:O	2:A:216:ASN:HA	2.18	0.44
2:C:114:ARG:HG3	2:C:114:ARG:O	2.10	0.44
2:E:45:LYS:O	2:E:48:GLN:HB2	2.17	0.44
2:E:9:SER:CB	4:N:38:GLU:O	2.66	0.44
3:H:153:GLU:HG2	3:H:173:ALA:CB	2.47	0.44
3:H:88:ASN:C	3:H:90:ASP:H	2.21	0.44
1:P:23:LYS:O	1:P:24:PHE:O	2.35	0.44
2:A:78:THR:HG22	2:A:79:LEU:N	2.26	0.44
2:C:139:VAL:CG1	2:C:140:CYS:N	2.81	0.44
2:C:155:LYS:CE	2:C:158:GLY:O	2.66	0.44
3:D:170:THR:O	3:D:170:THR:CG2	2.65	0.44
3:D:174:VAL:C	3:D:175:LEU:O	2.54	0.44
3:D:202:VAL:HG22	3:D:202:VAL:O	2.14	0.44
2:E:3:VAL:HB	2:E:26:SER:OG	2.18	0.44
3:F:20:ILE:CD1	3:F:112:THR:HB	2.45	0.44
3:F:157:VAL:HG11	3:F:184:SER:HB2	2.00	0.44
2:G:114:ARG:HB2	2:G:115:ALA:H	1.56	0.44
3:H:133:SER:HA	3:H:218:ARG:HH11	1.82	0.44
3:H:52:ASN:O	3:H:53:THR:C	2.54	0.44
4:L:41:GLY:C	4:L:46:ALA:HB2	2.38	0.44
4:M:32:GLY:C	4:M:33:LYS:O	2.51	0.44
4:N:21:VAL:CG1	4:N:22:THR:N	2.77	0.44
1:Q:40:ARG:NH2	1:Q:45:GLY:HA2	2.32	0.44
1:S:14:ASN:O	1:S:15:THR:HG23	2.18	0.44
2:A:49:SER:C	2:A:50:PRO:O	2.57	0.44
2:A:18:LYS:HA	2:A:82:SER:HA	1.99	0.44
3:B:159:TRP:CH2	3:B:200:CYS:HB3	2.53	0.44
3:B:28:THR:O	3:B:31:ASP:N	2.51	0.44
2:C:118:ALA:HA	2:C:206:THR:HG21	2.00	0.44
3:D:107:VAL:C	3:D:108:TRP:CD1	2.91	0.44
3:D:61:ALA:C	3:D:63:ASP:H	2.21	0.44
2:E:114:ARG:HB2	5:E:223:HOH:O	2.18	0.44
2:E:55:TYR:HE2	2:E:59:THR:CG2	2.31	0.44
3:F:48:MET:HG2	3:F:64:PHE:CE1	2.50	0.44
2:G:21:MET:HG2	2:G:108:THR:HB	2.00	0.44
3:H:36:TRP:O	3:H:37:VAL:CG2	2.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:25:PRO:HG3	1:Q:39:ARG:NE	2.33	0.44
2:A:116:ASP:N	2:A:116:ASP:OD2	2.51	0.43
2:A:60:ARG:NH2	2:A:68:PHE:O	2.51	0.43
3:B:134:ALA:O	3:B:135:ALA:HB2	2.18	0.43
3:D:168:VAL:C	3:D:169:HIS:ND1	2.72	0.43
2:G:182:SER:HB3	3:H:171:PHE:CD2	2.47	0.43
2:G:194:ARG:HE	2:G:194:ARG:C	2.21	0.43
2:G:21:MET:HG2	2:G:108:THR:CG2	2.48	0.43
3:H:98:ARG:O	3:H:100:LEU:N	2.51	0.43
1:S:30:ILE:HG21	3:H:101:LEU:HB3	1.99	0.43
3:H:177:SER:C	3:H:179:LEU:N	2.71	0.43
4:N:51:TYR:O	4:N:54:ALA:HB3	2.18	0.43
2:A:113:LYS:HA	2:A:146:TYR:OH	2.18	0.43
2:A:191:GLU:N	2:A:192:TYR:H	2.16	0.43
3:B:159:TRP:O	3:B:160:ASN:CB	2.66	0.43
2:C:187:LEU:HD23	2:C:187:LEU:HA	1.74	0.43
2:C:27:GLN:H	2:C:27:GLN:HG2	1.51	0.43
3:D:164:LEU:HD13	3:D:186:VAL:CG2	2.48	0.43
3:D:160:ASN:N	3:D:199:THR:O	2.37	0.43
3:D:24:ALA:HB1	3:D:27:TYR:CE1	2.53	0.43
2:G:169:TRP:HE3	2:G:169:TRP:H	1.63	0.43
2:G:55:TYR:CD1	2:G:55:TYR:N	2.86	0.43
2:G:7:SER:HB2	2:G:8:PRO:HA	2.00	0.43
4:N:29:PHE:CE1	4:N:61:ASN:ND2	2.86	0.43
2:A:113:LYS:O	2:A:114:ARG:HB3	2.17	0.43
3:B:149:GLY:C	3:B:179:LEU:CD2	2.86	0.43
2:C:140:CYS:HB2	2:C:154:TRP:CH2	2.53	0.43
3:D:35:HIS:NE2	3:D:99:PHE:HB3	2.33	0.43
2:E:36:LYS:HA	2:E:36:LYS:HE2	1.98	0.43
3:F:6:GLN:C	3:F:7:SER:O	2.53	0.43
2:G:126:PRO:CB	2:G:136:ALA:HB1	2.47	0.43
2:G:125:PRO:C	2:G:126:PRO:O	2.47	0.43
2:G:201:GLU:CA	2:G:201:GLU:CG	2.86	0.43
2:G:29:LEU:HD22	2:G:37:ASN:HB3	2.00	0.43
3:H:129:LEU:N	3:H:129:LEU:HD23	2.33	0.43
3:H:179:LEU:CG	3:H:180:TYR:H	2.14	0.43
3:H:174:VAL:HG23	3:H:182:LEU:HA	2.00	0.43
3:H:36:TRP:C	3:H:48:MET:HB2	2.38	0.43
4:L:29:PHE:CD1	4:L:29:PHE:N	2.85	0.43
1:S:23:LYS:HB3	1:S:24:PHE:H	1.39	0.43
1:S:38:PRO:O	1:S:39:ARG:HD2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:167:ASN:HB3	2:A:181:MET:CE	2.47	0.43
2:A:203:THR:HG22	2:A:204:HIS:N	2.33	0.43
2:A:37:ASN:O	2:A:56:TRP:HA	2.19	0.43
3:B:10:GLU:O	3:B:114:VAL:HA	2.19	0.43
2:C:67:ARG:O	2:C:80:THR:O	2.36	0.43
2:E:161:ARG:NH2	2:E:161:ARG:HG3	2.33	0.43
2:E:204:HIS:ND1	2:E:204:HIS:C	2.67	0.43
3:H:175:LEU:HG	3:H:175:LEU:CD2	2.23	0.43
2:A:138:VAL:HG21	2:A:198:TYR:HD1	1.84	0.43
2:A:46:PRO:O	2:A:46:PRO:CG	2.66	0.43
3:B:108:TRP:CD1	3:B:108:TRP:N	2.85	0.43
3:F:102:ARG:CG	3:F:102:ARG:NE	2.75	0.43
2:G:112:LEU:HG	2:G:113:LYS:N	2.32	0.43
2:G:53:LEU:HD12	2:G:53:LEU:N	2.34	0.43
2:G:67:ARG:C	2:G:69:THR:H	2.21	0.43
3:H:36:TRP:N	3:H:49:GLY:O	2.52	0.43
4:L:25:VAL:O	4:L:25:VAL:HG13	2.10	0.43
4:O:70:ASP:CB	4:O:73:ASN:HB3	2.44	0.43
2:A:43:GLN:HB2	2:A:53:LEU:HD21	2.00	0.43
2:C:150:ILE:HG21	2:C:150:ILE:HD13	1.73	0.43
2:C:30:LEU:HA	2:C:30:LEU:HD23	1.65	0.43
3:D:132:GLY:N	5:D:228:HOH:O	2.23	0.43
2:E:114:ARG:O	2:E:146:TYR:CE1	2.72	0.43
3:H:126:VAL:O	3:H:127:TYR:HD1	2.00	0.43
3:H:98:ARG:O	3:H:99:PHE:C	2.56	0.43
4:O:29:PHE:N	4:O:29:PHE:CD1	2.87	0.43
2:A:175:LYS:HA	2:A:175:LYS:HD2	1.88	0.43
2:A:89:GLN:HE22	2:A:172:GLN:CG	2.25	0.43
2:A:91:VAL:HG12	2:A:93:TYR:CE1	2.54	0.43
3:B:122:THR:HG23	3:B:122:THR:O	2.18	0.43
3:B:13:LYS:HG3	3:B:118:SER:HA	2.00	0.43
2:C:166:LEU:HD21	3:D:174:VAL:HG11	1.99	0.43
2:C:196:ASN:O	2:C:197:SER:C	2.56	0.43
3:D:49:GLY:O	3:D:50:TRP:HB3	2.19	0.43
2:E:182:SER:OG	2:E:182:SER:O	2.34	0.43
3:F:57:GLU:N	3:F:57:GLU:CD	2.71	0.43
2:G:56:TRP:CE3	2:G:59:THR:HG21	2.53	0.43
3:H:168:VAL:HG13	3:H:169:HIS:H	1.83	0.43
3:H:216:VAL:CA	3:H:216:VAL:CG1	2.89	0.43
2:A:157:ASP:O	2:A:159:SER:N	2.51	0.43
2:A:87:GLU:OE1	2:A:175:LYS:NZ	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:110:LEU:HG	2:C:111:GLU:O	2.18	0.43
2:C:16:GLY:O	2:C:17:GLU:HG3	2.18	0.43
2:C:30:LEU:HG	2:C:37:ASN:ND2	2.29	0.43
3:D:47:TRP:CZ3	3:D:49:GLY:HA2	2.53	0.43
2:E:204:HIS:C	2:E:206:THR:N	2.71	0.43
2:E:24:LYS:CE	2:E:76:ASP:CG	2.86	0.43
2:G:6:GLN:NE2	2:G:108:THR:OG1	2.41	0.43
2:G:123:ILE:H	2:G:213:LYS:HE3	1.83	0.43
3:H:201:ASN:OD1	3:H:212:ASP:OD1	2.36	0.43
4:M:47:THR:C	4:M:49:GLU:N	2.71	0.43
2:A:89:GLN:HE22	2:A:172:GLN:CB	2.31	0.43
2:C:127:SER:OG	2:C:130:GLN:HB3	2.19	0.43
2:G:127:SER:O	2:G:130:GLN:N	2.52	0.43
3:H:107:VAL:HG21	5:H:221:HOH:O	2.19	0.43
4:L:43:PHE:CE2	4:L:47:THR:OG1	2.70	0.43
1:Q:5:PRO:O	1:Q:6:LYS:CG	2.60	0.43
2:A:19:VAL:CG1	2:A:81:ILE:HD12	2.49	0.43
3:B:103:GLN:HA	3:B:103:GLN:OE1	2.16	0.43
3:D:198:VAL:O	3:D:215:ILE:CD1	2.57	0.43
2:E:139:VAL:HB	2:E:141:PHE:HE2	1.84	0.43
2:E:196:ASN:CG	2:E:196:ASN:O	2.57	0.43
2:G:178:THR:O	2:G:179:TYR:O	2.36	0.43
3:H:32:PHE:CD1	3:H:100:LEU:HA	2.54	0.43
4:O:42:THR:O	4:O:44:GLU:N	2.52	0.43
2:A:204:HIS:HB3	2:A:205:LYS:H	1.50	0.42
2:A:67:ARG:HH21	2:A:67:ARG:HG3	1.84	0.42
2:A:76:ASP:CG	2:A:76:ASP:CA	2.80	0.42
3:B:40:ALA:CB	3:B:41:PRO:CD	2.91	0.42
2:C:123:ILE:HD11	2:C:154:TRP:HZ3	1.84	0.42
2:E:191:GLU:CG	2:E:194:ARG:NH1	2.82	0.42
4:M:32:GLY:O	4:M:33:LYS:C	2.56	0.42
2:C:148:LYS:O	2:C:149:ASP:O	2.37	0.42
3:D:162:GLY:O	3:D:163:SER:C	2.57	0.42
2:E:45:LYS:HA	2:E:90:ALA:CB	2.50	0.42
3:F:182:LEU:C	3:F:182:LEU:CD2	2.82	0.42
3:F:52:ASN:CB	3:F:55:THR:OG1	2.63	0.42
2:G:19:VAL:HG22	2:G:20:THR:N	2.33	0.42
3:H:151:PHE:HB3	3:H:152:PRO:CD	2.44	0.42
3:H:91:THR:CG2	3:H:91:THR:O	2.66	0.42
2:C:153:LYS:O	2:C:201:GLU:N	2.30	0.42
2:C:199:THR:HB	2:C:214:SER:HB3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:132:GLY:C	3:D:134:ALA:N	2.73	0.42
3:F:106:ASP:OD2	3:F:107:VAL:HG12	2.19	0.42
3:F:7:SER:CB	3:F:20:ILE:HG13	2.39	0.42
4:M:24:LYS:CB	4:M:24:LYS:CD	2.91	0.42
4:O:65:THR:N	4:O:78:LYS:O	2.37	0.42
