



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 03:19 PM UTC

PDB ID : 4LVH / pdb_00004lvh
Title : Insight into highly conserved H1 subtype-specific epitopes in influenza virus hemagglutinin
Authors : Kim, K.H.; Cho, K.J.; Kim, S.; Seok, J.H.; Lee, J.-H.
Deposited on : 2013-07-26
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

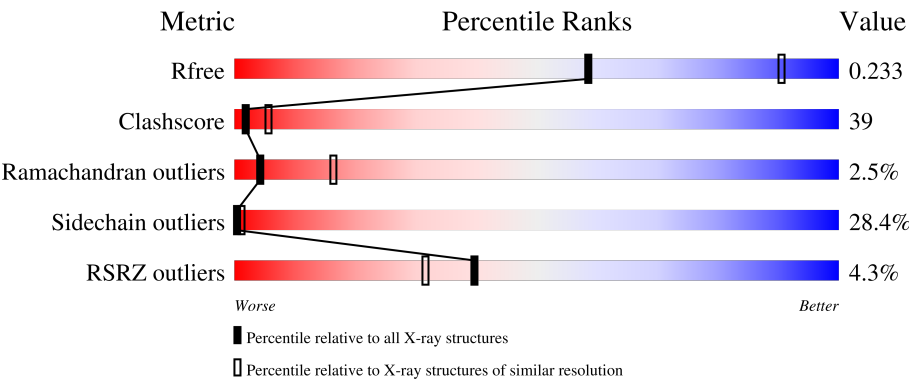
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	518	3% 15%22%8%54%
1	D	518	2% 15%20%7%57%
1	G	518	% 15%21%6%57%
1	J	518	2% 15%18%9%57%
2	B	222	3% 31%42%21%

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Mol	Chain	Length	Quality of chain
2	E	222	5% 35% 39% 20% 5%
2	H	222	5% 29% 42% 23% 5%
2	K	222	7% 29% 46% 20%
3	C	211	5% 26% 46% 20% 7%
3	F	211	2% 27% 41% 26% 5%
3	I	211	6% 29% 49% 18%
3	L	211	5% 30% 39% 26%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 20106 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 Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	236	Total	C	N	O	S	0	1	0
			1831	1162	311	352	6			
1	D	222	Total	C	N	O	S	0	1	0
			1762	1121	297	338	6			
1	G	222	Total	C	N	O	S	0	1	0
			1762	1121	297	338	6			
1	J	222	Total	C	N	O	S	0	1	0
			1762	1121	297	338	6			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	ALA	-	expression tag	UNP C5MQE6
A	-7	ASP	-	expression tag	UNP C5MQE6
A	-6	PRO	-	expression tag	UNP C5MQE6
A	-5	GLY	-	expression tag	UNP C5MQE6
A	-4	TYR	-	expression tag	UNP C5MQE6
A	-3	LEU	-	expression tag	UNP C5MQE6
A	-2	LEU	-	expression tag	UNP C5MQE6
A	-1	GLU	-	expression tag	UNP C5MQE6
A	0	PHE	-	expression tag	UNP C5MQE6
A	507	ARG	-	expression tag	UNP C5MQE6
A	508	SER	-	expression tag	UNP C5MQE6
A	509	LEU	-	expression tag	UNP C5MQE6
A	510	VAL	-	expression tag	UNP C5MQE6
A	511	PRO	-	expression tag	UNP C5MQE6
A	512	ARG	-	expression tag	UNP C5MQE6
D	-8	ALA	-	expression tag	UNP C5MQE6
D	-7	ASP	-	expression tag	UNP C5MQE6
D	-6	PRO	-	expression tag	UNP C5MQE6
D	-5	GLY	-	expression tag	UNP C5MQE6
D	-4	TYR	-	expression tag	UNP C5MQE6
D	-3	LEU	-	expression tag	UNP C5MQE6

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-2	LEU	-	expression tag	UNP C5MQE6
D	-1	GLU	-	expression tag	UNP C5MQE6
D	0	PHE	-	expression tag	UNP C5MQE6
D	504	ARG	-	expression tag	UNP C5MQE6
D	505	SER	-	expression tag	UNP C5MQE6
D	506	LEU	-	expression tag	UNP C5MQE6
D	507	VAL	-	expression tag	UNP C5MQE6
D	508	PRO	-	expression tag	UNP C5MQE6
D	509	ARG	-	expression tag	UNP C5MQE6
G	-8	ALA	-	expression tag	UNP C5MQE6
G	-7	ASP	-	expression tag	UNP C5MQE6
G	-6	PRO	-	expression tag	UNP C5MQE6
G	-5	GLY	-	expression tag	UNP C5MQE6
G	-4	TYR	-	expression tag	UNP C5MQE6
G	-3	LEU	-	expression tag	UNP C5MQE6
G	-2	LEU	-	expression tag	UNP C5MQE6
G	-1	GLU	-	expression tag	UNP C5MQE6
G	0	PHE	-	expression tag	UNP C5MQE6
G	504	ARG	-	expression tag	UNP C5MQE6
G	505	SER	-	expression tag	UNP C5MQE6
G	506	LEU	-	expression tag	UNP C5MQE6
G	507	VAL	-	expression tag	UNP C5MQE6
G	508	PRO	-	expression tag	UNP C5MQE6
G	509	ARG	-	expression tag	UNP C5MQE6
J	-8	ALA	-	expression tag	UNP C5MQE6
J	-7	ASP	-	expression tag	UNP C5MQE6
J	-6	PRO	-	expression tag	UNP C5MQE6
J	-5	GLY	-	expression tag	UNP C5MQE6
J	-4	TYR	-	expression tag	UNP C5MQE6
J	-3	LEU	-	expression tag	UNP C5MQE6
J	-2	LEU	-	expression tag	UNP C5MQE6
J	-1	GLU	-	expression tag	UNP C5MQE6
J	0	PHE	-	expression tag	UNP C5MQE6
J	504	ARG	-	expression tag	UNP C5MQE6
J	505	SER	-	expression tag	UNP C5MQE6
J	506	LEU	-	expression tag	UNP C5MQE6
J	507	VAL	-	expression tag	UNP C5MQE6
J	508	PRO	-	expression tag	UNP C5MQE6
J	509	ARG	-	expression tag	UNP C5MQE6

- Molecule 2 is a protein called MONOCLONAL ANTIBODY H-CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	218	Total	C	N	O	S	0	0	0
			1635	1028	280	319	8			
2	E	218	Total	C	N	O	S	0	0	0
			1635	1028	280	319	8			
2	H	218	Total	C	N	O	S	0	0	0
			1635	1028	280	319	8			
2	K	218	Total	C	N	O	S	0	0	0
			1635	1028	280	319	8			

- Molecule 3 is a protein called MONOCLONAL ANTIBODY L-CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	210	Total	C	N	O	S	0	0	0
			1610	1007	271	326	6			
3	F	210	Total	C	N	O	S	0	0	0
			1610	1007	271	326	6			
3	I	210	Total	C	N	O	S	0	0	0
			1610	1007	271	326	6			
3	L	209	Total	C	N	O	S	0	0	0
			1604	1004	270	324	6			

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Ca	0	0
			1	1		
4	D	1	Total	Ca	0	0
			1	1		
4	G	1	Total	Ca	0	0
			1	1		
4	J	1	Total	Ca	0	0
			1	1		

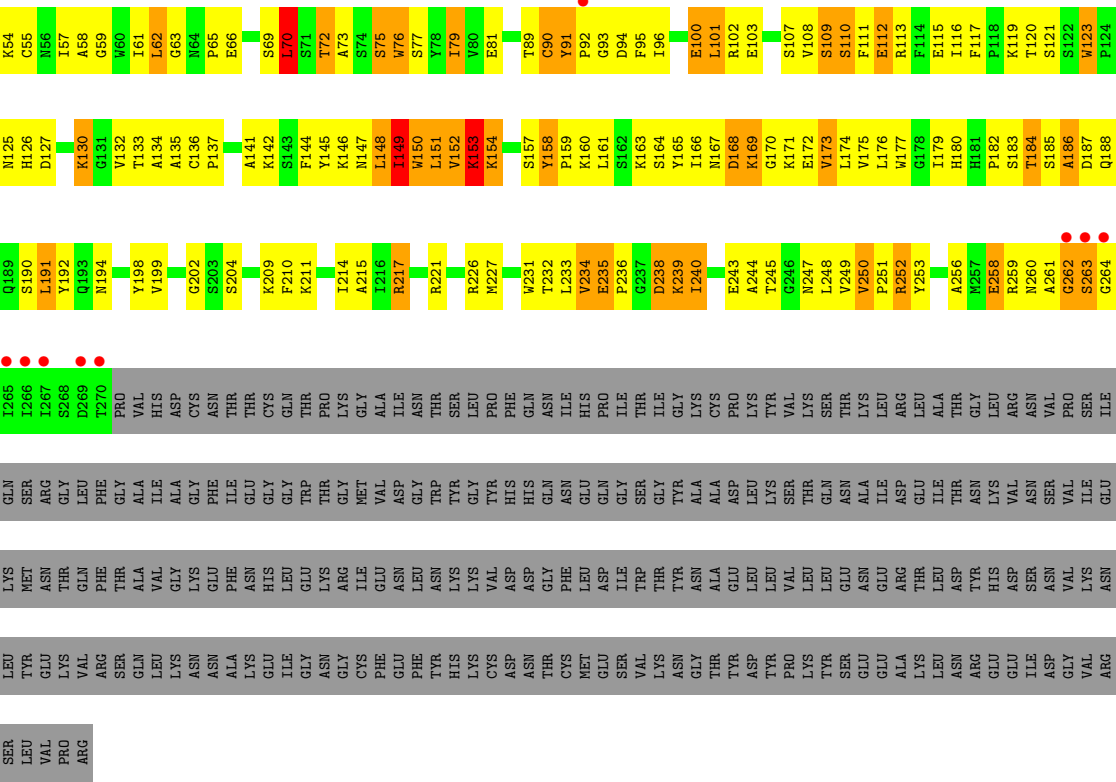
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	O	0	0
			1	1		
5	B	1	Total	O	0	0
			1	1		
5	F	1	Total	O	0	0
			1	1		

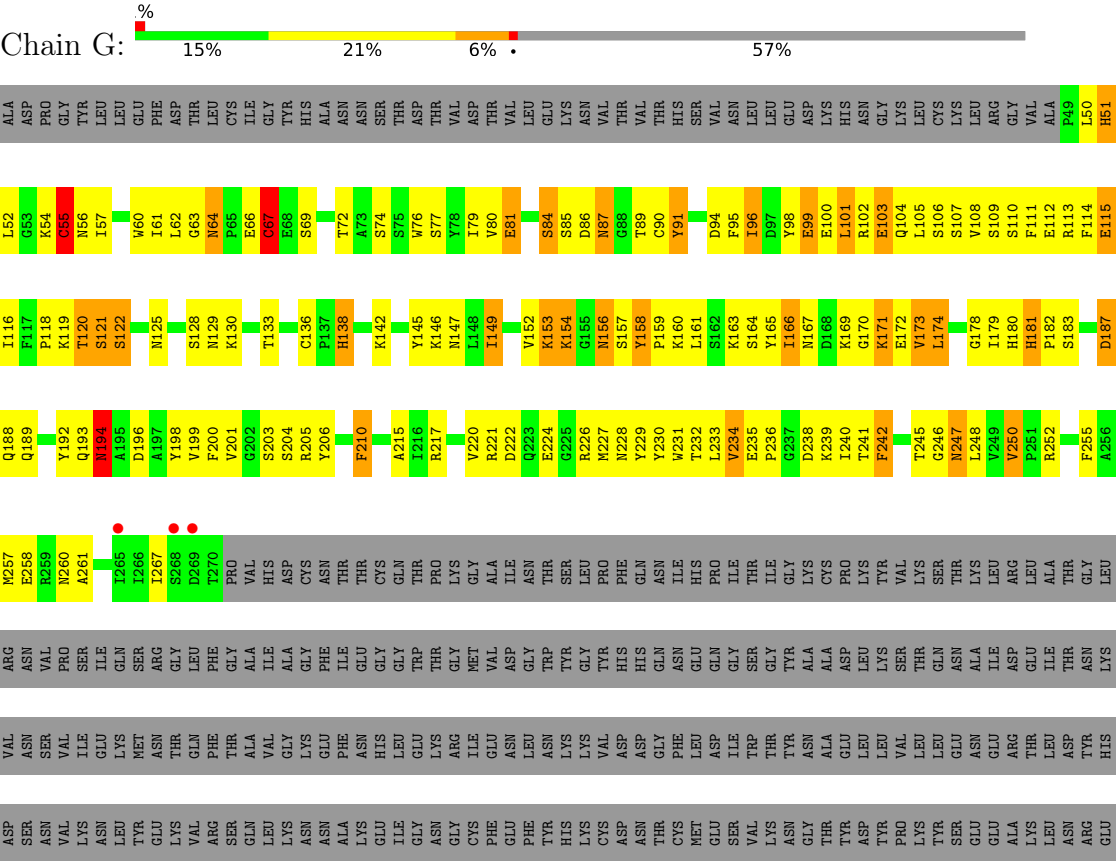
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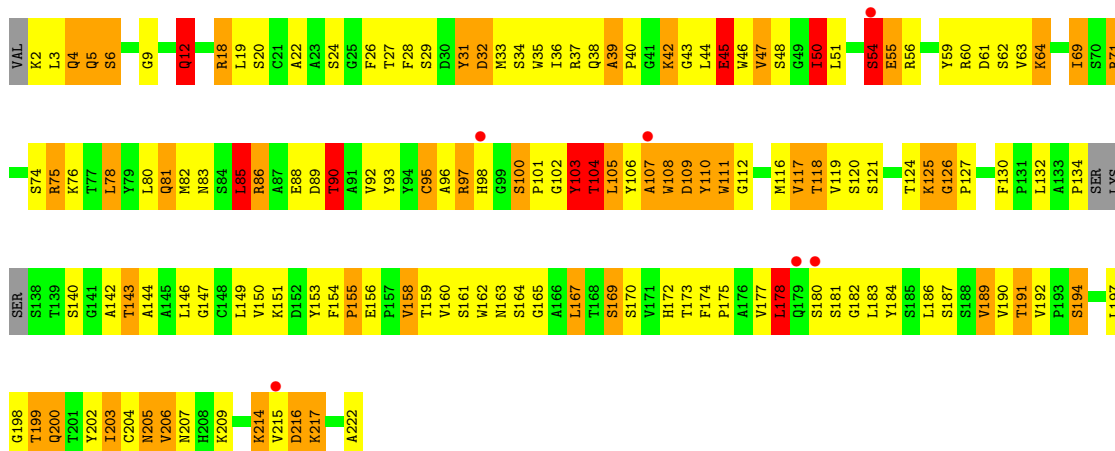
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	G	1	Total 1	O 1	0	0
5	H	3	Total 3	O 3	0	0
5	I	2	Total 2	O 2	0	0
5	K	1	Total 1	O 1	0	0
5	L	1	Total 1	O 1	0	0