1:Q:12:LYS:HG3	1:Q:13:ARG:HG2	2.01	0.42
2:A:118:ALA:CB	2:A:119:PRO:HD2	2.47	0.42
3:B:126:VAL:HG21	3:B:211:VAL:HG21	2.01	0.42
3:B:171:PHE:N	3:B:171:PHE:CD1	2.86	0.42
3:B:23:LYS:HA	3:B:78:THR:HA	2.02	0.42
2:C:148:LYS:CG	2:C:149:ASP:H	2.33	0.42
2:E:12:ALA:CB	2:E:12:ALA:N	2.67	0.42
2:E:12:ALA:CB	2:E:12:ALA:O	2.67	0.42
2:E:157:ASP:OD1	2:E:196:ASN:N	2.47	0.42
2:E:55:TYR:CD1	3:F:104:TYR:HE2	2.29	0.42
2:G:125:PRO:O	2:G:126:PRO:O	2.38	0.42
2:G:145:PHE:H	2:G:178:THR:HB	1.84	0.42
3:H:83:ILE:O	3:H:84:ASN:C	2.54	0.42
4:N:68:LEU:HG	4:N:75:MET:HE3	2.01	0.42
4:O:65:THR:HB	4:O:78:LYS:HG3	2.01	0.42
1:Q:19:PRO:O	1:Q:20:GLN:HG3	2.18	0.42
1:Q:40:ARG:CZ	1:Q:45:GLY:HA2	2.49	0.42
1:S:29:GLN:HA	3:H:101:LEU:CD2	2.49	0.42
1:S:6:LYS:HA	1:S:7:PRO:HD2	1.97	0.42
2:A:216:ASN:C	2:A:218:ASN:N	2.71	0.42
1:P:36:LEU:HD22	3:B:102:ARG:NH2	2.34	0.42
3:B:87:LYS:O	3:B:116:VAL:HG11	2.20	0.42
3:B:189:PRO:O	3:B:191:SER:N	2.52	0.42
3:B:4:LEU:HD23	3:B:34:MET:HE3	2.00	0.42
3:B:52:ASN:OD1	3:B:55:THR:N	2.52	0.42
2:C:4:MET:HE3	2:C:25:SER:HB3	2.01	0.42
2:G:54:ILE:HG22	2:G:60:ARG:CA	2.42	0.42
2:G:54:ILE:HG22	2:G:60:ARG:N	2.34	0.42
3:H:164:LEU:CD1	3:H:198:VAL:HG13	2.49	0.42
3:H:188:VAL:CB	3:H:189:PRO:CD	2.72	0.42
3:H:24:ALA:O	3:H:25:SER:CB	2.60	0.42
4:L:61:ASN:O	4:L:81:GLY:HA2	2.19	0.42
1:S:29:GLN:NE2	3:H:52:ASN:C	2.72	0.42
2:A:114:ARG:HG3	2:A:146:TYR:CG	2.54	0.42
2:A:28:SER:C	2:A:29:LEU:HD23	2.36	0.42
3:B:101:LEU:HD13	3:B:101:LEU:HA	1.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:157:VAL:C	3:B:158:THR:CG2	2.85	0.42
3:B:38:ASN:HB2	3:B:48:MET:SD	2.59	0.42
2:C:189:LYS:CG	2:C:189:LYS:CA	2.80	0.42
2:C:206:THR:H	2:C:206:THR:HG23	1.85	0.42
2:C:43:GLN:CD	2:C:45:LYS:NZ	2.73	0.42
2:E:215:PHE:HD1	2:E:215:PHE:C	2.18	0.42
2:E:89:GLN:OE1	2:E:177:SER:HB3	2.20	0.42
3:F:102:ARG:HH21	3:F:102:ARG:HG2	1.83	0.42
3:F:86:LEU:HD13	3:F:116:VAL:HG21	2.00	0.42
3:F:193:TRP:HA	3:F:194:PRO:HA	1.58	0.42
3:H:149:GLY:C	3:H:150:TYR:O	2.58	0.42
3:H:151:PHE:CB	3:H:152:PRO:CD	2.97	0.42
2:A:121:VAL:HG22	2:A:142:LEU:HD22	2.02	0.42
3:B:129:LEU:N	3:B:129:LEU:CD1	2.82	0.42
3:B:38:ASN:O	3:B:45:LEU:HA	2.20	0.42
2:C:95:LYS:HA	2:C:103:THR:O	2.20	0.42
2:C:117:ALA:O	2:C:145:PHE:HA	2.20	0.42
3:D:176:GLN:C	3:D:177:SER:HG	2.22	0.42
4:L:54:ALA:O	4:L:56:LEU:O	2.37	0.42
4:L:62:GLY:HA3	4:L:81:GLY:H	1.79	0.42
4:M:29:PHE:CD1	4:M:29:PHE:N	2.88	0.42
4:O:29:PHE:HD2	4:O:61:ASN:CG	2.23	0.42
4:O:59:LYS:CB	4:O:59:LYS:CD	2.90	0.42
1:P:25:PRO:HB2	1:P:26:GLY:H	1.55	0.42
1:S:13:ARG:CB	1:S:13:ARG:NH1	2.62	0.42
2:A:124:PHE:HA	2:A:125:PRO:HD3	1.75	0.42
2:C:155:LYS:HE3	2:C:158:GLY:HA2	2.01	0.42
2:G:148:LYS:O	2:G:149:ASP:C	2.51	0.42
2:G:16:GLY:C	2:G:83:SER:HA	2.40	0.42
4:O:29:PHE:CD2	4:O:79:PHE:CE2	3.08	0.42
2:A:54:ILE:HD12	2:A:70:GLY:CA	2.50	0.42
3:B:97:ALA:HA	3:B:108:TRP:HA	2.01	0.42
2:C:121:VAL:HG23	2:C:121:VAL:H	1.61	0.42
2:C:29:LEU:CD1	2:C:77:PHE:CZ	2.98	0.42
3:D:17:THR:OG1	3:D:17:THR:O	2.28	0.42
3:D:74:THR:O	3:D:77:SER:N	2.53	0.42
2:E:131:LEU:O	2:E:133:SER:N	2.48	0.42
2:E:49:SER:HA	2:E:50:PRO:HD3	1.85	0.42
3:F:17:THR:HG22	3:F:18:VAL:H	1.85	0.42
3:F:50:TRP:HE1	3:F:59:THR:HB	1.82	0.42
3:H:72:LEU:C	3:H:72:LEU:HD23	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:28:ILE:HA	4:M:34:ILE:HG12	2.02	0.42
4:N:21:VAL:O	4:N:40:LYS:HG3	2.20	0.42
1:P:38:PRO:O	3:F:32:PHE:CZ	2.72	0.42
1:Q:39:ARG:HA	1:Q:39:ARG:HD2	1.76	0.42
2:A:124:PHE:N	2:A:139:VAL:O	2.42	0.42
2:C:3:VAL:HB	2:C:26:SER:OG	2.20	0.42
3:D:11:LEU:C	3:D:11:LEU:HD13	2.40	0.42
3:D:200:CYS:N	3:D:213:LYS:O	2.50	0.42
3:D:52:ASN:O	3:D:53:THR:C	2.51	0.42
2:E:95:LYS:CB	2:E:104:PHE:CD2	3.00	0.42
2:E:165:VAL:O	2:E:166:LEU:CG	2.67	0.42
3:F:179:LEU:O	3:F:180:TYR:C	2.58	0.42
4:L:22:THR:HG22	4:L:23:ILE:N	2.34	0.42
4:M:28:ILE:HD11	4:M:76:ASN:HB3	2.01	0.42
1:Q:6:LYS:NZ	5:Q:54:HOH:O	2.53	0.42
2:A:114:ARG:NE	2:A:146:TYR:HB2	2.35	0.41
2:A:157:ASP:O	2:A:159:SER:HB2	2.20	0.41
3:D:11:LEU:HD23	3:D:115:THR:HG22	2.02	0.41
2:E:85:GLN:O	2:E:88:ASP:OD1	2.37	0.41
3:F:168:VAL:HG12	3:F:169:HIS:H	1.85	0.41
2:G:211:ILE:HD12	2:G:212:VAL:N	2.32	0.41
2:G:44:GLN:NE2	2:G:48:GLN:O	2.42	0.41
3:H:128:PRO:C	3:H:129:LEU:HD23	2.39	0.41
3:H:99:PHE:CB	3:H:99:PHE:N	2.69	0.41
4:M:39:PHE:O	4:M:40:LYS:C	2.57	0.41
4:O:21:VAL:C	4:O:22:THR:HG1	2.22	0.41
2:A:86:ALA:C	2:A:88:ASP:N	2.71	0.41
2:A:166:LEU:CD1	3:B:176:GLN:HE22	2.13	0.41
3:B:204:HIS:HA	3:B:205:PRO:HD2	1.61	0.41
2:C:199:THR:CB	2:C:214:SER:HB3	2.49	0.41
3:D:218:ARG:CG	3:D:218:ARG:HH21	2.33	0.41
3:D:64:PHE:HD2	3:D:68:PHE:CE2	2.39	0.41
3:F:87:LYS:O	3:F:116:VAL:HG11	2.20	0.41
2:G:62:SER:O	2:G:64:VAL:N	2.53	0.41
3:H:167:GLY:O	3:H:168:VAL:CG2	2.67	0.41
3:H:78:THR:CG2	3:H:79:ALA:N	2.83	0.41
4:L:44:GLU:C	4:L:46:ALA:N	2.71	0.41
2:A:20:THR:O	4:L:53:TYR:CE1	2.71	0.41
2:C:18:LYS:HE2	4:M:60:VAL:HG11	2.02	0.41
2:A:120:THR:HB	2:A:143:ASN:HB2	2.03	0.41
3:B:147:VAL:N	3:B:182:LEU:O	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:31:ASP:CG	2:E:33:ARG:HH11	2.23	0.41
2:C:188:THR:HG23	2:C:191:GLU:HB3	2.00	0.41
3:D:12:LYS:HD3	3:D:12:LYS:HA	1.75	0.41
3:D:138:ASN:CG	3:D:139:SER:N	2.56	0.41
3:D:214:LYS:CD	3:D:215:ILE:O	2.67	0.41
2:E:156:ILE:HG12	2:E:198:TYR:CD1	2.55	0.41
2:E:187:LEU:HB3	2:E:191:GLU:OE1	2.20	0.41
2:E:62:SER:C	2:E:64:VAL:H	2.23	0.41
2:E:65:PRO:HB3	2:E:67:ARG:CD	2.50	0.41
3:F:176:GLN:O	3:F:177:SER:C	2.58	0.41
2:G:102:LEU:CD2	3:H:105:PHE:HZ	2.30	0.41
2:G:199:THR:HG22	2:G:214:SER:CB	2.49	0.41
2:G:150:ILE:CD1	2:G:203:THR:O	2.69	0.41
3:H:12:LYS:CE	3:H:12:LYS:CA	2.96	0.41
4:N:77:ILE:O	4:N:79:PHE:CE1	2.69	0.41
4:O:31:ASP:OD2	4:O:33:LYS:HG2	2.20	0.41
2:A:2:ILE:O	2:A:3:VAL:C	2.57	0.41
2:A:61:GLU:HB3	2:A:64:VAL:HG23	2.02	0.41
3:B:6:GLN:NE2	3:B:111:GLY:CA	2.84	0.41
3:B:69:ALA:C	3:B:70:PHE:CD2	2.94	0.41
3:D:152:PRO:O	3:D:154:PRO:CG	2.68	0.41
3:D:1:GLN:NE2	1:Q:13:ARG:CD	2.81	0.41
3:F:215:ILE:HG23	3:F:215:ILE:HD12	1.55	0.41
3:F:216:VAL:O	3:F:217:PRO:C	2.58	0.41
2:G:112:LEU:CG	2:G:113:LYS:N	2.83	0.41
2:G:14:SER:HB3	2:G:17:GLU:OE1	2.21	0.41
2:G:152:VAL:HG21	2:G:202:ALA:HA	2.01	0.41
2:G:36:LYS:HD3	2:G:56:TRP:NE1	2.35	0.41
3:H:186:VAL:HG11	3:H:198:VAL:HG11	2.03	0.41
3:H:59:THR:CA	3:H:59:THR:CG2	2.89	0.41
4:L:25:VAL:CG2	4:L:26:ASN:N	2.75	0.41
4:N:20:GLU:HG2	4:N:41:GLY:O	2.20	0.41
1:S:14:ASN:O	1:S:15:THR:CG2	2.68	0.41
2:A:12:ALA:O	2:A:113:LYS:CG	2.62	0.41
2:A:14:SER:HB2	2:A:17:GLU:OE2	2.21	0.41
2:A:2:ILE:HD13	2:A:29:LEU:HD21	2.02	0.41
2:A:56:TRP:CH2	3:B:102:ARG:HD2	2.54	0.41
2:A:19:VAL:HG13	2:A:81:ILE:H	1.85	0.41
3:B:170:THR:O	3:B:170:THR:HG22	2.12	0.41
3:B:62:ASP:C	3:B:64:PHE:N	2.71	0.41
2:C:102:LEU:HD12	2:C:102:LEU:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:217:ARG:HD2	2:C:217:ARG:HH21	1.50	0.41
2:C:1:ASP:O	2:C:2:ILE:O	2.37	0.41
2:C:45:LYS:HA	2:C:90:ALA:CB	2.50	0.41
3:D:129:LEU:HB2	3:D:144:GLY:HA3	2.01	0.41