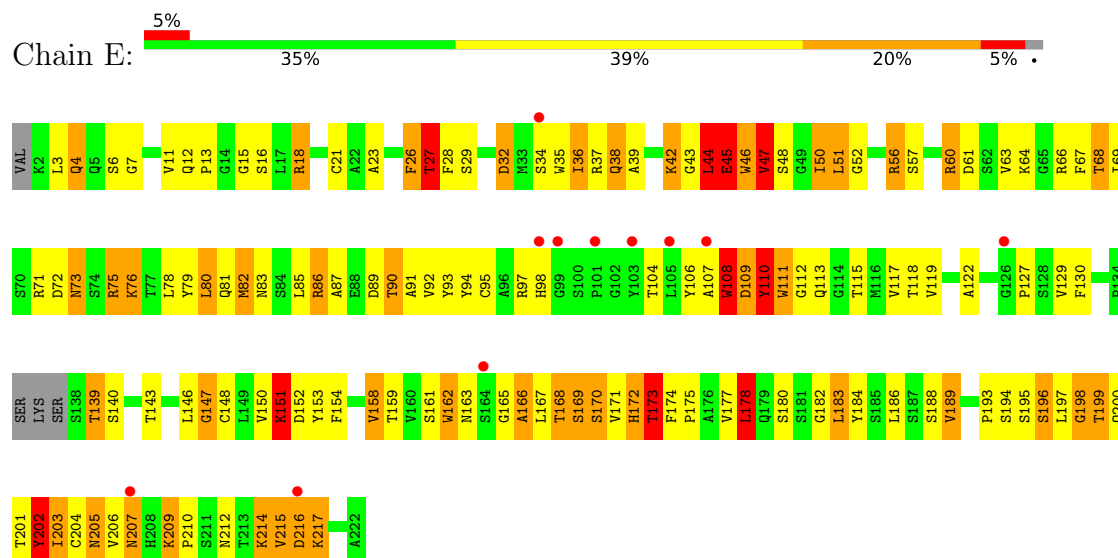


• Molecule 1: Hemagglutinin

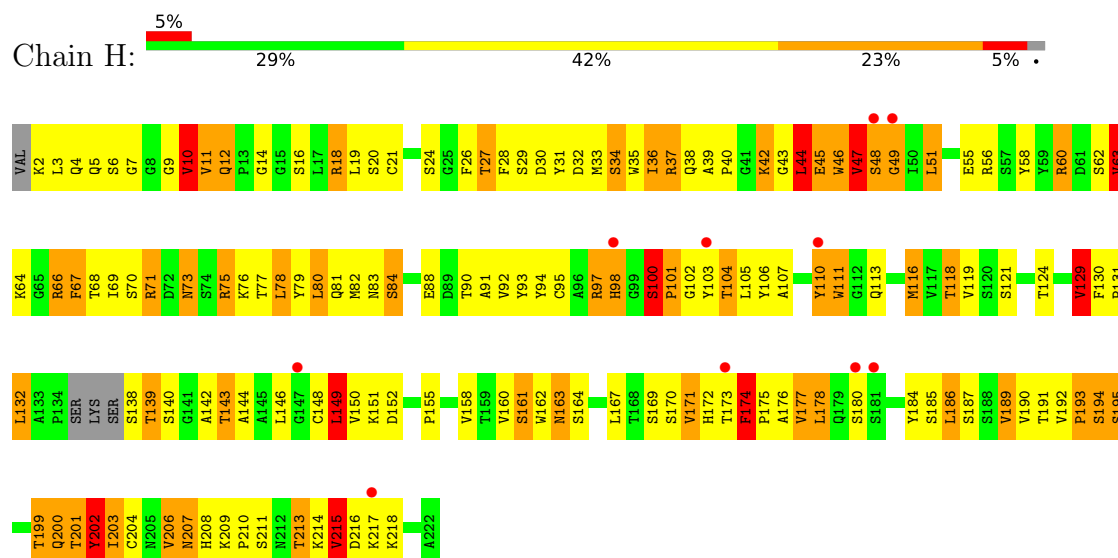




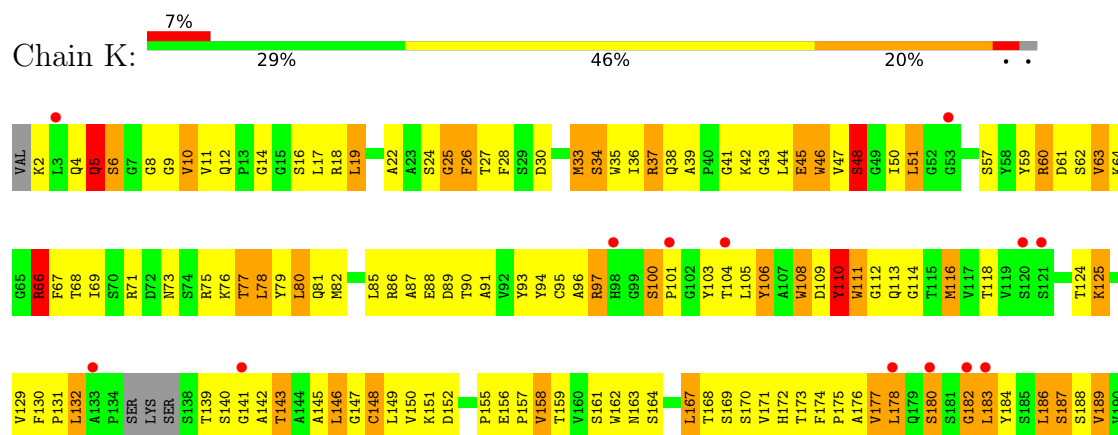
• Molecule 2: MONOCLONAL ANTIBODY H-CHAIN



• Molecule 2: MONOCLONAL ANTIBODY H-CHAIN

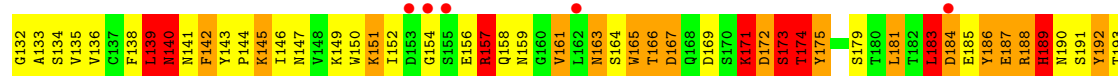


• Molecule 2: MONOCLONAL ANTIBODY H-CHAIN

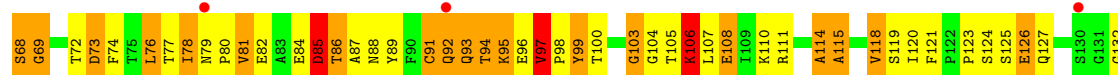
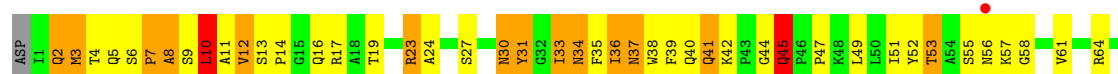




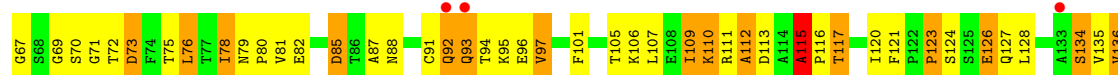
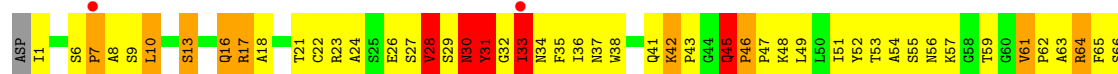
• Molecule 3: MONOCLONAL ANTIBODY L-CHAIN



• Molecule 3: MONOCLONAL ANTIBODY L-CHAIN

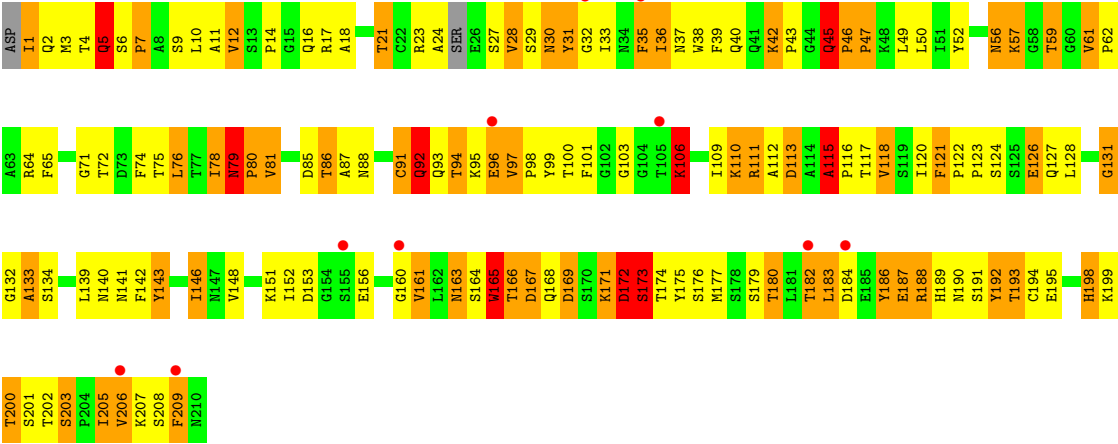


• Molecule 3: MONOCLONAL ANTIBODY L-CHAIN





● Molecule 3: MONOCLONAL ANTIBODY L-CHAIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	72.75Å 237.81Å 94.23Å 90.00° 110.31° 90.00°	Depositor
Resolution (Å)	43.49 – 2.80 43.49 – 2.80	Depositor EDS
% Data completeness (in resolution range)	76.8 (43.49-2.80) 92.6 (43.49-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.05 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.232 , 0.274 0.228 , 0.233	Depositor DCC
R_{free} test set	3559 reflections (4.31%)	wwPDB-VP
Wilson B-factor (Å ²)	36.9	Xtriage
Anisotropy	0.160	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 38.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.004 for h,-k,-h-l	Xtriage
Reported twinning fraction	0.844 for H, K, L 0.156 for -H, -K, H+L	Depositor
Outliers	0 of 69841 reflections	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	20106	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 22.72 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.3778e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.74	1/1879 (0.1%)	1.37	26/2549 (1.0%)
1	D	0.69	0/1811	1.28	25/2456 (1.0%)
1	G	0.74	0/1811	1.29	26/2456 (1.1%)
1	J	0.67	0/1811	1.30	24/2456 (1.0%)
2	B	0.76	0/1675	1.40	27/2277 (1.2%)
2	E	0.80	1/1675 (0.1%)	1.35	25/2277 (1.1%)
2	H	0.79	0/1675	1.33	24/2277 (1.1%)
2	K	0.75	0/1675	1.37	18/2277 (0.8%)
3	C	0.81	1/1648 (0.1%)	1.57	38/2242 (1.7%)
3	F	0.83	1/1648 (0.1%)	1.58	37/2242 (1.7%)
3	I	0.79	0/1648	1.53	40/2242 (1.8%)
3	L	0.81	1/1641 (0.1%)	1.56	38/2231 (1.7%)
All	All	0.76	5/20597 (0.0%)	1.41	348/27982 (1.2%)

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
1	A	0	6
1	D	0	1
1	G	0	1
1	J	0	3
2	B	0	7
2	E	0	2
2	H	0	5
2	K	0	6
3	C	0	7
3	F	0	6
3	I	0	4

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Mol	Chain	#Chirality outliers	#Planarity outliers
3	L	0	7
All	All	0	55

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	45	GLN	CA-C	6.52	1.61	1.52
1	A	70	LEU	CA-C	5.78	1.58	1.53
3	L	45	GLN	CA-C	5.46	1.59	1.52
3	F	202	THR	CA-CB	5.03	1.61	1.53
2	E	45	GLU	CA-C	5.01	1.58	1.52

All (348) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	97	VAL	CA-C-N	-14.77	104.04	119.99
3	L	97	VAL	C-N-CA	-14.77	104.04	119.99
1	D	235	GLU	CA-C-N	-11.85	109.68	121.65
1	D	235	GLU	C-N-CA	-11.85	109.68	121.65
3	F	97	VAL	CA-C-N	-11.79	107.53	119.90
3	F	97	VAL	C-N-CA	-11.79	107.53	119.90
3	I	31	TYR	N-CA-C	11.69	126.29	108.52
3	C	13	SER	CA-C-N	-11.02	106.07	119.84
3	C	13	SER	C-N-CA	-11.02	106.07	119.84
3	F	45	GLN	CA-C-N	10.81	131.52	120.38
3	F	45	GLN	C-N-CA	10.81	131.52	120.38
3	C	46	PRO	CA-C-N	10.61	130.71	119.89
3	C	46	PRO	C-N-CA	10.61	130.71	119.89
3	C	92	GLN	N-CA-C	10.53	126.56	108.76
2	K	110	TYR	N-CA-C	10.43	123.14	108.74
3	F	164	SER	N-CA-C	10.43	123.11	110.91
3	I	13	SER	CA-C-N	-10.31	111.23	121.65
3	I	13	SER	C-N-CA	-10.31	111.23	121.65
2	B	45	GLU	N-CA-C	10.31	122.29	108.38
2	K	5	GLN	N-CA-C	10.27	123.90	109.31
3	F	121	PHE	CA-C-N	10.22	130.91	120.38
3	F	121	PHE	C-N-CA	10.22	130.91	120.38
3	F	104	GLY	N-CA-C	10.05	122.92	110.96
2	B	102	GLY	N-CA-C	-9.87	98.35	112.17
1	A	262	GLY	N-CA-C	9.77	122.79	110.29
2	H	10	VAL	N-CA-C	9.51	121.30	108.27
3	I	28	VAL	N-CA-C	-9.48	94.48	108.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	92	GLN	N-CA-C	9.46	123.23	109.14
3	L	46	PRO	CA-C-N	9.41	129.53	120.31
3	L	46	PRO	C-N-CA	9.41	129.53	120.31
3	L	45	GLN	CA-C-N	9.40	130.06	120.38
3	L	45	GLN	C-N-CA	9.40	130.06	120.38
1	A	64	ASN	CA-C-N	-9.39	112.16	121.65
1	A	64	ASN	C-N-CA	-9.39	112.16	121.65
3	C	171	LYS	N-CA-C	9.36	125.89	113.72
2	H	39	ALA	CA-C-N	-9.21	111.12	120.98
2	H	39	ALA	C-N-CA	-9.21	111.12	120.98
2	H	7	GLY	N-CA-C	9.18	131.78	115.80
2	H	9	GLY	N-CA-C	9.11	134.76	113.18
1	D	55	CYS	N-CA-C	9.10	120.72	107.88
3	C	9	SER	N-CA-C	9.04	124.55	112.88
1	J	264	GLY	N-CA-C	9.01	127.25	114.64
2	K	6	SER	N-CA-C	9.01	119.81	108.19
2	H	45	GLU	N-CA-C	9.01	121.95	110.24
2	E	50	ILE	N-CA-C	8.63	120.61	109.30
3	I	33	ILE	N-CA-C	8.61	120.38	111.00
3	I	106	LYS	N-CA-C	8.59	121.88	111.40
3	F	92	GLN	N-CA-C	8.51	123.40	109.96
1	G	192	TYR	N-CA-C	8.43	124.60	113.30
3	I	10	LEU	N-CA-C	8.20	120.36	110.19
3	C	46	PRO	N-CA-C	8.20	120.70	110.70
3	I	61	VAL	N-CA-C	8.19	117.07	107.73
3	C	140	ASN	N-CA-C	8.18	120.87	110.24
2	K	194	SER	N-CA-C	8.11	124.67	111.37
3	I	35	PHE	N-CA-C	8.09	122.72	113.02
2	E	47	VAL	N-CA-C	8.05	120.11	111.58
1	D	91	TYR	CA-C-N	7.98	128.04	119.90
1	D	91	TYR	C-N-CA	7.98	128.04	119.90
3	L	16	GLN	N-CA-C	7.97	118.78	108.34
3	C	97	VAL	CA-C-N	-7.92	111.27	119.83
3	C	97	VAL	C-N-CA	-7.92	111.27	119.83
1	J	69	SER	N-CA-C	7.92	120.18	110.91
3	L	92	GLN	N-CA-C	7.83	121.22	109.95
1	J	55	CYS	N-CA-C	7.79	118.98	108.23
2	B	104	THR	N-CA-C	7.76	120.87	111.40
1	G	156	ASN	N-CA-C	7.72	122.04	111.54
1	G	194	ASN	N-CA-C	7.70	121.10	110.24
3	F	115	ALA	CA-C-N	7.68	145.43	127.00
3	F	115	ALA	C-N-CA	7.68	145.43	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	162	SER	N-CA-C	7.60	122.75	113.17
3	F	6	SER	CA-C-N	-7.59	109.30	120.46
3	F	6	SER	C-N-CA	-7.59	109.30	120.46
3	L	165	TRP	N-CA-C	7.57	121.24	108.90
1	A	91	TYR	CA-C-N	7.54	128.00	119.93
1	A	91	TYR	C-N-CA	7.54	128.00	119.93
3	F	69	GLY	N-CA-C	7.54	119.12	111.95
3	F	115	ALA	C-N-CD	-7.54	104.01	120.60
1	A	54	LYS	N-CA-C	7.52	122.65	113.17
1	G	247	ASN	N-CA-C	7.46	121.75	111.90
2	B	107	ALA	N-CA-C	7.44	117.70	107.73
3	I	46	PRO	CA-C-N	7.40	129.09	119.84
3	I	46	PRO	C-N-CA	7.40	129.09	119.84
2	E	198	GLY	N-CA-C	-7.39	105.89	114.69
2	B	9	GLY	N-CA-C	7.31	130.51	113.18
2	B	203	ILE	N-CA-C	7.26	118.57	111.67
3	F	203	SER	CA-C-N	7.25	128.90	119.84
3	F	203	SER	C-N-CA	7.25	128.90	119.84
1	A	110	SER	CB-CA-C	-7.24	107.17	115.79
3	F	103	GLY	N-CA-C	7.20	123.05	114.48
2	B	198	GLY	N-CA-C	-7.16	105.18	115.27
3	C	139	LEU	N-CA-C	7.13	121.69	112.92
3	C	122	PRO	CA-C-N	7.09	127.09	119.78
3	C	122	PRO	C-N-CA	7.09	127.09	119.78
3	L	46	PRO	N-CA-C	7.05	119.31	110.70
2	K	143	THR	N-CA-C	7.05	120.80	108.75
1	G	157	SER	N-CA-C	6.99	121.97	113.17
1	G	91	TYR	CA-C-N	6.98	126.95	119.76
1	G	91	TYR	C-N-CA	6.98	126.95	119.76
1	J	136	CYS	CA-C-N	6.97	127.14	120.31
1	J	136	CYS	C-N-CA	6.97	127.14	120.31
1	J	85	SER	N-CA-C	-6.96	103.13	111.69
1	D	238	ASP	N-CA-C	6.95	119.06	109.18
3	C	79	ASN	CA-C-N	-6.94	111.16	119.84
3	C	79	ASN	C-N-CA	-6.94	111.16	119.84
3	I	206	VAL	N-CA-C	6.94	117.00	108.53
1	G	121	SER	N-CA-C	6.91	121.87	113.17
3	L	96	GLU	N-CA-C	-6.88	95.89	107.80
1	A	100	GLU	N-CA-C	-6.88	103.56	112.23
1	A	125	ASN	N-CA-C	6.86	121.81	113.17
1	G	84	SER	N-CA-C	-6.85	104.80	113.02
3	I	185	GLU	N-CA-C	-6.82	105.04	113.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	146	ILE	N-CA-C	6.82	117.71	108.17
3	L	143	TYR	C-N-CD	-6.81	105.63	120.60
2	B	39	ALA	CA-C-N	-6.80	113.68	120.21
2	B	39	ALA	C-N-CA	-6.80	113.68	120.21
2	H	178	LEU	N-CA-C	-6.78	100.40	110.23
2	B	126	GLY	CA-C-N	6.75	126.51	119.76
2	B	126	GLY	C-N-CA	6.75	126.51	119.76
1	G	55	CYS	N-CA-C	6.75	119.66	109.41
3	C	172	ASP	N-CA-C	6.72	125.12	110.80
1	J	83	SER	N-CA-C	6.72	120.05	109.96
3	I	69	GLY	N-CA-C	6.69	118.30	111.95
3	I	121	PHE	CA-C-N	6.68	127.26	120.38
3	I	121	PHE	C-N-CA	6.68	127.26	120.38
1	J	215	ALA	N-CA-C	6.66	117.37	108.38
3	F	30	ASN	N-CA-C	-6.63	104.82	113.17
3	C	200	THR	N-CA-C	-6.61	98.67	108.79
3	L	143	TYR	CA-C-N	6.61	142.86	127.00
3	L	143	TYR	C-N-CA	6.61	142.86	127.00
3	C	32	GLY	N-CA-C	-6.60	104.74	114.90
3	C	174	THR	N-CA-C	6.58	124.81	110.80
3	I	7	PRO	N-CA-C	6.56	121.25	110.55
3	C	141	ASN	N-CA-C	6.56	120.71	111.92
3	I	164	SER	N-CA-C	6.55	118.98	110.53
3	I	136	VAL	N-CA-C	6.53	117.67	107.28
1	A	188	GLN	N-CA-C	6.53	118.28	111.03
1	J	123	TRP	CA-C-N	6.53	128.00	119.84
1	J	123	TRP	C-N-CA	6.53	128.00	119.84
1	A	55	CYS	N-CA-C	6.53	118.45	108.07
3	L	122	PRO	CA-C-N	6.52	126.48	119.76
3	L	122	PRO	C-N-CA	6.52	126.48	119.76
1	A	246	GLY	N-CA-C	6.45	119.27	110.69
2	H	144	ALA	N-CA-C	6.45	119.40	107.99
3	L	32	GLY	N-CA-C	-6.42	105.00	114.90
3	C	175	TYR	N-CA-C	6.41	124.45	110.80
3	I	203	SER	N-CA-C	6.40	117.98	108.76
2	K	182	GLY	N-CA-C	6.39	122.42	114.37
3	L	133	ALA	N-CA-C	6.39	118.86	108.26
2	K	45	GLU	N-CA-C	6.38	119.74	109.79
3	L	76	LEU	N-CA-C	-6.37	99.34	109.59
2	E	196	SER	N-CA-C	6.36	121.19	113.17
3	I	16	GLN	N-CA-C	6.35	116.45	108.45
2	B	178	LEU	N-CA-C	-6.35	100.88	110.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	7	PRO	N-CA-C	6.35	120.38	110.80
3	L	186	TYR	N-CA-C	-6.34	100.03	108.34
2	B	165	GLY	CA-C-N	-6.32	113.50	122.41
2	B	165	GLY	C-N-CA	-6.32	113.50	122.41
3	F	114	ALA	N-CA-C	6.32	118.29	109.31
3	I	141	ASN	N-CA-C	6.31	124.24	110.80
2	B	103	TYR	N-CA-C	6.31	119.45	111.69
2	H	213	THR	N-CA-C	6.29	116.75	107.88
3	F	179	SER	N-CA-C	6.28	118.72	109.24
2	K	141	GLY	N-CA-C	-6.28	104.88	115.80
1	A	203	SER	N-CA-C	6.26	124.14	110.80
3	L	172	ASP	N-CA-C	6.23	116.67	107.88
2	E	165	GLY	CA-C-N	-6.22	112.39	122.34
2	E	165	GLY	C-N-CA	-6.22	112.39	122.34
2	K	196	SER	N-CA-C	6.22	117.93	111.03
3	L	160	GLY	N-CA-C	6.22	121.43	110.80
2	B	5	GLN	N-CA-C	6.18	118.49	107.80
3	F	33	ILE	CA-C-N	6.17	133.32	121.54
3	F	33	ILE	C-N-CA	6.17	133.32	121.54
2	B	50	ILE	N-CA-C	6.17	122.16	109.34
1	G	173	VAL	N-CA-C	6.16	116.69	107.51
1	J	93	GLY	N-CA-C	-6.12	101.88	110.63
2	B	47	VAL	N-CA-C	6.12	120.74	113.22
2	K	66	ARG	N-CA-C	6.11	117.81	111.03
1	D	76	TRP	N-CA-C	6.11	118.36	109.07
3	I	85	ASP	CA-C-N	-6.08	113.47	122.41
3	I	85	ASP	C-N-CA	-6.08	113.47	122.41
2	H	11	VAL	N-CA-C	6.07	117.51	108.46
3	C	173	SER	N-CA-C	6.07	121.49	112.94
2	B	156	GLU	N-CA-C	6.05	113.67	108.22
3	C	19	THR	CB-CA-C	-6.02	101.53	110.62
2	K	34	SER	N-CA-C	6.01	118.20	109.07
1	D	123	TRP	CA-C-N	6.00	125.39	118.85
1	D	123	TRP	C-N-CA	6.00	125.39	118.85
1	D	173	VAL	N-CA-C	6.00	116.80	109.30
3	F	140	ASN	N-CA-C	5.99	123.55	110.80
2	K	191	THR	N-CA-C	-5.96	101.02	109.96
3	F	10	LEU	N-CA-C	5.96	118.13	109.07
2	H	174	PHE	N-CA-C	-5.95	96.67	109.81
1	D	261	ALA	N-CA-C	5.94	123.46	110.80
2	K	203	ILE	N-CA-C	5.92	121.65	109.34
3	C	47	PRO	N-CA-C	5.92	120.52	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	104	GLY	N-CA-C	5.91	121.55	112.81
3	F	201	SER	N-CA-C	5.90	120.65	112.45
3	I	152	ILE	N-CA-C	-5.90	106.49	111.56
3	C	106	LYS	N-CA-C	5.89	118.58	111.40
3	L	47	PRO	N-CA-C	5.88	120.51	111.57
3	L	106	LYS	N-CA-C	5.87	117.76	111.36
1	A	70	LEU	N-CA-C	5.86	117.99	108.08
1	A	127	ASP	N-CA-C	-5.84	101.00	109.59
1	G	158	TYR	CA-C-N	-5.84	113.76	119.90
1	G	158	TYR	C-N-CA	-5.84	113.76	119.90
2	K	33	MET	N-CA-C	5.84	117.84	109.14
2	H	100	SER	CA-C-N	5.84	127.14	119.84
2	H	100	SER	C-N-CA	5.84	127.14	119.84
2	H	149	LEU	N-CA-C	5.82	118.44	109.07
2	E	168	THR	N-CA-C	-5.81	101.81	110.23
1	G	130	LYS	CA-C-N	-5.81	115.75	120.98
1	G	130	LYS	C-N-CA	-5.81	115.75	120.98
2	E	34	SER	N-CA-C	5.80	117.35	108.42
3	I	186	TYR	N-CA-C	-5.79	106.56	113.21
3	F	33	ILE	N-CA-C	5.77	121.34	109.34
3	F	200	THR	N-CA-C	-5.77	98.51	110.80
1	J	234	VAL	N-CA-C	5.76	116.58	108.17
3	I	46	PRO	N-CA-C	5.76	117.73	110.70
2	K	14	GLY	N-CA-C	-5.76	107.43	114.92
3	L	115	ALA	CA-C-N	5.75	140.79	127.00
3	L	115	ALA	C-N-CA	5.75	140.79	127.00
3	F	145	LYS	N-CA-C	5.72	117.29	110.19
3	C	183	LEU	N-CA-C	5.69	118.75	109.59
3	C	115	ALA	C-N-CD	-5.69	108.09	120.60
2	B	110	TYR	N-CA-C	5.66	117.68	109.07
3	L	115	ALA	C-N-CD	-5.65	108.17	120.60
2	B	31	TYR	N-CA-C	5.64	117.57	110.24
1	J	194	ASN	N-CA-C	5.63	118.38	108.75
2	E	147	GLY	N-CA-C	5.61	119.27	110.91
1	D	100	GLU	N-CA-C	-5.60	105.26	111.36
1	A	257	MET	N-CA-C	5.59	117.48	109.14
2	H	170	SER	N-CA-C	5.59	117.45	110.91
2	E	130	PHE	CA-C-N	5.56	125.32	119.76
2	E	130	PHE	C-N-CA	5.56	125.32	119.76
3	C	156	GLU	N-CA-C	-5.56	101.28	109.18
1	J	227	MET	N-CA-C	5.54	117.70	108.99
1	G	100	GLU	N-CA-C	-5.53	105.25	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	6	SER	CA-C-N	5.52	126.37	120.13
3	I	6	SER	C-N-CA	5.52	126.37	120.13
1	J	171	LYS	N-CA-C	5.51	118.07	109.52
2	B	147	GLY	N-CA-C	5.50	118.76	110.18
3	F	99	TYR	N-CA-C	5.49	117.68	108.73
1	D	152	VAL	N-CA-C	5.49	120.75	109.34
1	G	210	PHE	N-CA-C	-5.49	101.79	109.69
1	G	64	ASN	CA-C-N	5.48	125.19	119.82
1	G	64	ASN	C-N-CA	5.48	125.19	119.82
1	A	75	SER	N-CA-C	-5.48	99.17	108.26
3	F	163	ASN	N-CA-C	5.47	115.35	108.45
3	F	86	THR	N-CA-C	5.47	117.31	110.91
3	C	17	ARG	N-CA-C	5.47	118.28	110.24
2	E	202	TYR	N-CA-C	-5.46	100.80	109.76
1	A	252	ARG	N-CA-C	-5.45	104.67	112.13
1	D	141	ALA	CA-C-N	-5.44	114.41	122.41
1	D	141	ALA	C-N-CA	-5.44	114.41	122.41
1	D	153	LYS	N-CA-C	5.44	118.27	108.48
1	G	238	ASP	N-CA-C	5.42	118.06	109.50
1	D	236	PRO	CA-C-O	-5.42	117.21	121.38
3	L	171	LYS	N-CA-C	5.41	120.75	113.72
3	L	203	SER	CA-C-N	5.41	125.83	119.99
3	L	203	SER	C-N-CA	5.41	125.83	119.99
1	J	212	PRO	CA-C-N	-5.40	115.19	123.07
1	J	212	PRO	C-N-CA	-5.40	115.19	123.07
3	C	61	VAL	CA-C-N	5.40	126.59	119.84
3	C	61	VAL	C-N-CA	5.40	126.59	119.84
1	J	64	ASN	CA-C-N	5.39	126.58	119.84
1	J	64	ASN	C-N-CA	5.39	126.58	119.84
2	E	162	TRP	CA-C-N	5.39	131.84	121.54
2	E	162	TRP	C-N-CA	5.39	131.84	121.54
2	H	64	LYS	N-CA-C	5.38	122.26	110.80
2	B	83	ASN	N-CA-C	5.37	118.32	109.72
1	J	202	GLY	N-CA-C	5.37	119.99	110.80
1	G	242	PHE	N-CA-C	5.37	117.76	110.35
2	E	48	SER	N-CA-C	5.37	117.93	108.75
2	B	89	ASP	N-CA-C	5.36	119.51	112.92
1	D	70	LEU	N-CA-C	5.35	117.13	108.08
3	I	32	GLY	N-CA-C	-5.35	107.13	114.67
2	E	46	TRP	N-CA-C	5.34	118.32	110.30
1	D	90	CYS	CB-CA-C	-5.34	109.97	117.23
1	D	186	ALA	N-CA-C	-5.34	105.51	112.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	207	LYS	N-CA-C	5.33	118.22	110.17
2	K	145	ALA	N-CA-C	5.33	118.80	112.72
1	A	129	ASN	N-CA-C	5.33	119.93	113.38
2	E	173	THR	N-CA-C	5.32	122.13	110.80
2	B	90	THR	CB-CA-C	-5.32	102.67	110.06
3	C	16	GLN	N-CA-C	5.32	114.85	107.73
2	H	14	GLY	N-CA-C	-5.32	101.67	111.34
3	L	121	PHE	N-CA-C	5.31	118.84	108.85
2	H	67	PHE	N-CA-C	5.31	117.61	109.07
2	H	152	ASP	N-CA-C	5.30	117.11	110.91
3	C	97	VAL	CB-CA-C	5.29	120.99	111.36
1	G	261	ALA	N-CA-C	5.29	117.10	110.91
3	L	161	VAL	N-CA-C	-5.29	101.37	108.35
3	C	181	LEU	N-CA-C	5.29	117.04	108.26
2	E	108	TRP	N-CA-C	5.28	117.57	109.07
1	J	156	ASN	N-CA-C	5.27	118.71	111.54
3	I	115	ALA	CA-C-N	5.27	139.64	127.00
3	I	115	ALA	C-N-CA	5.27	139.64	127.00
2	K	97	ARG	N-CA-C	-5.25	102.97	110.59
1	G	206	TYR	N-CA-C	-5.25	99.61	110.80
3	I	151	LYS	N-CA-C	5.24	116.97	108.26
1	J	94	ASP	N-CA-C	5.22	117.12	109.24
3	C	20	ILE	N-CA-C	-5.20	102.37	109.55
1	G	64	ASN	N-CA-C	5.19	116.19	109.65
3	F	141	ASN	N-CA-C	5.19	121.86	110.80
1	D	149	ILE	N-CA-C	-5.18	102.91	109.80
2	H	63	VAL	N-CA-C	5.18	120.11	109.34
3	L	59	THR	N-CA-C	5.18	117.20	109.59
2	E	169	SER	CB-CA-C	-5.17	110.19	117.23
1	D	262	GLY	N-CA-C	5.17	121.64	112.64
1	D	247	ASN	N-CA-C	5.16	118.71	111.90
3	F	94	THR	N-CA-C	-5.15	100.37	108.00
3	I	61	VAL	CA-C-N	5.15	125.44	119.93
3	I	61	VAL	C-N-CA	5.15	125.44	119.93
3	F	106	LYS	N-CA-C	5.14	117.87	111.24
3	F	139	LEU	N-CA-C	5.13	119.64	113.17
2	E	44	LEU	N-CA-C	5.13	115.31	108.23
2	E	183	LEU	N-CA-C	5.12	121.70	110.80
3	L	173	SER	N-CA-C	5.12	118.55	112.72
3	C	103	GLY	N-CA-C	5.11	121.80	114.64
2	E	162	TRP	CB-CA-C	5.11	119.37	110.94
2	E	178	LEU	N-CA-C	-5.11	102.49	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	140	ASN	N-CA-C	5.11	117.81	109.59
1	J	88	GLY	N-CA-C	5.11	118.42	112.50
1	A	199	VAL	CB-CA-C	-5.10	103.19	110.12
1	J	122	SER	N-CA-C	5.09	117.22	111.11
2	K	147	GLY	N-CA-C	5.09	119.77	111.27
2	H	37	ARG	N-CA-C	5.08	117.85	109.72
1	D	70	LEU	CA-CB-CG	5.08	134.06	116.30
3	I	18	ALA	N-CA-C	-5.06	101.44	109.59
3	F	148	VAL	N-CA-C	5.06	115.87	108.53
2	E	82	MET	N-CA-C	-5.05	101.47	109.96
1	A	131	GLY	N-CA-C	5.05	118.85	110.97
2	H	3	LEU	N-CA-C	5.05	116.86	109.24
2	H	129	VAL	N-CA-C	5.05	115.12	107.80
3	I	112	ALA	N-CA-C	5.04	119.12	112.92
2	B	85	LEU	N-CA-C	5.04	117.45	109.24
2	H	47	VAL	N-CA-C	5.04	119.50	112.50
1	A	171	LYS	N-CA-C	-5.03	101.10	108.79
1	A	72	THR	CA-C-N	5.02	131.13	121.54
1	A	72	THR	C-N-CA	5.02	131.13	121.54
1	A	255	PHE	N-CA-C	5.02	117.24	108.76
2	B	26	PHE	CB-CA-C	-5.02	100.44	110.42
1	D	252	ARG	N-CA-C	-5.02	105.40	112.12
2	E	151	LYS	N-CA-C	5.01	116.58	108.41
3	I	124	SER	N-CA-C	5.01	117.61	109.24
3	L	131	GLY	N-CA-C	5.01	125.05	113.18
1	G	181	HIS	CA-C-N	5.01	125.72	120.11
1	G	181	HIS	C-N-CA	5.01	125.72	120.11