3:D:140:MET:CE	3:D:187:THR:OG1	2.68	0.41
3:D:2:ILE:HG12	3:D:26:GLY:O	2.21	0.41
2:E:55:TYR:HD2	2:E:56:TRP:N	2.17	0.41
3:F:141:VAL:HG12	3:F:190:SER:HA	2.03	0.41
2:G:155:LYS:HE2	2:G:201:GLU:CD	2.39	0.41
2:G:19:VAL:CG1	2:G:81:ILE:CB	2.88	0.41
3:H:122:THR:HA	3:H:123:PRO:HD3	1.87	0.41
3:H:48:MET:HE2	3:H:64:PHE:CD1	2.55	0.41
4:M:63:GLU:OE2	4:M:63:GLU:N	2.41	0.41
4:O:58:ALA:CB	4:O:59:LYS:N	2.83	0.41
1:Q:33:GLY:CA	1:Q:36:LEU:HB3	2.22	0.41
3:B:182:LEU:CD2	3:B:183:SER:O	2.69	0.41
3:B:215:ILE:CG2	3:B:215:ILE:O	2.67	0.41
2:C:219:GLU:O	2:C:220:CYS:HB3	2.21	0.41
2:C:61:GLU:H	2:C:64:VAL:CG2	2.32	0.41
3:F:13:LYS:HA	3:F:117:SER:O	2.20	0.41
3:F:6:GLN:O	3:F:7:SER:C	2.59	0.41
3:F:73:GLU:HB3	3:F:78:THR:HB	2.02	0.41
2:G:64:VAL:HG22	2:G:65:PRO:HD2	2.02	0.41
3:H:100:LEU:N	3:H:100:LEU:HD23	2.34	0.41
1:S:30:ILE:HG22	3:H:101:LEU:HD22	2.02	0.41
3:H:197:THR:CG2	3:H:214:LYS:HE3	2.50	0.41
4:L:76:ASN:O	4:L:77:ILE:C	2.59	0.41
4:N:28:ILE:CG1	4:N:28:ILE:CG2	2.86	0.41
1:S:9:ARG:HH21	1:S:10:LYS:H	1.68	0.41
1:S:11:THR:HB	1:S:12:LYS:HD2	2.02	0.41
3:B:60:TYR:CZ	3:B:69:ALA:HA	2.55	0.41
2:C:161:ARG:NE	2:C:161:ARG:CG	2.72	0.41
3:D:20:ILE:HG21	3:D:20:ILE:HD13	1.83	0.41
3:F:211:VAL:HG22	3:F:212:ASP:C	2.40	0.41
3:B:176:GLN:O	3:B:177:SER:HB2	2.20	0.41
2:C:54:ILE:CG2	2:C:55:TYR:N	2.83	0.41
3:D:39:GLN:HA	3:D:44:GLY:O	2.21	0.41
3:D:52:ASN:HD21	3:D:54:GLU:HB2	1.86	0.41
3:D:83:ILE:HG22	3:D:86:LEU:HD23	2.01	0.41
2:E:175:LYS:O	2:E:176:ASP:CB	2.66	0.41
2:G:198:TYR:O	2:G:214:SER:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:123:ILE:HG22	2:G:213:LYS:HD2	2.02	0.41
2:G:53:LEU:HB3	2:G:54:ILE:CD1	2.51	0.41
2:G:53:LEU:N	2:G:53:LEU:CD1	2.83	0.41
2:G:55:TYR:O	2:G:56:TRP:HB2	2.20	0.41
3:H:186:VAL:HG22	3:H:187:THR:N	2.35	0.41
3:H:67:ARG:CG	3:H:68:PHE:CE2	3.00	0.41
3:H:18:VAL:HG11	3:H:86:LEU:HD21	2.02	0.41
2:A:112:LEU:HD23	2:A:113:LYS:O	2.19	0.41
2:A:220:CYS:HA	3:B:133:SER:HB3	2.02	0.41
2:A:55:TYR:O	2:A:56:TRP:C	2.55	0.41
2:A:89:GLN:HE22	2:A:172:GLN:C	2.24	0.41
2:C:31:ASN:HD21	2:C:33:ARG:HB2	1.85	0.41
2:C:43:GLN:O	2:C:51:LYS:N	2.54	0.41
3:D:125:SER:O	3:D:126:VAL:HG23	2.20	0.41
3:D:175:LEU:HD12	3:D:180:TYR:CD1	2.56	0.41
3:D:160:ASN:HA	3:D:199:THR:OG1	2.19	0.41
3:D:72:LEU:HA	3:D:72:LEU:HD12	1.71	0.41
2:E:71:ARG:CD	2:E:71:ARG:CB	2.79	0.41
3:F:35:HIS:CD2	3:F:50:TRP:CB	3.03	0.41
2:G:109:LYS:CD	2:G:109:LYS:CB	2.81	0.41
3:H:58:PRO:HB2	3:H:60:TYR:CE2	2.55	0.41
4:M:45:GLU:HB3	4:M:46:ALA:H	1.71	0.41
3:B:117:SER:OG	3:B:118:SER:N	2.54	0.41
3:B:143:LEU:HD12	3:B:198:VAL:HG11	2.03	0.41
3:D:170:THR:O	3:D:171:PHE:C	2.59	0.41
3:D:142:THR:OG1	3:D:187:THR:HB	2.21	0.41
3:D:20:ILE:HG13	3:D:81:LEU:HB3	2.02	0.41
2:E:11:LEU:HD11	2:E:21:MET:SD	2.61	0.41
2:E:157:ASP:OD1	2:E:195:HIS:HB3	2.21	0.41
2:E:102:LEU:HD12	3:F:47:TRP:NE1	2.36	0.41
3:F:57:GLU:HA	3:F:58:PRO:HD2	1.98	0.41
3:F:39:GLN:O	3:F:92:ALA:HB1	2.20	0.41
2:G:188:THR:OG1	2:G:191:GLU:HB3	2.21	0.41
3:H:46:ASN:O	3:H:47:TRP:C	2.55	0.41
1:S:24:PHE:CZ	3:H:32:PHE:CZ	3.09	0.41
2:A:45:LYS:CB	2:A:46:PRO:HD2	2.41	0.41
3:B:94:TYR:O	3:B:111:GLY:CA	2.69	0.41
2:C:70:GLY:C	2:C:71:ARG:HG3	2.42	0.41
3:D:135:ALA:C	3:D:137:THR:N	2.70	0.41
2:E:172:GLN:HE21	2:E:177:SER:CB	2.29	0.41
2:E:155:LYS:NZ	2:E:201:GLU:OE2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:65:PRO:O	2:E:66:ASP:C	2.59	0.41
3:F:117:SER:OG	3:F:118:SER:N	2.54	0.41
3:F:199:THR:CG2	3:F:214:LYS:HB2	2.49	0.41
3:F:51:VAL:HG22	3:F:70:PHE:HB3	2.02	0.41
3:H:116:VAL:O	3:H:117:SER:CB	2.63	0.41
3:H:37:VAL:C	3:H:48:MET:HG3	2.39	0.41
3:H:53:THR:H	3:H:53:THR:HG23	1.35	0.41
3:H:78:THR:HG22	3:H:79:ALA:N	2.35	0.41
3:H:70:PHE:CD2	3:H:81:LEU:HD23	2.56	0.41
2:A:173:ASP:CG	2:A:174:SER:H	2.25	0.40
3:B:151:PHE:CE1	3:B:152:PRO:HB3	2.57	0.40
3:B:204:HIS:C	3:B:206:ALA:N	2.69	0.40
3:D:136:GLN:O	3:D:137:THR:O	2.39	0.40
2:E:174:SER:OG	2:E:174:SER:O	2.33	0.40
3:F:78:THR:CG2	3:F:79:ALA:H	2.32	0.40
2:G:123:ILE:O	2:G:123:ILE:CG2	2.65	0.40
3:H:10:GLU:HB2	3:H:114:VAL:HA	2.03	0.40
3:H:126:VAL:C	3:H:127:TYR:CD1	2.95	0.40
4:M:21:VAL:O	4:M:41:GLY:O	2.39	0.40
2:A:166:LEU:O	2:A:184:THR:N	2.51	0.40
2:A:145:PHE:N	2:A:179:TYR:O	2.52	0.40
2:A:20:THR:HG22	2:A:20:THR:O	2.20	0.40
2:A:44:GLN:HB2	2:A:50:PRO:HA	2.02	0.40
2:C:54:ILE:C	2:C:55:TYR:HD1	2.23	0.40
2:C:86:ALA:O	2:C:88:ASP:N	2.47	0.40
2:E:69:THR:N	2:E:80:THR:O	2.53	0.40
2:E:19:VAL:HG11	2:E:84:VAL:CG2	2.51	0.40
3:F:13:LYS:O	3:F:14:PRO:C	2.58	0.40
2:G:211:ILE:HG13	2:G:212:VAL:N	2.35	0.40
2:G:219:GLU:OE2	3:H:134:ALA:CB	2.69	0.40
3:H:169:HIS:HB2	3:H:171:PHE:HE1	1.87	0.40
4:M:75:MET:HG2	4:M:77:ILE:CD1	2.51	0.40
4:N:53:TYR:OH	4:N:57:HIS:CE1	2.75	0.40
4:O:57:HIS:HB2	4:O:58:ALA:H	1.04	0.40
1:S:36:LEU:HD13	1:S:36:LEU:HA	2.02	0.40
2:A:127:SER:O	2:A:128:SER:C	2.59	0.40
2:A:69:THR:O	2:A:79:LEU:HA	2.22	0.40
2:A:97:ALA:O	2:A:98:TYR:C	2.57	0.40
3:D:11:LEU:O	3:D:11:LEU:HD13	2.21	0.40
3:D:15:GLY:C	3:D:86:LEU:H	2.24	0.40
2:E:122:SER:O	2:E:141:PHE:N	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:139:VAL:O	2:E:139:VAL:HG23	2.13	0.40
2:E:63:GLY:O	2:E:65:PRO:HD3	2.22	0.40
3:F:196:GLU:O	3:F:197:THR:CG2	2.57	0.40
2:G:102:LEU:HD23	3:H:105:PHE:HZ	1.81	0.40
2:G:123:ILE:HA	2:G:140:CYS:HA	2.04	0.40
2:G:67:ARG:HB2	2:G:82:SER:HG	1.86	0.40
2:A:77:PHE:N	2:A:77:PHE:CD2	2.88	0.40
3:B:89:GLU:N	3:B:89:GLU:CD	2.75	0.40
3:B:94:TYR:O	3:B:111:GLY:HA2	2.22	0.40
2:C:129:GLU:CA	2:C:129:GLU:CG	2.89	0.40
2:C:173:ASP:OD1	2:C:175:LYS:CD	2.66	0.40
2:C:53:LEU:O	2:C:54:ILE:HD13	2.22	0.40
3:D:174:VAL:HG12	3:D:175:LEU:O	2.21	0.40
3:D:196:GLU:O	3:D:198:VAL:HG23	2.22	0.40
3:D:67:ARG:CD	3:D:85:SER:HG	2.35	0.40
2:G:173:ASP:CB	2:G:176:ASP:HB3	2.50	0.40
2:G:203:THR:HA	2:G:210:PRO:HG3	2.03	0.40
2:G:61:GLU:OE1	3:H:104:TYR:OH	2.39	0.40
3:H:29:PHE:HE2	3:H:72:LEU:HD11	1.87	0.40
4:O:64:TRP:CZ3	4:O:66:ALA:CB	3.05	0.40
1:Q:37:LEU:H	1:Q:38:PRO:CD	2.34	0.40
1:Q:40:ARG:NE	1:Q:45:GLY:O	2.55	0.40
3:B:118:SER:O	3:B:119:ALA:O	2.39	0.40
3:B:98:ARG:HH21	3:B:98:ARG:HD2	1.35	0.40
2:C:157:ASP:CB	2:C:196:ASN:H	2.27	0.40
2:C:51:LYS:HA	2:C:51:LYS:HD3	1.75	0.40
2:C:16:GLY:CA	2:C:84:VAL:O	2.69	0.40
3:D:20:ILE:HD11	3:D:81:LEU:HD22	2.04	0.40
3:D:96:CYS:O	3:D:109:GLY:N	2.52	0.40
2:E:124:PHE:HA	2:E:125:PRO:HD3	1.88	0.40
2:E:173:ASP:OD1	2:E:175:LYS:HG2	2.21	0.40
2:E:191:GLU:O	2:E:194:ARG:NH1	2.54	0.40
2:E:155:LYS:CB	2:E:199:THR:OG1	2.70	0.40
3:F:20:ILE:CD1	3:F:112:THR:CB	2.99	0.40
3:F:126:VAL:O	3:F:213:LYS:NZ	2.43	0.40
3:F:17:THR:CG2	3:F:18:VAL:N	2.85	0.40
2:G:22:SER:CB	2:G:78:THR:HG22	2.51	0.40
3:H:207:SER:HB2	3:H:209:THR:HG23	2.02	0.40
3:H:51:VAL:HG23	3:H:52:ASN:H	1.86	0.40
4:L:39:PHE:HB3	4:L:49:GLU:OE2	2.21	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:149:ASP:OD1	1:Q:10:LYS:O[1_455]	2.02	0.18
2:C:171:ASP:OD1	1:Q:18:ARG:NH1[1_455]	2.11	0.09
1:S:21:ASP:OD2	4:O:22:THR:OG1[1_655]	2.12	0.08