There are no chirality outliers.

All (55) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	156	ASN	Peptide
1	A	203	SER	Peptide
1	A	221	ARG	Sidechain
1	A	421	ILE	Peptide
1	A	65	PRO	Peptide
1	A	74	SER	Peptide
2	B	100	SER	Peptide
2	B	101	PRO	Peptide
2	B	12	GLN	Peptide
2	B	178	LEU	Peptide

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Mol	Chain	Res	Type	Group
2	B	24	SER	Peptide
2	B	54	SER	Peptide
2	B	6	SER	Peptide
3	C	114	ALA	Peptide
3	C	145	LYS	Peptide
3	C	173	SER	Peptide
3	C	174	THR	Peptide
3	C	189	HIS	Peptide
3	C	207	LYS	Peptide
3	C	30	ASN	Peptide
1	D	244	ALA	Peptide
2	E	166	ALA	Peptide
2	E	173	THR	Peptide
3	F	157	ARG	Peptide
3	F	174	THR	Peptide
3	F	45	GLN	Peptide
3	F	7	PRO	Peptide
3	F	8	ALA	Peptide
3	F	91	CYS	Peptide
1	G	160	LYS	Peptide
2	H	100	SER	Peptide
2	H	202	TYR	Peptide
2	H	42	LYS	Peptide
2	H	48	SER	Peptide
2	H	71	ARG	Sidechain
3	I	173	SER	Peptide
3	I	30	ASN	Peptide
3	I	45	GLN	Peptide
3	I	9	SER	Peptide
1	J	138	HIS	Peptide
1	J	213	GLU	Peptide
1	J	68	GLU	Peptide
2	K	100	SER	Peptide
2	K	106	TYR	Peptide
2	K	193	PRO	Peptide
2	K	202	TYR	Peptide
2	K	25	GLY	Peptide
2	K	66	ARG	Sidechain
3	L	198	HIS	Peptide
3	L	206	VAL	Peptide
3	L	30	ASN	Peptide
3	L	45	GLN	Peptide

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Mol	Chain	Res	Type	Group
3	L	79	ASN	Peptide
3	L	92	GLN	Peptide
3	L	94	THR	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1831	0	1725	142	0
1	D	1762	0	1694	110	0
1	G	1762	0	1694	114	0
1	J	1762	0	1694	114	0
2	B	1635	0	1587	138	0
2	E	1635	0	1587	153	0
2	H	1635	0	1587	153	0
2	K	1635	0	1587	142	0
3	C	1610	0	1549	173	0
3	F	1610	0	1549	165	0
3	I	1610	0	1549	140	0
3	L	1604	0	1543	127	0
4	A	1	0	0	0	0
4	D	1	0	0	0	0
4	G	1	0	0	0	0
4	J	1	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	F	1	0	0	0	0
5	G	1	0	0	0	0
5	H	3	0	0	0	0
5	I	2	0	0	0	0
5	K	1	0	0	0	0
5	L	1	0	0	0	0
All	All	20106	0	19345	1554	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 39.

All (1554) 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:G:115:GLU:HB3	3:I:96:GLU:HB3	1.37	1.07
2:H:216:ASP:O	2:H:217:LYS:HG3	1.56	1.06
2:K:63:VAL:HA	2:K:66:ARG:NH2	1.71	1.02
2:K:63:VAL:HA	2:K:66:ARG:HH21	1.18	1.02
2:E:39:ALA:HB2	2:E:44:LEU:HB2	1.42	1.01
2:E:162:TRP:HA	2:E:204:CYS:HA	1.40	1.01
3:C:9:SER:HB3	3:C:106:LYS:HG2	1.40	1.00
1:A:73:ALA:H	3:C:31:TYR:HB3	1.27	0.97
3:I:57:LYS:HE2	3:I:63:ALA:HA	1.45	0.96
2:E:204:CYS:SG	2:E:217:LYS:NZ	2.38	0.96
1:A:221:ARG:HB2	1:A:221:ARG:HH11	1.33	0.93
1:A:221:ARG:HB2	1:A:221:ARG:NH1	1.82	0.93
2:B:143:THR:HG21	2:B:191:THR:HG23	1.53	0.91
3:I:151:LYS:HB3	3:I:193:THR:HB	1.52	0.90
2:B:169:SER:OG	2:B:170:SER:N	2.02	0.90
3:L:111:ARG:NH1	3:L:112:ALA:O	2.05	0.90
2:E:7:GLY:HA2	2:E:115:THR:HG21	1.52	0.89
3:C:3:MET:SD	3:C:5:GLN:NE2	2.44	0.89
2:K:60:ARG:CZ	3:L:98:PRO:HB2	2.02	0.89
1:G:169:LYS:HZ2	2:H:103:TYR:HD2	1.21	0.89
1:A:137:PRO:HA	1:A:143:SER:H	1.37	0.89
2:B:173:THR:HG22	2:B:174:PHE:H	1.36	0.89
1:G:101:LEU:HB2	1:G:231:TRP:HE1	1.36	0.88
1:G:119:LYS:H	1:G:252:ARG:NH1	1.72	0.88
1:D:90:CYS:SG	1:D:91:TYR:N	2.46	0.87
2:H:162:TRP:H	2:H:167:LEU:HD11	1.37	0.87
2:H:173:THR:HB	2:H:186:LEU:HB2	1.55	0.87
2:H:173:THR:HG22	2:H:174:PHE:H	1.40	0.86
3:I:111:ARG:HD2	3:I:172:ASP:HA	1.57	0.85
2:K:42:LYS:HE3	3:L:103:GLY:HA2	1.59	0.84
3:L:115:ALA:HB1	3:L:116:PRO:HA	1.57	0.84
2:K:82:MET:HE2	2:K:85:LEU:HD21	1.59	0.84
1:A:112:GLU:HG3	2:B:103:TYR:HD2	1.42	0.84
1:A:153:LYS:NZ	1:A:154:LYS:O	2.10	0.83
1:G:149:ILE:HG13	1:G:250:VAL:HG23	1.60	0.83
2:K:196:SER:HA	2:K:200:GLN:HE22	1.44	0.82
3:L:92:GLN:HG3	3:L:101:PHE:HE1	1.43	0.82
2:B:60:ARG:HG3	2:B:62:SER:H	1.44	0.82
2:H:189:VAL:HG13	3:I:175:TYR:HE2	1.45	0.82
2:K:175:PRO:HB2	2:K:184:TYR:HB3	1.62	0.82
1:J:64:ASN:ND2	1:J:90:CYS:SG	2.52	0.81
2:H:189:VAL:HG13	3:I:175:TYR:CE2	2.16	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:132:LEU:HD22	3:I:136:VAL:HG21	1.63	0.81
2:E:162:TRP:CE3	2:E:204:CYS:HB3	2.16	0.81
2:K:176:ALA:HB2	3:L:165:TRP:CD1	2.16	0.81
1:G:153:LYS:HD2	1:G:158:TYR:H	1.46	0.81
1:A:169:LYS:HZ1	2:B:103:TYR:HD1	1.26	0.81
2:H:174:PHE:CE2	3:I:167:ASP:HB3	2.17	0.80
2:K:199:THR:OG1	2:K:200:GLN:NE2	2.15	0.80
2:B:146:LEU:HD21	2:B:197:LEU:HD22	1.63	0.80
1:G:153:LYS:HE2	1:G:154:LYS:H	1.46	0.80
2:K:94:TYR:HA	2:K:114:GLY:HA2	1.64	0.80
2:K:176:ALA:HB2	3:L:165:TRP:HD1	1.45	0.79
1:D:166:ILE:HG12	1:D:239:LYS:HB3	1.65	0.79
3:C:140:ASN:OD1	3:C:175:TYR:HD1	1.65	0.79
2:K:96:ALA:HB1	2:K:108:TRP:HB3	1.63	0.79
1:G:101:LEU:HB2	1:G:231:TRP:NE1	1.99	0.78
1:J:196:ASP:OD1	1:J:196:ASP:N	2.17	0.78
3:C:37:ASN:HD22	3:C:93:GLN:HE21	1.32	0.78
3:F:14:PRO:HA	3:F:81:VAL:HG12	1.66	0.77
2:K:86:ARG:HB2	2:K:88:GLU:HG2	1.64	0.77
1:D:153:LYS:HZ1	1:D:154:LYS:H	1.32	0.77
1:G:72:THR:HA	3:I:31:TYR:HB3	1.66	0.77
2:B:5:GLN:HB2	2:B:22:ALA:HB3	1.64	0.77
1:J:222:ASP:O	1:J:223:GLN:NE2	2.18	0.77
2:K:10:VAL:HG23	2:K:118:THR:HB	1.66	0.77
3:L:86:THR:HB	3:L:109:ILE:HG12	1.65	0.77
1:D:169:LYS:HD2	1:D:170:GLY:H	1.49	0.77
2:K:163:ASN:HB2	2:K:203:ILE:HD13	1.64	0.77
1:A:166:ILE:HG23	1:A:239:LYS:HB3	1.65	0.76
1:D:92:PRO:HB2	1:D:226:ARG:HD3	1.65	0.76
3:L:37:ASN:HD22	3:L:52:TYR:HA	1.50	0.76
2:B:160:VAL:HB	2:B:172:HIS:CE1	2.20	0.76
3:L:93:GLN:HB2	3:L:99:TYR:HB3	1.67	0.76
2:H:70:SER:HB3	2:H:79:TYR:HB2	1.68	0.76
3:C:64:ARG:HB3	3:C:80:PRO:HD2	1.68	0.76
3:C:45:GLN:HB3	3:C:46:PRO:HD3	1.67	0.76
1:J:221:ARG:HB2	1:J:221:ARG:HH11	1.51	0.76
2:K:146:LEU:H	2:K:146:LEU:HD23	1.51	0.76
3:C:17:ARG:HH22	3:C:19:THR:HG23	1.50	0.75
1:G:153:LYS:NZ	1:G:154:LYS:O	2.19	0.75
3:I:143:TYR:H	3:I:198:HIS:HE1	1.33	0.75
2:B:173:THR:HG22	2:B:174:PHE:N	2.02	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:172:ASP:OD1	3:I:173:SER:N	2.19	0.75
1:A:221:ARG:HH11	1:A:221:ARG:CB	2.00	0.75
2:B:190:VAL:HB	2:B:202:TYR:OH	1.87	0.75
1:G:64:ASN:HD21	1:G:90:CYS:HB2	1.49	0.75
3:F:166:THR:HG22	3:F:167:ASP:H	1.52	0.74
2:K:4:GLN:NE2	2:K:95:CYS:SG	2.60	0.74
3:L:115:ALA:HB3	3:L:142:PHE:HA	1.69	0.74
3:L:62:PRO:HB2	3:L:64:ARG:HG3	1.68	0.74
1:D:90:CYS:O	1:D:221:ARG:NH1	2.21	0.74
1:G:166:ILE:HG13	1:G:239:LYS:HB3	1.70	0.74
2:H:138:SER:OG	2:H:139:THR:N	2.19	0.74
1:A:165:TYR:HE1	1:A:167:ASN:HA	1.53	0.73
3:F:96:GLU:HA	3:F:99:TYR:CE2	2.23	0.73
3:F:157:ARG:HB3	3:F:159:ASN:H	1.53	0.73
2:H:28:PHE:HB3	2:H:76:LYS:HE3	1.70	0.73
2:H:66:ARG:NH1	2:H:84:SER:O	2.21	0.73
3:C:64:ARG:NH2	3:C:85:ASP:OD1	2.20	0.73
3:F:146:ILE:HG12	3:F:147:ASN:H	1.53	0.73
3:L:166:THR:HG23	3:L:176:SER:HA	1.70	0.73
1:D:50:LEU:HD22	1:D:76:TRP:CG	2.24	0.73
2:K:180:SER:HB2	2:K:183:LEU:HG	1.71	0.73
2:E:60:ARG:HH21	3:F:98:PRO:HB2	1.53	0.72
1:A:203:SER:HB3	1:A:206:TYR:H	1.53	0.72
2:H:2:LYS:N	2:H:24:SER:O	2.22	0.72
3:C:96:GLU:HA	3:C:99:TYR:CE1	2.24	0.72
3:C:161:VAL:HG11	3:C:181:LEU:H	1.54	0.72
2:H:32:ASP:HB3	2:H:98:HIS:CE1	2.25	0.72
3:I:142:PHE:HB2	3:I:198:HIS:CE1	2.24	0.72
2:E:146:LEU:HD21	2:E:197:LEU:HD22	1.71	0.72
2:H:171:VAL:HG23	3:I:175:TYR:HD2	1.53	0.71
3:C:118:VAL:HB	3:C:205:ILE:HG13	1.72	0.71
2:H:161:SER:HA	2:H:167:LEU:HD21	1.73	0.71
1:G:115:GLU:H	3:I:96:GLU:HG2	1.52	0.71
1:A:115:GLU:HB2	3:C:96:GLU:HB2	1.73	0.71
3:I:95:LYS:HG2	3:I:96:GLU:H	1.54	0.71
2:H:162:TRP:CZ3	2:H:204:CYS:HB2	2.26	0.71
3:I:115:ALA:HB1	3:I:116:PRO:HA	1.71	0.71
3:F:161:VAL:HG11	3:F:181:LEU:H	1.55	0.71
3:L:201:SER:O	3:L:202:THR:OG1	2.09	0.71
1:A:153:LYS:HE2	1:A:154:LYS:H	1.56	0.71
2:B:163:ASN:HA	2:B:205:ASN:HD21	1.55	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:51:ILE:HG13	3:I:76:LEU:HD21	1.72	0.71
1:A:56[A]:ASN:HA	1:A:81:GLU:HG2	1.73	0.70
1:A:204:SER:OG	1:A:205:ARG:N	2.18	0.70
2:H:11:VAL:O	2:H:119:VAL:HA	1.91	0.70
1:J:123:TRP:CZ2	1:J:250:VAL:HG11	2.25	0.70
1:G:113:ARG:HH12	3:I:95:LYS:HE2	1.54	0.70
3:C:190:ASN:HB3	3:C:208:SER:O	1.92	0.70
2:H:37:ARG:HD2	2:H:93:TYR:CZ	2.27	0.70
1:J:106:SER:O	1:J:259:ARG:NH1	2.24	0.70
2:H:163:ASN:HB2	2:H:203:ILE:HD13	1.74	0.70
2:E:195:SER:O	2:E:199:THR:HG21	1.92	0.70
2:H:81:GLN:HG3	2:H:83:ASN:HD21	1.57	0.70
1:D:123:TRP:HE1	1:D:149:ILE:HD13	1.56	0.70
2:E:90:THR:HB	2:E:118:THR:HA	1.71	0.70
3:F:95:LYS:CG	3:F:96:GLU:H	2.04	0.70
1:A:60:TRP:HE1	1:A:70:LEU:HD22	1.57	0.69
2:B:86:ARG:HH11	2:B:86:ARG:HB3	1.56	0.69
2:H:199:THR:OG1	2:H:200:GLN:N	2.17	0.69
2:H:31:TYR:O	2:H:71:ARG:NH2	2.24	0.69
3:C:4:THR:OG1	3:C:22:CYS:SG	2.50	0.69
1:A:119:LYS:HB3	1:A:252:ARG:HH11	1.55	0.69
2:K:77:THR:HB	2:K:79:TYR:CE1	2.28	0.69
1:A:234:VAL:HG23	1:A:238:ASP:HB2	1.74	0.69
3:F:4:THR:HG21	3:F:36:ILE:HD11	1.75	0.69
2:B:97:ARG:O	2:B:108:TRP:HB3	1.93	0.69
3:L:10:LEU:HG	3:L:11:ALA:H	1.57	0.69
3:F:79:ASN:HB3	3:F:80:PRO:HD3	1.75	0.69
1:D:108:VAL:HA	1:D:259:ARG:HA	1.73	0.68
1:A:99:GLU:OE2	1:A:102:ARG:NH1	2.27	0.68
1:A:180:HIS:HA	1:A:227:MET:HG2	1.73	0.68
2:B:175:PRO:HB3	2:B:184:TYR:HB3	1.75	0.68
1:D:63:GLY:HA3	1:D:146:LYS:HB3	1.75	0.68
1:J:91:TYR:HH	1:J:180:HIS:HE2	1.39	0.68
1:D:109:SER:N	1:D:258:GLU:O	2.26	0.68
2:H:201:THR:HG23	2:H:218:LYS:HD2	1.74	0.68
3:L:14:PRO:HA	3:L:81:VAL:HG12	1.75	0.68
2:E:162:TRP:CZ3	2:E:202:TYR:HE1	2.11	0.68
1:D:182:PRO:HB3	1:D:187:ASP:HB3	1.74	0.68
3:F:151:LYS:HG3	3:F:153:ASP:HA	1.76	0.68
1:G:252:ARG:NH2	3:I:97:VAL:HA	2.09	0.68
3:I:169:ASP:OD1	3:I:171:LYS:N	2.27	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:152:VAL:HG23	1:G:153:LYS:H	1.59	0.68
3:C:192:TYR:H	3:C:207:LYS:HG2	1.59	0.68
3:I:23:ARG:HH21	2:K:75:ARG:HD2	1.57	0.68
3:L:163:ASN:OD1	3:L:163:ASN:N	2.27	0.68
1:A:112:GLU:HG3	2:B:103:TYR:CD2	2.28	0.67
3:L:93:GLN:CD	3:L:93:GLN:H	2.02	0.67
2:B:3:LEU:O	2:B:4:GLN:NE2	2.27	0.67
1:D:101:LEU:HB2	1:D:231:TRP:NE1	2.08	0.67
3:C:161:VAL:HG21	3:C:181:LEU:HB3	1.77	0.67
2:H:60:ARG:HG2	2:H:62:SER:H	1.59	0.67
3:L:120:ILE:HD12	3:L:194:CYS:HB2	1.75	0.67
1:D:182:PRO:HG2	1:D:188:GLN:OE1	1.93	0.67
2:E:197:LEU:HG	2:E:198:GLY:N	2.08	0.67
2:K:116:MET:HG3	2:K:157:PRO:HD3	1.77	0.67
2:B:189:VAL:HG21	3:C:140:ASN:HD21	1.58	0.67
1:D:177:TRP:HE1	1:D:210:PHE:HE2	1.43	0.67
3:C:157:ARG:HG2	3:C:158:GLN:H	1.58	0.67
3:F:118:VAL:HG13	3:F:139:LEU:HG	1.77	0.67
1:G:120:THR:OG1	1:G:121:SER:N	2.27	0.67
3:I:57:LYS:HE3	3:I:61:VAL:O	1.95	0.67
2:K:97:ARG:HB3	2:K:109:ASP:OD1	1.95	0.67
2:B:38:GLN:NE2	3:C:41:GLN:OE1	2.23	0.66
1:D:167:ASN:OD1	1:D:168:ASP:N	2.27	0.66
3:F:3:MET:HE2	3:F:3:MET:H	1.60	0.66
2:H:36:ILE:O	2:H:94:TYR:N	2.28	0.66
2:E:4:GLN:HG3	2:E:23:ALA:HB2	1.76	0.66
1:G:228:ASN:HB3	1:G:230:TYR:HE1	1.61	0.66
1:J:56[B]:ASN:ND2	1:J:84:SER:O	2.27	0.66
2:K:202:TYR:HD2	2:K:219:SER:HB2	1.59	0.66
3:L:92:GLN:HG3	3:L:101:PHE:CE1	2.28	0.66
3:L:118:VAL:HB	3:L:205:ILE:HD13	1.77	0.66
1:A:218:PRO:O	1:A:226:ARG:NH2	2.29	0.66
2:B:36:ILE:HD13	2:B:111:TRP:CZ3	2.31	0.66
3:I:13:SER:HA	3:I:110:LYS:HB2	1.77	0.66
2:K:45:GLU:OE2	2:K:46:TRP:N	2.28	0.66
1:A:87:ASN:OD1	1:A:87:ASN:N	2.28	0.66
3:C:16:GLN:NE2	2:E:210:PRO:O	2.28	0.66
2:B:108:TRP:H	2:B:108:TRP:CD1	2.12	0.66
1:J:171:LYS:HZ3	1:J:171:LYS:HA	1.59	0.66
2:K:50:ILE:HD12	2:K:71:ARG:HE	1.59	0.66
2:K:35:TRP:CD1	2:K:80:LEU:HB2	2.31	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:62:SER:O	2:K:66:ARG:NH2	2.29	0.66
1:A:165:TYR:H	1:A:240:ILE:HG22	1.61	0.66
3:C:86:THR:HA	3:C:107:LEU:HD23	1.77	0.66
3:L:151:LYS:NZ	3:L:195:GLU:OE2	2.29	0.66
1:J:169:LYS:HD2	1:J:171:LYS:HB3	1.78	0.65
2:K:125:LYS:NZ	2:K:152:ASP:O	2.27	0.65
2:B:35:TRP:CD1	2:B:80:LEU:HD13	2.31	0.65
2:E:35:TRP:NE1	2:E:79:TYR:O	2.29	0.65
3:F:126:GLU:H	3:F:126:GLU:CD	2.04	0.65
2:H:173:THR:HG21	3:I:177:MET:HE2	1.79	0.65
2:K:46:TRP:NE1	2:K:48:SER:O	2.29	0.65
2:E:217:LYS:H	2:E:217:LYS:HZ2	1.44	0.65
3:F:163:ASN:N	3:F:163:ASN:OD1	2.28	0.65
2:B:90:THR:CG2	2:B:119:VAL:H	2.09	0.65
1:D:110:SER:HB3	1:D:258:GLU:HB2	1.78	0.65
2:E:16:SER:OG	2:E:81:GLN:NE2	2.30	0.65
2:E:81:GLN:NE2	2:E:82:MET:O	2.30	0.65
1:D:61:ILE:O	1:D:147:ASN:ND2	2.28	0.65