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	P	22/44 (50%)	5 (23%)	4 (18%)	13 (59%)	0	0
1	Q	42/44 (96%)	14 (33%)	15 (36%)	13 (31%)	0	0
1	S	42/44 (96%)	10 (24%)	14 (33%)	18 (43%)	0	0
2	A	218/220 (99%)	158 (72%)	38 (17%)	22 (10%)	0	7
2	C	218/220 (99%)	147 (67%)	35 (16%)	36 (16%)	0	2
2	E	218/220 (99%)	163 (75%)	34 (16%)	21 (10%)	0	8
2	G	217/220 (99%)	147 (68%)	38 (18%)	32 (15%)	0	3
3	B	216/218 (99%)	144 (67%)	39 (18%)	33 (15%)	0	3
3	D	216/218 (99%)	142 (66%)	40 (18%)	34 (16%)	0	2
3	F	216/218 (99%)	149 (69%)	39 (18%)	28 (13%)	0	4
3	H	216/218 (99%)	138 (64%)	51 (24%)	27 (12%)	0	5
4	L	64/80 (80%)	47 (73%)	8 (12%)	9 (14%)	0	3
4	M	60/80 (75%)	33 (55%)	19 (32%)	8 (13%)	0	4
4	N	62/80 (78%)	39 (63%)	13 (21%)	10 (16%)	0	2
4	O	60/80 (75%)	37 (62%)	16 (27%)	7 (12%)	0	5
All	All	2087/2204 (95%)	1373 (66%)	403 (19%)	311 (15%)	0	3