2:K:161:SER:O	2:K:205:ASN:ND2	2.30	0.65
2:K:187:SER:OG	3:L:177:MET:SD	2.55	0.65
3:C:17:ARG:HB3	3:C:79:ASN:HA	1.79	0.65
3:I:173:SER:O	3:I:173:SER:OG	2.12	0.65
2:E:161:SER:HA	2:E:167:LEU:HD11	1.78	0.65
3:F:127:GLN:NE2	3:F:134:SER:OG	2.28	0.65
3:L:182:THR:OG1	3:L:183:LEU:N	2.29	0.65
2:B:161:SER:HA	2:B:167:LEU:HD11	1.79	0.64
1:D:192:TYR:O	1:D:194:ASN:ND2	2.30	0.64
1:A:167:ASN:OD1	1:A:168:ASP:N	2.30	0.64
2:B:2:LYS:HZ2	2:B:97:ARG:HH12	1.44	0.64
3:F:5:GLN:NE2	3:F:23:ARG:HG2	2.13	0.64
3:C:92:GLN:O	3:C:94:THR:N	2.28	0.64
3:C:96:GLU:HA	3:C:99:TYR:HE1	1.61	0.64
2:H:111:TRP:CD1	2:H:111:TRP:N	2.64	0.64
1:J:95:PHE:HD2	1:J:98:TYR:HD2	1.46	0.64
3:C:92:GLN:C	3:C:94:THR:H	2.06	0.64
3:F:168:GLN:NE2	3:F:169:ASP:O	2.30	0.64
3:C:145:LYS:HG2	3:C:146:ILE:H	1.63	0.63
1:D:173:VAL:HG22	1:D:256:ALA:HA	1.80	0.63
1:J:150:TRP:C	1:J:150:TRP:CD1	2.77	0.63
2:B:173:THR:OG1	3:C:175:TYR:HE2	1.82	0.63
2:K:162:TRP:HA	2:K:204:CYS:HA	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:140:ASN:HA	3:C:175:TYR:HA	1.81	0.63
2:E:72:ASP:OD2	2:E:75:ARG:NH1	2.32	0.63
1:A:109:SER:HB3	1:A:258:GLU:HG3	1.79	0.63
3:C:172:ASP:CG	3:C:173:SER:H	2.06	0.63
2:K:101:PRO:C	2:K:103:TYR:H	2.05	0.63
2:B:173:THR:CG2	2:B:174:PHE:H	2.09	0.63
3:C:15:GLY:O	2:E:212:ASN:HB2	1.99	0.63
2:E:162:TRP:CD2	2:E:204:CYS:HB3	2.32	0.63
2:H:160:VAL:HG22	2:H:206:VAL:HG22	1.81	0.63
3:L:39:PHE:CD1	3:L:92:GLN:HG2	2.33	0.63
1:A:179:ILE:HD11	1:A:199:VAL:HG11	1.81	0.63
3:C:166:THR:HG22	3:C:167:ASP:H	1.62	0.63
1:J:178:GLY:O	1:J:179:ILE:HD12	1.99	0.63
2:K:33:MET:HG2	2:K:97:ARG:HA	1.81	0.63
2:B:174:PHE:CE1	3:C:167:ASP:HB3	2.34	0.62
2:B:217:LYS:NZ	2:B:217:LYS:H	1.97	0.62
3:C:28:VAL:HG12	3:C:95:LYS:HG3	1.81	0.62
2:K:129:VAL:HG11	2:K:217:LYS:HD2	1.82	0.62
3:F:111:ARG:NE	3:F:171:LYS:O	2.32	0.62
3:F:133:ALA:N	3:F:182:THR:O	2.29	0.62
2:K:142:ALA:C	2:K:194:SER:HG	2.07	0.62
1:G:87:ASN:HA	1:G:221:ARG:NH2	2.15	0.62
2:H:160:VAL:HB	2:H:172:HIS:NE2	2.13	0.62
3:I:190:ASN:O	3:I:207:LYS:NZ	2.31	0.62
3:F:146:ILE:HG13	3:F:198:HIS:CD2	2.34	0.62
3:F:146:ILE:HG13	3:F:198:HIS:HD2	1.64	0.62
2:K:162:TRP:H	2:K:167:LEU:HG	1.65	0.62
3:C:7:PRO:HG3	3:C:21:THR:HG23	1.79	0.62
1:A:185:SER:HA	1:A:188:GLN:HB3	1.81	0.62
2:B:158:VAL:HG12	2:B:186:LEU:HD21	1.82	0.62
3:I:200:THR:OG1	3:I:201:SER:N	2.31	0.62
2:E:204:CYS:O	2:E:216:ASP:HB3	2.00	0.62
3:F:89:TYR:HE2	3:F:107:LEU:HD22	1.64	0.62
2:K:59:TYR:OH	2:K:69:ILE:HG22	2.00	0.62
1:A:173:VAL:HA	1:A:255:PHE:O	2.00	0.61
3:I:37:ASN:ND2	3:I:93:GLN:HE21	1.98	0.61
3:I:157:ARG:HG3	3:I:159:ASN:H	1.65	0.61
2:E:68:THR:HB	2:E:81:GLN:HB3	1.81	0.61
2:E:110:TYR:C	2:E:111:TRP:CD1	2.78	0.61
2:E:143:THR:HA	2:E:193:PRO:HA	1.81	0.61
3:F:159:ASN:O	3:F:161:VAL:N	2.32	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:143:THR:CG2	2:B:191:THR:HG23	2.27	0.61
2:E:177:VAL:HG22	2:E:184:TYR:CE2	2.35	0.61
3:C:16:GLN:HG2	3:C:17:ARG:HG3	1.81	0.61
3:F:5:GLN:NE2	3:F:23:ARG:O	2.33	0.61
2:H:36:ILE:HB	2:H:46:TRP:HA	1.83	0.61
3:I:95:LYS:HB3	3:I:97:VAL:HG22	1.82	0.61
1:J:117:PHE:CE1	1:J:163:LYS:HG2	2.35	0.61
3:L:38:TRP:CE2	3:L:76:LEU:HB2	2.35	0.61
3:C:192:TYR:N	3:C:207:LYS:HG2	2.15	0.61
1:G:228:ASN:HB3	1:G:230:TYR:CE1	2.35	0.61
2:K:47:VAL:O	2:K:48:SER:HB3	1.99	0.61
2:B:18:ARG:HG3	2:B:81:GLN:HG2	1.82	0.61
2:B:100:SER:HB2	2:B:105:LEU:HD23	1.83	0.61
3:C:172:ASP:OD2	3:C:173:SER:N	2.28	0.61
2:E:38:GLN:NE2	3:F:41:GLN:OE1	2.33	0.61
2:E:66:ARG:NH1	2:E:89:ASP:OD2	2.33	0.61
2:E:127:PRO:HB3	2:E:153:TYR:HB3	1.82	0.61
3:I:37:ASN:HD21	3:I:93:GLN:HE21	1.48	0.61
3:F:141:ASN:HA	3:F:174:THR:HA	1.83	0.60
2:K:139:THR:OG1	2:K:140:SER:N	2.32	0.60
2:B:90:THR:HG22	2:B:118:THR:HA	1.83	0.60
3:F:42:LYS:O	3:F:44:GLY:N	2.34	0.60
1:J:64:ASN:O	1:J:67:CYS:N	2.33	0.60
3:F:36:ILE:HB	3:F:74:PHE:CE2	2.36	0.60
1:J:95:PHE:CD1	1:J:229:TYR:HB2	2.37	0.60
1:J:112:GLU:HB3	1:J:256:ALA:HB3	1.82	0.60
2:K:36:ILE:HD11	3:L:101:PHE:HE2	1.65	0.60
2:B:59:TYR:HB2	2:B:64:LYS:HE3	1.82	0.60
2:B:146:LEU:HD22	2:B:202:TYR:CD2	2.36	0.60
3:C:39:PHE:CD2	3:C:92:GLN:HG3	2.37	0.60
2:E:205:ASN:HB3	2:E:216:ASP:OD1	2.02	0.60
3:F:92:GLN:HG3	3:F:93:GLN:NE2	2.16	0.60
3:L:50:LEU:C	3:L:57:LYS:HZ3	2.09	0.60
2:K:202:TYR:CD2	2:K:219:SER:HB2	2.36	0.60
3:L:81:VAL:HG13	3:L:109:ILE:HD12	1.84	0.60
3:C:41:GLN:O	3:C:87:ALA:HB1	2.02	0.60
1:D:191:LEU:HB3	1:D:192:TYR:CD1	2.36	0.60
1:A:174:LEU:HD23	1:A:233:LEU:HD22	1.82	0.60
2:E:108:TRP:H	2:E:108:TRP:CD1	2.20	0.60
2:H:81:GLN:HG3	2:H:83:ASN:ND2	2.17	0.60
2:H:143:THR:HA	2:H:194:SER:N	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:75:ARG:HB2	2:K:77:THR:OG1	2.01	0.60
3:L:57:LYS:HE2	3:L:65:PHE:HB2	1.84	0.60
3:L:95:LYS:HG3	3:L:96:GLU:H	1.67	0.60
1:J:123:TRP:HH2	1:J:250:VAL:HG21	1.65	0.60
3:F:9:SER:HB3	3:F:106:LYS:HG2	1.85	0.59
1:J:211:LYS:HG3	1:J:212:PRO:HD2	1.83	0.59
3:L:35:PHE:O	3:L:94:THR:HA	2.02	0.59
1:A:204:SER:O	1:A:206:TYR:N	2.35	0.59
3:C:17:ARG:HG2	3:C:79:ASN:ND2	2.17	0.59
1:D:154:LYS:O	1:D:154:LYS:HD3	2.02	0.59
3:F:11:ALA:HB3	3:F:110:LYS:HE2	1.82	0.59
3:F:17:ARG:HH21	3:F:77:THR:HG21	1.67	0.59
1:J:176:LEU:HA	1:J:231:TRP:HA	1.85	0.59
2:B:36:ILE:HD11	2:B:108:TRP:CH2	2.38	0.59
3:C:167:ASP:OD1	3:C:167:ASP:N	2.36	0.59
2:E:169:SER:OG	2:E:170:SER:N	2.33	0.59
3:F:164:SER:HA	3:F:177:MET:O	2.03	0.59
1:G:163:LYS:O	1:G:241:THR:HA	2.03	0.59
2:H:47:VAL:O	2:H:60:ARG:NH1	2.34	0.59
1:J:194:ASN:HD21	1:J:245:THR:HG22	1.67	0.59
1:A:110:SER:OG	1:A:111:PHE:N	2.33	0.59
1:A:133:THR:HG23	1:A:136:CYS:H	1.67	0.59
1:G:153:LYS:CD	1:G:158:TYR:H	2.15	0.59
1:J:123:TRP:CH2	1:J:250:VAL:HG21	2.37	0.59
3:C:140:ASN:OD1	3:C:140:ASN:N	2.33	0.59
3:F:42:LYS:NZ	3:F:84:GLU:O	2.36	0.59
2:H:98:HIS:ND1	2:H:98:HIS:N	2.50	0.59
3:I:27:SER:O	3:I:95:LYS:NZ	2.25	0.59
1:J:123:TRP:H	1:J:123:TRP:CD1	2.19	0.59
2:K:97:ARG:O	2:K:108:TRP:HA	2.03	0.59
2:B:111:TRP:N	2:B:111:TRP:CD1	2.70	0.59
2:B:162:TRP:CD1	2:B:170:SER:HG	2.21	0.59
2:K:217:LYS:H	2:K:217:LYS:NZ	2.01	0.59
3:L:37:ASN:OD1	3:L:93:GLN:NE2	2.36	0.59
1:A:215:ALA:HB1	1:G:96:ILE:HD13	1.84	0.59
3:C:134:SER:HB3	3:C:181:LEU:HD13	1.85	0.59
3:F:93:GLN:HB3	3:F:99:TYR:HB3	1.85	0.59
2:H:60:ARG:HD2	2:H:63:VAL:HB	1.84	0.59
3:I:117:THR:O	3:I:139:LEU:HA	2.03	0.59
2:B:189:VAL:HG21	3:C:140:ASN:ND2	2.18	0.59
1:J:101:LEU:HD23	1:J:231:TRP:CE2	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:161:SER:HB2	2:K:167:LEU:HD11	1.85	0.58
3:C:42:LYS:HA	3:C:87:ALA:HB1	1.85	0.58
2:E:177:VAL:HA	2:E:184:TYR:HA	1.85	0.58
3:F:207:LYS:HG3	3:F:209:PHE:HB3	1.84	0.58
2:H:216:ASP:O	2:H:217:LYS:CG	2.41	0.58
3:L:133:ALA:HB3	3:L:182:THR:HG23	1.84	0.58
3:L:79:ASN:HB3	3:L:80:PRO:HD3	1.86	0.58
1:A:73:ALA:H	3:C:31:TYR:CB	2.09	0.58
3:F:37:ASN:HB3	3:F:52:TYR:HA	1.84	0.58
2:B:162:TRP:NE1	2:B:170:SER:OG	2.36	0.58
2:E:178:LEU:O	2:E:180:SER:N	2.36	0.58
2:H:143:THR:HA	2:H:194:SER:H	1.69	0.58
2:H:174:PHE:CE1	3:I:165:TRP:HB3	2.38	0.58
1:J:150:TRP:NE1	1:J:192:TYR:OH	2.37	0.58
2:K:60:ARG:HH21	3:L:1:ILE:HG12	1.68	0.58
2:K:196:SER:HA	2:K:200:GLN:NE2	2.17	0.58
3:L:50:LEU:O	3:L:57:LYS:NZ	2.37	0.58
3:L:151:LYS:O	3:L:192:TYR:HA	2.03	0.58
2:E:60:ARG:HE	3:F:98:PRO:HB2	1.69	0.58
3:F:68:SER:OG	3:F:69:GLY:N	2.33	0.58
3:C:14:PRO:HA	3:C:81:VAL:HG12	1.86	0.58
3:C:19:THR:OG1	2:E:12:GLN:NE2	2.35	0.58
3:C:28:VAL:HG11	3:C:94:THR:HB	1.86	0.58
1:G:180:HIS:O	1:G:247:ASN:ND2	2.37	0.58
3:I:28:VAL:HA	3:I:95:LYS:HE3	1.85	0.58
2:B:33:MET:HB2	2:B:78:LEU:HD23	1.84	0.58
2:B:160:VAL:HB	2:B:172:HIS:HE1	1.68	0.58
3:C:37:ASN:O	3:C:92:GLN:HB2	2.03	0.58
3:F:42:LYS:NZ	3:F:85:ASP:O	2.36	0.58
3:I:62:PRO:HG2	3:I:65:PHE:CE1	2.38	0.58
1:A:104:GLN:O	1:A:259:ARG:HD2	2.04	0.58
3:C:92:GLN:HB3	3:C:93:GLN:CD	2.29	0.58
2:H:111:TRP:CD1	2:H:111:TRP:H	2.22	0.58
3:I:168:GLN:HG3	3:I:169:ASP:H	1.68	0.58
2:K:161:SER:OG	2:K:205:ASN:ND2	2.33	0.58
3:F:161:VAL:HG11	3:F:181:LEU:N	2.18	0.58
2:H:73:ASN:OD1	2:H:73:ASN:N	2.35	0.58
1:J:148:LEU:HD23	1:J:251:PRO:HA	1.86	0.58
2:E:159:THR:OG1	2:E:207:ASN:O	2.20	0.57
3:L:184:ASP:HB3	3:L:186:TYR:CE1	2.38	0.57
3:C:189:HIS:HB3	3:C:191:SER:N	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:152:ASP:HA	2:E:184:TYR:O	2.04	0.57
2:H:149:LEU:HD11	3:I:136:VAL:HG11	1.85	0.57
2:K:174:PHE:CE1	3:L:167:ASP:HB3	2.39	0.57
2:E:45:GLU:OE2	3:F:100:THR:HA	2.05	0.57
1:J:59:GLY:HA2	1:J:62:LEU:HB2	1.86	0.57
2:K:63:VAL:HG22	2:K:66:ARG:HH22	1.69	0.57
1:A:116:ILE:HG13	1:A:165:TYR:HD2	1.69	0.57
3:C:7:PRO:CD	3:C:21:THR:H	2.17	0.57
3:F:69:GLY:HA3	3:F:74:PHE:HA	1.85	0.57
1:G:79:ILE:HD12	1:G:79:ILE:H	1.69	0.57
2:H:46:TRP:NE1	2:H:48:SER:O	2.38	0.57
1:J:123:TRP:CZ3	1:J:163:LYS:HD2	2.40	0.57
1:D:153:LYS:HE2	1:D:157:SER:N	2.20	0.57
2:E:32:ASP:HA	2:E:71:ARG:HH22	1.70	0.57
3:F:151:LYS:HG2	3:F:193:THR:HB	1.86	0.57
2:H:29:SER:HA	2:H:73:ASN:HD22	1.68	0.57
2:H:208:HIS:CE1	2:H:211:SER:HB3	2.40	0.57
3:C:9:SER:HB3	3:C:106:LYS:CG	2.27	0.57
1:J:216:ILE:HG23	1:J:224:GLU:HG3	1.87	0.57
3:L:42:LYS:HD3	3:L:43:PRO:HD2	1.87	0.57
2:B:39:ALA:N	2:B:43:GLY:HA2	2.19	0.57
2:B:180:SER:C	2:B:182:GLY:H	2.13	0.57
3:C:16:GLN:HG2	3:C:17:ARG:H	1.68	0.57
1:D:119:LYS:HB2	1:D:252:ARG:HD3	1.87	0.57
2:E:37:ARG:HD2	2:E:93:TYR:CZ	2.39	0.57
2:K:208:HIS:CD2	2:K:210:PRO:HG2	2.40	0.57
2:B:45:GLU:OE2	2:B:46:TRP:N	2.37	0.57
2:B:178:LEU:O	2:B:180:SER:N	2.38	0.57
2:E:32:ASP:N	2:E:32:ASP:OD1	2.38	0.57
2:H:44:LEU:HD23	2:H:45:GLU:HG3	1.86	0.57
2:K:109:ASP:OD1	2:K:110:TYR:N	2.38	0.57
3:F:184:ASP:HB3	3:F:186:TYR:CE1	2.39	0.57
3:I:45:GLN:HB3	3:I:46:PRO:HD3	1.86	0.57
2:K:95:CYS:O	2:K:111:TRP:HA	2.05	0.57
3:F:133:ALA:HB3	3:F:182:THR:HG23	1.87	0.56
1:A:182:PRO:HG2	1:A:188:GLN:OE1	2.05	0.56
1:D:119:LYS:HG3	1:D:149:ILE:HG12	1.87	0.56
2:E:26:PHE:C	2:E:28:PHE:H	2.13	0.56
2:E:36:ILE:HG22	2:E:94:TYR:HB2	1.86	0.56
3:F:111:ARG:HH12	3:F:114:ALA:HB2	1.70	0.56