All (311) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	P	20	GLN
1	P	25	PRO
1	P	34	VAL
1	P	35	TYR
1	P	37	LEU
1	P	38	PRO
1	P	39	ARG
2	A	25	SER
2	A	56	TRP
2	A	133	SER
2	A	144	ASN
2	A	191	GLU
2	A	217	ARG
3	B	40	ALA
3	B	53	THR
3	B	74	THR
3	B	103	GLN
3	B	119	ALA
3	B	141	VAL
3	B	163	SER
3	B	178	ASP
3	B	195	SER
3	B	210	LYS
4	L	19	GLU
4	L	66	ALA
4	L	67	ASP
4	L	77	ILE
2	C	2	ILE
2	C	14	SER
2	C	28	SER
2	C	34	THR
2	C	50	PRO
2	C	63	GLY
2	C	73	SER
2	C	83	SER
2	C	84	VAL
2	C	89	GLN
2	C	106	ALA
2	C	133	SER
2	C	149	ASP
2	C	189	LYS
2	C	194	ARG
2	C	195	HIS

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Mol	Chain	Res	Type
3	D	16	GLU
3	D	53	THR
3	D	74	THR
3	D	75	SER
3	D	77	SER
3	D	91	THR
3	D	112	THR
3	D	113	THR
3	D	119	ALA
3	D	135	ALA
3	D	137	THR
3	D	151	PHE
3	D	160	ASN
3	D	171	PHE
3	D	186	VAL
3	D	206	ALA
1	Q	5	PRO
1	Q	19	PRO
1	Q	39	ARG
4	M	40	LYS
4	M	58	ALA
4	M	59	LYS
4	M	60	VAL
2	E	28	SER
2	E	46	PRO
2	E	50	PRO
2	E	56	TRP
2	E	84	VAL
2	E	144	ASN
2	E	176	ASP
3	F	14	PRO
3	F	54	GLU
3	F	63	ASP
3	F	74	THR
3	F	149	GLY
4	N	21	VAL
4	N	43	PHE
4	N	59	LYS
4	N	68	LEU
4	N	69	GLU
1	S	7	PRO
1	S	10	LYS

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Mol	Chain	Res	Type
1	S	23	LYS
1	S	30	ILE
1	S	31	VAL
1	S	38	PRO
2	G	25	SER
2	G	28	SER
2	G	35	ARG
2	G	62	SER
2	G	72	GLY
2	G	98	TYR
2	G	111	GLU
2	G	162	GLN
2	G	179	TYR
2	G	188	THR
3	H	2	ILE
3	H	52	ASN
3	H	92	ALA
3	H	139	SER
3	H	150	TYR
3	H	161	SER
3	H	165	SER
3	H	166	SER
4	O	33	LYS
4	O	56	LEU
4	O	60	VAL
1	P	24	PHE
2	A	66	ASP
2	A	114	ARG
2	A	158	GLY
2	A	194	ARG
2	A	195	HIS
2	A	205	LYS
3	B	28	THR
3	B	118	SER
3	B	135	ALA
3	B	149	GLY
3	B	197	THR
3	B	217	PRO
4	L	20	GLU
2	C	87	GLU
2	C	148	LYS
2	C	162	GLN

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Mol	Chain	Res	Type
2	C	187	LEU
2	C	219	GLU
3	D	8	GLY
3	D	62	ASP
3	D	103	GLN
3	D	133	SER
3	D	152	PRO
3	D	175	LEU
3	D	176	GLN
1	Q	13	ARG
1	Q	16	ASN
1	Q	21	ASP
4	M	80	ALA
2	E	66	ASP
2	E	86	ALA
2	E	129	GLU
2	E	134	GLY
2	E	157	ASP
2	E	171	ASP
3	F	7	SER
3	F	15	GLY
3	F	32	PHE
3	F	77	SER
3	F	86	LEU
3	F	103	GLN
3	F	110	ALA
3	F	135	ALA
3	F	197	THR
4	N	20	GLU
4	N	44	GLU
1	S	5	PRO
1	S	36	LEU
1	S	40	ARG
1	S	43	ARG
2	G	16	GLY
2	G	32	SER
2	G	60	ARG
2	G	83	SER
2	G	131	LEU
2	G	132	THR
2	G	144	ASN
2	G	161	ARG