3:F:141:ASN:H	3:F:175:TYR:H	1.53	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:203:SER:HB2	1:G:240:ILE:HA	1.86	0.56
2:H:33:MET:HB3	2:H:78:LEU:HD22	1.87	0.56
3:L:96:GLU:HA	3:L:99:TYR:HE1	1.69	0.56
1:G:122:SER:HB3	1:G:163:LYS:HE2	1.86	0.56
2:H:71:ARG:HH11	2:H:73:ASN:HD21	1.54	0.56
1:J:70:LEU:HB3	3:L:30:ASN:O	2.05	0.56
1:J:166:ILE:HD13	1:J:239:LYS:HB3	1.87	0.56
3:L:127:GLN:HG2	3:L:132:GLY:O	2.06	0.56
1:A:116:ILE:HG23	1:A:117:PHE:H	1.70	0.56
2:E:110:TYR:CG	2:E:111:TRP:N	2.74	0.56
2:K:77:THR:HB	2:K:79:TYR:HE1	1.67	0.56
2:K:177:VAL:HG12	2:K:182:GLY:O	2.05	0.56
2:B:28:PHE:HB3	2:B:76:LYS:HE2	1.88	0.56
3:C:21:THR:HG22	3:C:75:THR:HG23	1.87	0.56
3:C:50:LEU:HA	3:C:61:VAL:HG21	1.88	0.56
1:G:164:SER:H	2:H:56:ARG:HH12	1.53	0.56
2:H:81:GLN:CG	2:H:83:ASN:HD21	2.18	0.56
3:I:43:PRO:HD3	3:I:87:ALA:HB2	1.87	0.56
3:I:170:SER:O	3:I:170:SER:OG	2.17	0.56
2:K:50:ILE:C	2:K:51:LEU:HD13	2.30	0.56
2:K:161:SER:HB2	2:K:167:LEU:HD21	1.88	0.56
1:A:56[B]:ASN:HA	1:A:81:GLU:HG2	1.87	0.56
2:B:160:VAL:HG13	2:B:206:VAL:HG23	1.88	0.56
3:F:151:LYS:C	3:F:153:ASP:H	2.13	0.56
2:K:26:PHE:O	2:K:27:THR:HG22	2.04	0.56
2:K:173:THR:HG22	2:K:186:LEU:HG	1.87	0.56
1:A:109:SER:N	1:A:258:GLU:O	2.36	0.56
1:A:177:TRP:CZ3	1:A:232:THR:HG22	2.41	0.56
3:F:166:THR:HG22	3:F:167:ASP:N	2.20	0.56
2:K:50:ILE:HD11	2:K:78:LEU:HD13	1.88	0.56
2:B:32:ASP:OD1	2:B:51:LEU:HA	2.06	0.55
3:F:17:ARG:NH2	3:F:77:THR:HG21	2.21	0.55
3:F:96:GLU:HA	3:F:99:TYR:HE2	1.69	0.55
2:H:10:VAL:HG21	2:H:155:PRO:HG3	1.87	0.55
2:K:87:ALA:O	2:K:90:THR:HG22	2.06	0.55
3:C:86:THR:HB	3:C:109:ILE:HD13	1.87	0.55
3:C:115:ALA:HB1	3:C:116:PRO:O	2.06	0.55
2:E:47:VAL:HG22	2:E:63:VAL:HG21	1.87	0.55
3:L:167:ASP:OD1	3:L:175:TYR:HB3	2.06	0.55
3:C:38:TRP:N	3:C:51:ILE:O	2.38	0.55
3:C:140:ASN:OD1	3:C:175:TYR:CD1	2.54	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:64:ARG:HB3	3:F:78:ILE:HD12	1.88	0.55
1:G:153:LYS:CE	1:G:154:LYS:H	2.17	0.55
2:H:175:PRO:HG3	2:H:186:LEU:HD12	1.88	0.55
3:C:45:GLN:HB3	3:C:46:PRO:CD	2.35	0.55
3:F:78:ILE:O	3:F:78:ILE:HG13	2.06	0.55
3:L:187:GLU:HB3	3:L:188:ARG:NH2	2.21	0.55
3:C:39:PHE:HD2	3:C:92:GLN:HG3	1.71	0.55
3:C:143:TYR:HD2	3:C:173:SER:HB2	1.72	0.55
3:C:191:SER:HA	3:C:207:LYS:HD3	1.88	0.55
1:D:123:TRP:CD1	1:D:151:LEU:HD21	2.42	0.55
2:K:163:ASN:ND2	2:K:203:ILE:HG12	2.21	0.55
1:A:96:ILE:HG12	1:A:230:TYR:CE2	2.42	0.55
1:A:156:ASN:HB2	1:A:193:GLN:NE2	2.21	0.55
2:B:54:SER:O	2:B:56:ARG:HG2	2.06	0.55
3:C:45:GLN:CB	3:C:46:PRO:HD3	2.36	0.55
1:D:184:THR:HG1	1:D:186:ALA:H	1.51	0.55
3:F:37:ASN:HD22	3:F:53:THR:H	1.55	0.55
1:J:116:ILE:HD11	1:J:165:TYR:CG	2.42	0.55
1:A:153:LYS:HG2	1:A:156:ASN:HA	1.88	0.55
2:K:42:LYS:O	2:K:42:LYS:HG2	2.06	0.55
2:B:162:TRP:HD1	2:B:167:LEU:HG	1.71	0.55
3:C:7:PRO:HD3	3:C:21:THR:O	2.07	0.55
1:D:126:HIS:HE1	1:D:161:LEU:HB2	1.72	0.55
2:E:6:SER:HB2	2:E:115:THR:HG23	1.89	0.55
2:E:143:THR:HG22	2:E:193:PRO:HD3	1.88	0.55
1:G:50:LEU:HD21	1:G:79:ILE:HG13	1.89	0.55
3:I:41:GLN:O	3:I:87:ALA:HB1	2.07	0.55
3:I:64:ARG:HE	3:I:78:ILE:HD11	1.71	0.55
2:B:32:ASP:CG	2:B:51:LEU:HA	2.32	0.54
2:B:217:LYS:H	2:B:217:LYS:HZ2	1.52	0.54
3:C:35:PHE:HB3	3:C:94:THR:O	2.07	0.54
2:E:60:ARG:NH2	3:F:98:PRO:O	2.40	0.54
3:I:115:ALA:HB3	3:I:142:PHE:HA	1.88	0.54
1:J:123:TRP:CD1	1:J:123:TRP:N	2.74	0.54
2:B:42:LYS:HE3	3:C:103:GLY:O	2.07	0.54
3:C:57:LYS:NZ	3:C:62:PRO:O	2.27	0.54
3:C:183:LEU:O	3:C:186:TYR:HB2	2.08	0.54
1:D:248:LEU:HG	1:D:250:VAL:HG13	1.88	0.54
1:A:91:TYR:CE2	1:A:227:MET:HG3	2.43	0.54
1:A:111:PHE:O	1:A:112:GLU:HG2	2.08	0.54
1:A:172:GLU:HB3	1:A:233:LEU:HD11	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:187:SER:HG	3:C:138:PHE:HE1	1.56	0.54
1:D:59:GLY:O	1:D:63:GLY:N	2.40	0.54
3:L:153:ASP:HB2	3:L:189:HIS:CE1	2.41	0.54
1:D:50:LEU:HD22	1:D:76:TRP:CD1	2.42	0.54
3:F:52:TYR:CE1	3:F:56:ASN:HB3	2.42	0.54
3:F:169:ASP:OD2	3:F:171:LYS:HD2	2.06	0.54
1:G:113:ARG:HD3	3:I:30:ASN:HB2	1.90	0.54
1:A:153:LYS:NZ	1:A:157:SER:O	2.35	0.54
2:B:125:LYS:HD2	2:B:126:GLY:O	2.08	0.54
1:D:123:TRP:HE1	1:D:149:ILE:CD1	2.21	0.54
2:E:129:VAL:HG11	2:E:217:LYS:HE2	1.89	0.54
2:H:27:THR:O	2:H:27:THR:HG22	2.06	0.54
3:I:64:ARG:NH2	3:I:85:ASP:HB3	2.23	0.54
1:J:112:GLU:HA	3:L:33:ILE:HD11	1.88	0.54
2:K:206:VAL:HG22	2:K:215:VAL:O	2.07	0.54
3:L:92:GLN:N	3:L:92:GLN:OE1	2.41	0.54
3:C:123:PRO:HD3	3:C:135:VAL:HG22	1.90	0.54
3:F:38:TRP:HA	3:F:92:GLN:OE1	2.08	0.54
2:H:111:TRP:N	2:H:111:TRP:HD1	2.05	0.54
3:I:166:THR:HG22	3:I:167:ASP:H	1.73	0.54
2:B:55:GLU:O	2:B:56:ARG:NE	2.40	0.54
2:E:18:ARG:NE	2:E:81:GLN:HG2	2.22	0.54
3:F:185:GLU:C	3:F:186:TYR:HD1	2.15	0.54
1:G:235:GLU:HB3	1:G:236:PRO:HD2	1.90	0.54
2:H:178:LEU:O	2:H:180:SER:OG	2.26	0.54
1:A:210:PHE:HE2	1:A:230:TYR:CE2	2.25	0.54
2:B:4:GLN:HB3	2:B:112:GLY:CA	2.38	0.54
2:K:47:VAL:HG11	2:K:63:VAL:HG21	1.89	0.54
2:H:162:TRP:C	2:H:164:SER:H	2.16	0.54
3:I:64:ARG:HB3	3:I:80:PRO:HD2	1.89	0.54
2:B:125:LYS:HG3	2:B:153:TYR:HA	1.90	0.54
2:B:144:ALA:N	2:B:192:VAL:O	2.37	0.54
2:B:173:THR:OG1	3:C:175:TYR:CE2	2.61	0.54
2:E:26:PHE:C	2:E:28:PHE:N	2.64	0.54
3:F:93:GLN:O	3:F:94:THR:OG1	2.20	0.54
3:L:183:LEU:O	3:L:186:TYR:HB2	2.08	0.54
1:G:227:MET:HE3	1:G:229:TYR:HE1	1.74	0.53
2:H:28:PHE:H	2:H:76:LYS:HE3	1.72	0.53
3:L:153:ASP:HB2	3:L:189:HIS:HE1	1.73	0.53
2:B:18:ARG:HD2	2:B:18:ARG:N	2.24	0.53
2:E:60:ARG:HE	3:F:98:PRO:CB	2.21	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:29:SER:HB2	3:I:34:ASN:H	1.73	0.53
1:J:133:THR:HG23	1:J:135:ALA:H	1.73	0.53
1:J:240:ILE:HG12	1:J:241:THR:H	1.73	0.53
1:A:91:TYR:HD2	1:A:227:MET:HE2	1.73	0.53
1:A:221:ARG:O	1:A:223:GLN:HG2	2.07	0.53
2:B:96:ALA:HB2	2:B:111:TRP:HB3	1.91	0.53
2:B:190:VAL:HG22	2:B:191:THR:N	2.23	0.53
2:E:38:GLN:O	2:E:91:ALA:HB1	2.09	0.53
3:F:163:ASN:HB3	3:F:179:SER:H	1.72	0.53
1:G:115:GLU:H	3:I:96:GLU:CG	2.19	0.53
2:K:204:CYS:SG	2:K:205:ASN:N	2.81	0.53
2:B:48:SER:OG	2:B:69:ILE:HG21	2.07	0.53
2:B:205:ASN:HA	2:B:216:ASP:HB3	1.90	0.53
1:J:153:LYS:HD2	1:J:156:ASN:HA	1.90	0.53
2:B:109:ASP:OD1	2:B:109:ASP:N	2.30	0.53
3:C:126:GLU:OE1	3:C:126:GLU:N	2.35	0.53
2:E:32:ASP:HB3	2:E:51:LEU:HA	1.91	0.53
2:H:106:TYR:HD1	2:H:107:ALA:HB3	1.73	0.53
2:H:143:THR:OG1	2:H:193:PRO:HA	2.08	0.53
2:H:207:ASN:HD21	2:H:214:LYS:HB3	1.73	0.53
2:K:47:VAL:O	2:K:47:VAL:HG12	2.08	0.53
2:K:202:TYR:O	2:K:218:LYS:HG2	2.08	0.53
3:L:4:THR:O	3:L:5:GLN:HB3	2.08	0.53
1:D:147:ASN:HA	1:D:253:TYR:HB2	1.90	0.53
1:D:184:THR:OG1	1:D:186:ALA:N	2.32	0.53
2:E:106:TYR:CD2	2:E:107:ALA:N	2.76	0.53
1:G:171:LYS:HE3	1:G:258:GLU:HB2	1.91	0.53
2:H:178:LEU:O	2:H:180:SER:N	2.42	0.53
2:K:71:ARG:HD3	2:K:73:ASN:OD1	2.09	0.53
2:K:218:LYS:NZ	2:K:218:LYS:HB3	2.24	0.53
3:L:116:PRO:HB2	3:L:139:LEU:HB3	1.89	0.53
1:A:170:GLY:O	1:A:171:LYS:HG2	2.08	0.53
3:F:73:ASP:C	3:F:74:PHE:HD1	2.16	0.53
1:G:169:LYS:HG2	2:H:103:TYR:HB3	1.89	0.53
1:J:161:LEU:O	1:J:243:GLU:HA	2.08	0.53
3:L:172:ASP:OD1	3:L:174:THR:N	2.39	0.53
2:B:142:ALA:O	2:B:194:SER:HB2	2.09	0.53
3:C:191:SER:HA	3:C:207:LYS:HG2	1.91	0.53
1:D:177:TRP:HB3	1:D:251:PRO:HD3	1.91	0.53
2:E:106:TYR:CE2	3:F:52:TYR:HB2	2.44	0.53
3:F:17:ARG:HB2	3:F:79:ASN:HA	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:183:SER:HB2	1:G:224:GLU:HB2	1.90	0.53
2:H:63:VAL:HG13	2:H:67:PHE:HB2	1.91	0.53
1:J:133:THR:HG23	1:J:136:CYS:H	1.74	0.53
3:L:164:SER:HA	3:L:177:MET:O	2.08	0.53
1:D:57:ILE:N	1:D:81:GLU:OE1	2.32	0.53
2:E:180:SER:C	2:E:182:GLY:H	2.15	0.53
3:F:209:PHE:CG	3:F:210:ASN:N	2.77	0.53
3:I:136:VAL:HG12	3:I:179:SER:HB3	1.91	0.53
3:I:143:TYR:H	3:I:198:HIS:CE1	2.21	0.53
2:E:51:LEU:HD13	2:E:52:GLY:N	2.24	0.53
2:E:207:ASN:OD1	2:E:214:LYS:HB3	2.09	0.53
3:F:82:GLU:O	3:F:85:ASP:HB2	2.09	0.53
1:G:72:THR:HG22	3:I:31:TYR:CG	2.44	0.53
2:H:40:PRO:O	2:H:42:LYS:N	2.41	0.53
2:H:110:TYR:O	2:H:110:TYR:CD1	2.61	0.53
3:I:23:ARG:NH2	2:K:75:ARG:HH11	2.07	0.53
3:I:191:SER:HA	3:I:207:LYS:CE	2.39	0.53
1:J:91:TYR:OH	1:J:180:HIS:NE2	2.28	0.53
2:K:39:ALA:N	2:K:43:GLY:HA2	2.24	0.53
1:A:217:ARG:HG2	1:A:226:ARG:HG3	1.91	0.52
2:B:4:GLN:HE22	2:B:110:TYR:HE1	1.56	0.52
1:D:58:ALA:O	1:D:62:LEU:HD12	2.08	0.52
3:F:156:GLU:CD	3:F:188:ARG:HD3	2.33	0.52
3:F:157:ARG:CB	3:F:159:ASN:H	2.21	0.52
3:F:159:ASN:C	3:F:161:VAL:H	2.16	0.52
3:F:184:ASP:HB3	3:F:186:TYR:CD1	2.45	0.52
1:J:191:LEU:HB3	1:J:192:TYR:CD1	2.44	0.52
1:A:173:VAL:HG12	1:A:234:VAL:HG13	1.91	0.52
3:F:27:SER:HA	3:F:72:THR:HG22	1.90	0.52
3:I:7:PRO:HD2	3:I:21:THR:O	2.08	0.52
2:K:39:ALA:H	2:K:43:GLY:HA2	1.73	0.52
3:L:14:PRO:HD3	3:L:110:LYS:O	2.09	0.52
3:C:1:ILE:O	3:C:100:THR:HG21	2.09	0.52
3:C:13:SER:C	3:C:15:GLY:H	2.17	0.52
3:C:146:ILE:HG13	3:C:198:HIS:CD2	2.45	0.52
3:F:124:SER:OG	3:F:126:GLU:OE1	2.27	0.52
1:G:165:TYR:O	1:G:239:LYS:HA	2.09	0.52
3:I:167:ASP:OD1	3:I:167:ASP:N	2.41	0.52
1:A:165:TYR:HD1	1:A:165:TYR:C	2.18	0.52
1:A:175:VAL:HG13	1:A:232:THR:HG23	1.90	0.52
2:B:4:GLN:NE2	2:B:110:TYR:HE1	2.07	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:167:ASP:OD2	3:C:174:THR:OG1	2.24	0.52
1:D:91:TYR:CD1	1:D:92:PRO:HD2	2.45	0.52
1:G:62:LEU:O	1:G:145:TYR:HB3	2.09	0.52
2:H:38:GLN:O	2:H:91:ALA:HB1	2.10	0.52
2:H:130:PHE:HB2	2:H:149:LEU:HB3	1.92	0.52
1:J:146:LYS:HD3	1:J:252:ARG:NH2	2.24	0.52
1:A:219:LYS:NZ	1:A:222:ASP:HA	2.24	0.52
3:C:207:LYS:HD2	3:C:208:SER:N	2.23	0.52
2:E:109:ASP:O	2:E:110:TYR:HD1	1.92	0.52
1:A:112:GLU:O	1:A:255:PHE:HA	2.10	0.52
1:A:112:GLU:OE1	2:B:104:THR:OG1	2.23	0.52
1:A:165:TYR:C	1:A:165:TYR:CD1	2.88	0.52
1:A:203:SER:HB3	1:A:206:TYR:N	2.24	0.52
1:D:101:LEU:HB2	1:D:231:TRP:HE1	1.73	0.52
2:E:60:ARG:NH2	3:F:98:PRO:HB2	2.22	0.52
1:J:87:ASN:HA	1:J:221:ARG:HH21	1.75	0.52
3:L:23:ARG:HD3	3:L:24:ALA:N	2.25	0.52
2:B:82:MET:HE3	2:B:85:LEU:HD21	1.90	0.52
3:C:115:ALA:HB1	3:C:116:PRO:C	2.35	0.52
1:D:170:GLY:O	1:D:171:LYS:HB2	2.08	0.52
3:F:16:GLN:O	3:F:81:VAL:HB	2.09	0.52