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Mol	Chain	Res	Type
2	G	206	THR
3	H	20	ILE
3	H	60	TYR
3	H	62	ASP
3	H	89	GLU
3	H	113	THR
3	H	176	GLN
3	H	190	SER
3	H	210	LYS
4	O	54	ALA
4	O	59	LYS
1	P	30	ILE
2	A	88	ASP
2	A	129	GLU
2	A	157	ASP
3	B	14	PRO
3	B	29	PHE
3	B	52	ASN
3	B	145	CYS
3	B	177	SER
3	B	190	SER
3	B	215	ILE
4	L	44	GLU
4	L	59	LYS
2	C	16	GLY
2	C	33	ARG
2	C	57	ALA
2	C	65	PRO
2	C	86	ALA
2	C	197	SER
2	C	214	SER
2	C	218	ASN
3	D	14	PRO
3	D	73	GLU
3	D	85	SER
3	D	177	SER
3	D	205	PRO
1	Q	10	LYS
1	Q	28	GLY
1	Q	37	LEU
2	E	89	GLN
2	E	218	ASN

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Mol	Chain	Res	Type
3	F	47	TRP
3	F	65	LYS
3	F	190	SER
4	N	72	GLY
1	S	14	ASN
1	S	18	ARG
2	G	128	SER
2	G	217	ARG
3	H	74	THR
3	H	141	VAL
4	O	58	ALA
2	A	2	ILE
2	A	57	ALA
2	A	215	PHE
3	B	88	ASN
2	C	8	PRO
2	C	82	SER
2	C	206	THR
3	D	134	ALA
3	D	149	GLY
1	Q	22	VAL
4	M	44	GLU
2	E	73	SER
2	E	189	LYS
2	E	194	ARG
3	F	31	ASP
3	F	76	ALA
3	F	138	ASN
3	F	150	TYR
3	F	191	SER
4	N	70	ASP
1	S	11	THR
1	S	19	PRO
1	S	44	LEU
2	G	38	TYR
2	G	114	ARG
3	H	7	SER
3	H	151	PHE
2	A	75	THR
2	A	117	ALA
2	A	148	LYS
3	B	7	SER

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Mol	Chain	Res	Type
3	B	22	CYS
3	B	76	ALA
3	B	85	SER
3	B	114	VAL
3	B	170	THR
3	B	205	PRO
4	L	18	LYS
4	L	60	VAL
2	C	126	PRO
2	C	136	ALA
2	C	144	ASN
3	D	57	GLU
3	D	162	GLY
3	D	209	THR
1	Q	4	ASN
1	Q	40	ARG
4	M	25	VAL
4	M	35	GLN
3	F	18	VAL
3	F	55	THR
3	F	151	PHE
4	N	60	VAL
2	G	30	LEU
2	G	90	ALA
2	G	157	ASP
3	H	31	ASP
3	H	58	PRO
3	H	94	TYR
3	H	153	GLU
3	D	104	TYR
1	Q	42	PRO
2	E	65	PRO
3	F	215	ILE
1	S	6	LYS
1	S	42	PRO
2	G	3	VAL
2	G	196	ASN
3	H	51	VAL
3	H	66	GLY
3	B	132	GLY
2	E	150	ILE
2	G	13	VAL

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Mol	Chain	Res	Type
2	G	46	PRO
2	G	65	PRO
3	H	171	PHE
1	P	22	VAL
1	P	32	GLY
3	F	9	PRO
1	S	33	GLY
2	A	84	VAL
2	C	135	GLY
2	G	84	VAL
1	P	28	GLY
3	B	172	PRO
2	E	210	PRO
4	O	21	VAL
1	P	26	GLY
3	F	152	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	P	15/37 (40%)	13 (87%)	2 (13%)	4 21
1	Q	37/37 (100%)	29 (78%)	8 (22%)	1 5
1	S	37/37 (100%)	25 (68%)	12 (32%)	0 2
2	A	195/195 (100%)	171 (88%)	24 (12%)	4 23
2	C	195/195 (100%)	167 (86%)	28 (14%)	3 18
2	E	195/195 (100%)	161 (83%)	34 (17%)	2 11
2	G	194/195 (100%)	165 (85%)	29 (15%)	3 17
3	B	187/187 (100%)	156 (83%)	31 (17%)	2 13
3	D	187/187 (100%)	165 (88%)	22 (12%)	5 25
3	F	187/187 (100%)	155 (83%)	32 (17%)	2 12
3	H	187/187 (100%)	161 (86%)	26 (14%)	3 20

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	L	48/62 (77%)	41 (85%)	7 (15%)	3 18
4	M	46/62 (74%)	37 (80%)	9 (20%)	1 7
4	N	46/62 (74%)	38 (83%)	8 (17%)	2 11
4	O	46/62 (74%)	42 (91%)	4 (9%)	10 38
All	All	1802/1887 (96%)	1526 (85%)	276 (15%)	2 17

All (276) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	P	21	ASP
1	P	38	PRO
2	A	3	VAL
2	A	9	SER
2	A	24	LYS
2	A	31	ASN
2	A	39	LEU
2	A	48	GLN
2	A	53	LEU
2	A	55	TYR
2	A	79	LEU
2	A	84	VAL
2	A	99	ILE
2	A	112	LEU
2	A	116	ASP
2	A	122	SER
2	A	142	LEU
2	A	147	PRO
2	A	180	SER
2	A	184	THR
2	A	187	LEU
2	A	205	LYS
2	A	210	PRO
2	A	212	VAL
2	A	215	PHE
2	A	216	ASN
3	B	5	VAL
3	B	10	GLU
3	B	11	LEU
3	B	20	ILE
3	B	31	ASP
3	B	39	GLN

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Mol	Chain	Res	Type
3	B	51	VAL
3	B	58	PRO
3	B	59	THR
3	B	62	ASP
3	B	65	LYS
3	B	72	LEU
3	B	73	GLU
3	B	74	THR
3	B	85	SER
3	B	90	ASP
3	B	108	TRP
3	B	113	THR
3	B	115	THR
3	B	120	LYS
3	B	128	PRO
3	B	136	GLN
3	B	179	LEU
3	B	182	LEU
3	B	186	VAL
3	B	194	PRO
3	B	196	GLU
3	B	202	VAL
3	B	211	VAL
3	B	212	ASP
3	B	215	ILE
4	L	25	VAL
4	L	26	ASN
4	L	43	PHE
4	L	47	THR
4	L	63	GLU
4	L	67	ASP
4	L	75	MET
2	C	2	ILE
2	C	27	GLN
2	C	35	ARG
2	C	39	LEU
2	C	49	SER
2	C	50	PRO
2	C	55	TYR
2	C	67	ARG
2	C	76	ASP
2	C	77	PHE

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Mol	Chain	Res	Type
2	C	96	GLN
2	C	120	THR
2	C	126	PRO
2	C	131	LEU
2	C	133	SER
2	C	137	SER
2	C	144	ASN
2	C	148	LYS
2	C	151	ASN
2	C	155	LYS
2	C	161	ARG
2	C	165	VAL
2	C	166	LEU
2	C	176	ASP
2	C	188	THR
2	C	210	PRO
2	C	215	PHE
2	C	218	ASN
3	D	9	PRO
3	D	27	TYR
3	D	43	LYS
3	D	46	ASN
3	D	52	ASN
3	D	89	GLU
3	D	115	THR
3	D	122	THR
3	D	124	PRO
3	D	141	VAL
3	D	153	GLU
3	D	156	THR
3	D	176	GLN
3	D	178	ASP
3	D	187	THR
3	D	197	THR
3	D	201	ASN
3	D	202	VAL
3	D	212	ASP
3	D	213	LYS
3	D	215	ILE
3	D	218	ARG
1	Q	5	PRO
1	Q	8	GLN

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Mol	Chain	Res	Type
1	Q	9	ARG
1	Q	13	ARG
1	Q	19	PRO
1	Q	36	LEU
1	Q	40	ARG
1	Q	44	LEU
4	M	23	ILE
4	M	31	ASP
4	M	34	ILE
4	M	36	THR
4	M	42	THR
4	M	52	ARG
4	M	65	THR
4	M	74	HIS
4	M	79	PHE
2	E	13	VAL
2	E	30	LEU
2	E	31	ASN
2	E	36	LYS
2	E	39	LEU
2	E	44	GLN
2	E	50	PRO
2	E	52	VAL
2	E	56	TRP
2	E	59	THR
2	E	66	ASP
2	E	69	THR
2	E	80	THR
2	E	88	ASP
2	E	89	GLN
2	E	96	GLN
2	E	101	PRO
2	E	114	ARG
2	E	144	ASN
2	E	149	ASP
2	E	150	ILE
2	E	151	ASN
2	E	166	LEU
2	E	179	TYR
2	E	180	SER
2	E	181	MET
2	E	185	LEU

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Mol	Chain	Res	Type
2	E	188	THR
2	E	199	THR
2	E	203	THR
2	E	205	LYS
2	E	208	THR
2	E	209	SER
2	E	215	PHE
3	F	7	SER
3	F	11	LEU
3	F	20	ILE
3	F	25	SER
3	F	33	SER
3	F	34	MET
3	F	38	ASN
3	F	57	GLU
3	F	58	PRO
3	F	63	ASP
3	F	67	ARG
3	F	71	SER
3	F	102	ARG
3	F	103	GLN
3	F	115	THR
3	F	118	SER
3	F	139	SER
3	F	140	MET
3	F	154	PRO
3	F	158	THR
3	F	160	ASN
3	F	171	PHE
3	F	176	GLN
3	F	178	ASP
3	F	182	LEU
3	F	188	VAL
3	F	197	THR
3	F	200	CYS
3	F	202	VAL
3	F	212	ASP
3	F	214	LYS
3	F	217	PRO
4	N	20	GLU
4	N	26	ASN
4	N	27	LEU

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Mol	Chain	Res	Type
4	N	43	PHE
4	N	49	GLU
4	N	57	HIS
4	N	65	THR
4	N	79	PHE
1	S	9	ARG
1	S	10	LYS
1	S	13	ARG
1	S	16	ASN
1	S	19	PRO
1	S	23	LYS
1	S	24	PHE
1	S	25	PRO
1	S	30	ILE
1	S	31	VAL
1	S	39	ARG
1	S	44	LEU
2	G	10	SER
2	G	20	THR
2	G	24	LYS
2	G	39	LEU
2	G	42	TYR
2	G	43	GLN
2	G	44	GLN
2	G	46	PRO
2	G	54	ILE
2	G	65	PRO
2	G	71	ARG
2	G	75	THR
2	G	87	GLU
2	G	96	GLN
2	G	102	LEU
2	G	125	PRO
2	G	126	PRO
2	G	137	SER
2	G	150	ILE
2	G	151	ASN
2	G	160	GLU
2	G	162	GLN
2	G	167	ASN
2	G	194	ARG
2	G	196	ASN

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Mol	Chain	Res	Type
2	G	213	LYS
2	G	215	PHE
2	G	217	ARG
2	G	218	ASN
3	H	2	ILE
3	H	9	PRO
3	H	17	THR
3	H	31	ASP
3	H	41	PRO
3	H	50	TRP
3	H	52	ASN
3	H	54	GLU
3	H	59	THR
3	H	62	ASP
3	H	65	LYS
3	H	67	ARG
3	H	93	THR
3	H	95	PHE
3	H	104	TYR
3	H	114	VAL
3	H	122	THR
3	H	125	SER
3	H	129	LEU
3	H	136	GLN
3	H	175	LEU
3	H	176	GLN
3	H	181	THR
3	H	187	THR
3	H	209	THR
3	H	211	VAL
4	O	52	ARG
4	O	61	ASN
4	O	65	THR
4	O	70	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (64) such sidechains are listed below:

Mol	Chain	Res	Type
1	P	20	GLN
2	A	6	GLN
2	A	31	ASN
2	A	37	ASN

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Mol	Chain	Res	Type
2	A	43	GLN
2	A	48	GLN
2	A	172	GLN
2	A	195	HIS
3	B	6	GLN
3	B	39	GLN
3	B	136	GLN
3	B	160	ASN
3	B	176	GLN
3	B	201	ASN
4	L	35	GLN
4	L	61	ASN
2	C	6	GLN
2	C	27	GLN
2	C	31	ASN
2	C	37	ASN
2	C	43	GLN
2	C	130	GLN
2	C	144	ASN
2	C	162	GLN
2	C	167	ASN
2	C	218	ASN
3	D	3	GLN
3	D	52	ASN
3	D	82	GLN
3	D	138	ASN
3	D	201	ASN
1	Q	8	GLN
1	Q	14	ASN
1	Q	16	ASN
4	M	35	GLN
2	E	31	ASN
2	E	37	ASN
2	E	96	GLN
2	E	130	GLN
2	E	144	ASN
2	E	151	ASN
3	F	3	GLN
3	F	52	ASN
3	F	136	GLN
3	F	176	GLN
3	F	201	ASN

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Mol	Chain	Res	Type
4	N	26	ASN
4	N	35	GLN
1	S	16	ASN
1	S	20	GLN
1	S	29	GLN
2	G	6	GLN
2	G	27	GLN
2	G	43	GLN
2	G	48	GLN
2	G	130	GLN
2	G	151	ASN
2	G	167	ASN
2	G	196	ASN
2	G	204	HIS
2	G	216	ASN
3	H	136	GLN
4	O	57	HIS
4	O	76	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	F	3
2	G	2
3	B	1
2	A	1
3	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	212:ASP	C	213:LYS	N	1.19
1	F	113:THR	C	114:VAL	N	1.19
1	F	131:PRO	C	132:GLY	N	1.19
1	F	193:TRP	C	194:PRO	N	1.19
1	A	171:ASP	C	172:GLN	N	1.17
1	G	110:LEU	C	111:GLU	N	1.17
1	D	169:HIS	C	170:THR	N	1.15
1	G	146:TYR	C	147:PRO	N	1.15

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	P	24/44 (54%)	-0.45	0 100 100	88, 139, 163, 172	0
1	Q	44/44 (100%)	-0.11	3 (6%) 17 16	63, 126, 196, 211	0
1	S	44/44 (100%)	-0.11	1 (2%) 60 54	69, 131, 193, 203	0
2	A	220/220 (100%)	-1.12	0 100 100	29, 41, 78, 152	0
2	C	220/220 (100%)	-1.01	0 100 100	29, 53, 109, 182	0
2	E	220/220 (100%)	-1.13	0 100 100	27, 40, 81, 135	0
2	G	219/220 (99%)	-1.04	0 100 100	28, 54, 107, 158	0
3	B	218/218 (100%)	-1.05	0 100 100	27, 40, 85, 180	0
3	D	218/218 (100%)	-1.08	0 100 100	26, 47, 115, 165	0
3	F	218/218 (100%)	-1.11	0 100 100	26, 39, 78, 143	0
3	H	218/218 (100%)	-0.97	0 100 100	27, 48, 111, 164	0
4	L	66/80 (82%)	-1.04	0 100 100	27, 49, 99, 163	0
4	M	62/80 (77%)	-1.08	0 100 100	29, 46, 84, 115	0
4	N	64/80 (80%)	-0.96	0 100 100	27, 50, 110, 151	0
4	O	62/80 (77%)	-1.14	0 100 100	30, 47, 81, 103	0
All	All	2117/2204 (96%)	-1.02	4 (0%) 95 93	26, 47, 126, 211	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Q	38	PRO	3.3
1	Q	21	ASP	2.4
1	S	39	ARG	2.1
1	Q	5	PRO	2.0

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.