2:B:127:PRO:HB3	2:B:153:TYR:HB3	1.92	0.52
1:G:91:TYR:HE2	1:G:180:HIS:HD2	1.57	0.52
2:K:178:LEU:HB3	2:K:183:LEU:CD1	2.40	0.52
3:F:182:THR:HG21	3:F:187:GLU:HG3	1.91	0.52
2:H:2:LYS:O	2:H:110:TYR:HE2	1.92	0.52
1:J:54:LYS:HD2	1:J:66:GLU:HB2	1.91	0.52
1:J:95:PHE:HD1	1:J:229:TYR:HB2	1.75	0.52
1:J:177:TRP:HZ3	1:J:232:THR:HG22	1.74	0.52
3:C:2:GLN:HG2	3:C:97:VAL:HG11	1.92	0.52
3:C:16:GLN:HA	3:C:81:VAL:H	1.75	0.52
1:G:107:SER:HB3	1:G:260:ASN:OD1	2.10	0.52
1:A:73:ALA:HA	3:C:31:TYR:C	2.35	0.51
2:B:159:THR:O	2:B:206:VAL:HA	2.10	0.51
3:C:120:ILE:HG12	3:C:121:PHE:H	1.75	0.51
3:C:158:GLN:O	3:C:159:ASN:HB2	2.10	0.51
1:D:65:PRO:HG2	1:D:136:CYS:HB3	1.91	0.51
2:E:15:GLY:O	2:E:85:LEU:HD12	2.10	0.51
2:E:63:VAL:CG1	2:E:67:PHE:HB2	2.41	0.51
1:G:51:HIS:ND1	1:G:51:HIS:N	2.57	0.51
3:I:142:PHE:O	3:I:173:SER:HB3	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:172:HIS:N	2:E:172:HIS:CD2	2.77	0.51
1:G:169:LYS:HG2	2:H:103:TYR:HD2	1.76	0.51
1:J:135:ALA:O	1:J:137:PRO:HD3	2.10	0.51
3:C:36:ILE:HB	3:C:74:PHE:CD2	2.44	0.51
2:E:162:TRP:O	2:E:163:ASN:HB2	2.08	0.51
3:F:118:VAL:HB	3:F:205:ILE:HD13	1.92	0.51
1:G:182:PRO:HG2	1:G:188:GLN:HB2	1.91	0.51
2:H:208:HIS:CD2	2:H:210:PRO:HG2	2.46	0.51
2:K:86:ARG:HD2	2:K:88:GLU:OE2	2.11	0.51
1:A:183:SER:OG	1:A:184:THR:HG23	2.10	0.51
3:F:156:GLU:OE1	3:F:188:ARG:NH1	2.43	0.51
2:H:130:PHE:CE2	3:I:127:GLN:HG3	2.46	0.51
2:K:130:PHE:CE2	3:L:127:GLN:HG3	2.45	0.51
2:B:34:SER:OG	2:B:48:SER:O	2.24	0.51
1:D:232:THR:OG1	1:D:233:LEU:N	2.44	0.51
3:F:5:GLN:O	3:F:7:PRO:HD3	2.10	0.51
3:F:19:THR:HG22	3:F:77:THR:OG1	2.11	0.51
3:F:182:THR:OG1	3:F:183:LEU:N	2.40	0.51
1:J:250:VAL:HG22	1:J:251:PRO:HD2	1.93	0.51
2:H:37:ARG:HH11	2:H:47:VAL:HG23	1.76	0.51
2:B:37:ARG:HB3	2:B:93:TYR:CE2	2.46	0.51
3:C:110:LYS:HD2	3:C:143:TYR:OH	2.10	0.51
1:D:91:TYR:CE2	1:D:227:MET:HB2	2.46	0.51
1:G:109:SER:HB3	1:G:258:GLU:HB3	1.93	0.51
2:H:175:PRO:HB2	2:H:184:TYR:HD2	1.76	0.51
1:J:147:ASN:HA	1:J:253:TYR:HB2	1.93	0.51
2:B:44:LEU:HG	2:B:45:GLU:HB3	1.92	0.51
3:C:19:THR:OG1	3:C:19:THR:O	2.27	0.51
1:D:49:PRO:N	1:D:77:SER:H	2.09	0.51
1:D:113:ARG:NH1	3:F:30:ASN:OD1	2.44	0.51
2:E:106:TYR:CG	2:E:107:ALA:N	2.79	0.51
1:G:163:LYS:HA	2:H:56:ARG:NH2	2.26	0.51
3:I:172:ASP:CG	3:I:173:SER:H	2.11	0.51
3:L:209:PHE:HD1	3:L:209:PHE:H	1.59	0.51
3:L:52:TYR:CZ	3:L:56:ASN:HB2	2.45	0.51
2:B:146:LEU:HD22	2:B:202:TYR:HD2	1.76	0.51
3:C:31:TYR:O	3:C:33:ILE:HG12	2.10	0.51
3:C:92:GLN:HB3	3:C:93:GLN:OE1	2.10	0.51
2:E:151:LYS:HD3	2:E:152:ASP:N	2.26	0.51
2:E:199:THR:HG23	2:E:200:GLN:H	1.76	0.51
1:J:180:HIS:CD2	1:J:227:MET:HG3	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:GLU:CD	1:A:118:PRO:HB3	2.35	0.50
1:A:163:LYS:HG3	1:A:164:SER:N	2.26	0.50
2:B:34:SER:HB2	2:B:98:HIS:HE1	1.76	0.50
2:B:132:LEU:HD11	3:C:136:VAL:HG21	1.92	0.50
1:J:153:LYS:HD3	1:J:193:GLN:HB2	1.92	0.50
2:B:31:TYR:O	2:B:71:ARG:NH2	2.44	0.50
2:E:205:ASN:HA	2:E:216:ASP:HA	1.91	0.50
2:H:51:LEU:HD22	2:H:56:ARG:HB2	1.92	0.50
2:H:101:PRO:C	2:H:103:TYR:H	2.20	0.50
2:H:129:VAL:HA	2:H:149:LEU:O	2.10	0.50
1:D:147:ASN:O	1:D:252:ARG:N	2.33	0.50
2:E:26:PHE:O	2:E:28:PHE:N	2.44	0.50
2:K:50:ILE:HG22	2:K:57:SER:HB3	1.92	0.50
3:C:110:LYS:HA	3:C:143:TYR:OH	2.11	0.50
2:E:69:ILE:HD11	2:E:78:LEU:HD11	1.92	0.50
2:E:172:HIS:CD2	2:E:172:HIS:H	2.29	0.50
3:C:161:VAL:O	3:C:163:ASN:ND2	2.45	0.50
1:D:50:LEU:HD13	1:D:76:TRP:CE2	2.47	0.50
2:E:21:CYS:N	2:E:78:LEU:O	2.45	0.50
2:E:122:ALA:HB3	2:E:154:PHE:CE2	2.47	0.50
2:E:161:SER:HB3	2:E:205:ASN:ND2	2.27	0.50
3:F:175:TYR:CZ	3:F:177:MET:HB3	2.46	0.50
1:G:152:VAL:HG23	1:G:153:LYS:N	2.26	0.50
2:H:75:ARG:HB2	2:H:77:THR:HG22	1.93	0.50
3:I:38:TRP:CD1	3:I:76:LEU:HD23	2.47	0.50
1:J:179:ILE:HD11	1:J:199:VAL:HG11	1.93	0.50
2:K:97:ARG:HB3	2:K:109:ASP:CG	2.36	0.50
3:L:186:TYR:C	3:L:187:GLU:HG3	2.36	0.50
1:A:91:TYR:CD2	1:A:227:MET:HE2	2.46	0.50
2:E:153:TYR:CZ	2:E:158:VAL:HB	2.46	0.50
2:H:16:SER:O	2:H:18:ARG:NH1	2.45	0.50
1:A:76:TRP:CE2	1:A:108:VAL:HG11	2.46	0.50
1:A:217:ARG:O	1:A:224:GLU:HG2	2.12	0.50
1:A:232:THR:OG1	1:A:233:LEU:N	2.43	0.50
3:F:33:ILE:HG23	3:F:34:ASN:N	2.27	0.50
3:F:40:GLN:O	3:F:47:PRO:HA	2.12	0.50
1:A:177:TRP:HZ3	1:A:232:THR:HG22	1.77	0.50
2:B:134:PRO:O	2:B:222:ALA:HB3	2.11	0.50
1:J:86:ASP:O	1:J:221:ARG:NH2	2.45	0.50
1:A:179:ILE:O	1:A:228:ASN:N	2.38	0.50
2:B:46:TRP:HE1	2:B:48:SER:C	2.20	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:180:SER:O	2:B:182:GLY:N	2.45	0.50
1:D:127:ASP:OD2	1:D:130:LYS:HG3	2.11	0.50
2:E:7:GLY:CA	2:E:115:THR:HG21	2.35	0.50
3:F:93:GLN:HA	3:F:100:THR:O	2.12	0.50
1:G:174:LEU:N	1:G:255:PHE:O	2.43	0.50
1:G:203:SER:OG	1:G:204:SER:N	2.43	0.50
3:L:165:TRP:HE3	3:L:166:THR:H	1.59	0.50
1:A:153:LYS:HE2	1:A:153:LYS:HA	1.93	0.49
1:A:153:LYS:HD3	1:A:157:SER:C	2.37	0.49
2:B:90:THR:HG23	2:B:119:VAL:H	1.77	0.49
3:C:17:ARG:NH2	3:C:19:THR:HG23	2.23	0.49
3:C:76:LEU:HD13	3:C:77:THR:N	2.27	0.49
3:C:89:TYR:O	3:C:104:GLY:HA2	2.11	0.49
3:F:5:GLN:HE21	3:F:23:ARG:HG2	1.76	0.49
1:J:216:ILE:HG23	1:J:224:GLU:CG	2.41	0.49
1:A:93:GLY:HA3	1:A:227:MET:O	2.12	0.49
1:A:153:LYS:HE3	1:A:158:TYR:HA	1.93	0.49
2:B:82:MET:HE1	2:B:117:VAL:HG11	1.94	0.49
3:C:152:ILE:HG13	3:C:154:GLY:H	1.76	0.49
1:J:160:LYS:HA	1:J:244:ALA:O	2.12	0.49
2:K:193:PRO:O	2:K:196:SER:OG	2.29	0.49
3:C:10:LEU:HG	3:C:11:ALA:H	1.77	0.49
1:D:260:ASN:OD1	1:D:260:ASN:N	2.46	0.49
1:G:115:GLU:HB3	3:I:96:GLU:CB	2.24	0.49
3:L:168:GLN:HG3	3:L:169:ASP:H	1.77	0.49
3:L:209:PHE:CD1	3:L:209:PHE:N	2.80	0.49
1:A:174:LEU:HD21	1:A:231:TRP:CE3	2.47	0.49
1:D:202:GLY:O	1:D:240:ILE:HA	2.11	0.49
3:I:38:TRP:CZ3	3:I:91:CYS:HB3	2.48	0.49
3:L:115:ALA:HB3	3:L:142:PHE:CA	2.41	0.49
3:C:111:ARG:NE	3:C:172:ASP:HA	2.28	0.49
2:E:146:LEU:HD13	2:E:202:TYR:CE2	2.48	0.49
3:F:42:LYS:C	3:F:44:GLY:N	2.70	0.49
1:G:63:GLY:N	1:G:147:ASN:OD1	2.45	0.49
1:G:181:HIS:N	1:G:226:ARG:O	2.43	0.49
3:I:54:ALA:O	3:I:67:GLY:HA3	2.11	0.49
1:J:191:LEU:HB3	1:J:192:TYR:CE1	2.47	0.49
2:K:28:PHE:HE2	2:K:73:ASN:HA	1.78	0.49
2:B:175:PRO:HG3	2:B:186:LEU:HD23	1.94	0.49
3:F:10:LEU:HD22	3:F:11:ALA:H	1.78	0.49
2:H:173:THR:HG22	2:H:174:PHE:N	2.19	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:71:GLY:O	3:I:72:THR:OG1	2.31	0.49
1:G:114:PHE:HZ	1:G:173:VAL:HG13	1.78	0.49
3:I:42:LYS:HG3	3:I:45:GLN:O	2.13	0.49
2:K:6:SER:OG	2:K:113:GLN:OE1	2.24	0.49
2:K:146:LEU:HA	3:L:121:PHE:CZ	2.48	0.49
2:K:217:LYS:H	2:K:217:LYS:HZ2	1.61	0.49
3:L:85:ASP:HB2	3:L:109:ILE:HD11	1.93	0.49
1:D:116:ILE:HD11	1:D:165:TYR:CD2	2.48	0.49
1:D:191:LEU:HD23	1:D:192:TYR:CE1	2.48	0.49
2:E:4:GLN:HG2	2:E:95:CYS:SG	2.53	0.49
2:H:162:TRP:C	2:H:164:SER:N	2.71	0.49
2:H:216:ASP:OD1	2:H:217:LYS:N	2.41	0.49
3:I:23:ARG:HD3	3:I:73:ASP:HB3	1.95	0.49
2:K:130:PHE:O	2:K:149:LEU:HB3	2.12	0.49
3:C:115:ALA:HB3	3:C:142:PHE:HA	1.94	0.49
1:D:95:PHE:HE1	1:D:231:TRP:HD1	1.59	0.49
2:E:18:ARG:HG3	2:E:81:GLN:HG2	1.95	0.49
3:F:139:LEU:HD22	3:F:146:ILE:HD13	1.94	0.49
1:G:217:ARG:HB2	1:G:224:GLU:O	2.13	0.49
3:I:38:TRP:CH2	3:I:91:CYS:HB3	2.48	0.49
3:I:120:ILE:HD11	3:I:150:TRP:CZ3	2.48	0.49
1:J:180:HIS:HD2	1:J:227:MET:HG3	1.76	0.49
1:A:421:ILE:O	1:A:423:THR:N	2.46	0.48
2:B:40:PRO:C	2:B:42:LYS:H	2.20	0.48
3:C:120:ILE:HD13	3:C:207:LYS:HA	1.95	0.48
3:F:156:GLU:OE2	3:F:188:ARG:HD3	2.12	0.48
1:J:103:GLU:HG3	1:J:104:GLN:N	2.26	0.48
3:L:93:GLN:HA	3:L:100:THR:O	2.13	0.48
2:E:42:LYS:NZ	3:F:103:GLY:O	2.43	0.48
1:J:194:ASN:ND2	1:J:245:THR:HG22	2.27	0.48
1:D:100:GLU:O	1:D:103:GLU:HB3	2.13	0.48
2:E:60:ARG:HH22	3:F:100:THR:CG2	2.27	0.48
2:H:142:ALA:C	2:H:194:SER:HB3	2.37	0.48
2:K:175:PRO:O	2:K:184:TYR:HD1	1.97	0.48
1:A:70:LEU:HD12	1:A:71:SER:H	1.77	0.48
1:A:149:ILE:HD12	1:A:250:VAL:HG23	1.95	0.48
1:A:172:GLU:N	1:A:257:MET:O	2.38	0.48
2:B:36:ILE:HD11	2:B:108:TRP:CZ3	2.49	0.48
2:B:36:ILE:HG12	3:C:101:PHE:CZ	2.48	0.48
1:D:123:TRP:NE1	1:D:149:ILE:HD13	2.27	0.48
1:G:119:LYS:H	1:G:252:ARG:HH12	1.56	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:34:ASN:O	3:I:53:THR:HA	2.12	0.48
3:I:168:GLN:HG3	3:I:169:ASP:N	2.27	0.48
2:K:41:GLY:O	2:K:42:LYS:HB3	2.12	0.48
3:L:42:LYS:HG2	3:L:87:ALA:HB2	1.94	0.48
3:L:92:GLN:HB3	3:L:93:GLN:OE1	2.13	0.48
3:C:31:TYR:C	3:C:33:ILE:HG12	2.38	0.48
3:C:37:ASN:HA	3:C:52:TYR:HA	1.96	0.48
2:E:108:TRP:HD1	3:F:39:PHE:CZ	2.32	0.48
3:F:41:GLN:C	3:F:87:ALA:HB1	2.37	0.48
1:J:171:LYS:HG3	1:J:257:MET:O	2.13	0.48
3:C:6:SER:HA	3:C:21:THR:O	2.14	0.48
3:C:165:TRP:HA	3:C:165:TRP:CE3	2.48	0.48
2:E:80:LEU:HD23	2:E:82:MET:HG3	1.95	0.48
3:F:37:ASN:H	3:F:92:GLN:HB2	1.77	0.48
2:H:111:TRP:H	2:H:111:TRP:HD1	1.60	0.48
2:K:19:LEU:HD11	2:K:82:MET:SD	2.54	0.48
2:K:28:PHE:HD2	2:K:76:LYS:HD2	1.78	0.48
1:A:211:LYS:HG3	1:A:212:PRO:HD2	1.95	0.48
3:C:12:VAL:O	3:C:109:ILE:HA	2.13	0.48
1:D:50:LEU:HD21	1:D:79:ILE:HG12	1.94	0.48
3:F:27:SER:CA	3:F:72:THR:HG22	2.43	0.48
3:F:91:CYS:HA	3:F:92:GLN:OE1	2.13	0.48
1:G:248:LEU:HG	1:G:250:VAL:HG13	1.95	0.48
2:H:71:ARG:HH11	2:H:73:ASN:ND2	2.11	0.48
1:J:182:PRO:O	1:J:214:ILE:HG22	2.14	0.48
3:L:71:GLY:HA2	3:L:74:PHE:CZ	2.49	0.48
1:A:70:LEU:CG	1:A:71:SER:H	2.27	0.48
1:D:126:HIS:CE1	1:D:161:LEU:HB2	2.47	0.48
2:E:178:LEU:C	2:E:180:SER:H	2.22	0.48
1:J:56[A]:ASN:HD21	1:J:88:GLY:HA3	1.79	0.48
2:K:5:GLN:HG3	2:K:22:ALA:HB3	1.94	0.48
3:C:7:PRO:HD3	3:C:21:THR:H	1.77	0.48
2:E:66:ARG:CZ	2:E:86:ARG:HD3	2.43	0.48
3:F:24:ALA:N	3:F:72:THR:O	2.46	0.48
3:I:23:ARG:HA	3:I:73:ASP:HA	1.94	0.48
1:J:174:LEU:HD11	1:J:176:LEU:HD13	1.96	0.48
3:L:38:TRP:CD2	3:L:76:LEU:HD22	2.49	0.48
1:A:56[B]:ASN:OD1	1:A:56[B]:ASN:N	2.47	0.48
1:A:228:ASN:HB3	1:A:230:TYR:CE1	2.49	0.48
2:E:107:ALA:HB2	3:F:93:GLN:OE1	2.14	0.48
2:H:35:TRP:H	2:H:48:SER:HB3	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:173:THR:C	2:H:174:PHE:CD2	2.92	0.48
1:J:173:VAL:HB	1:J:234:VAL:HG23	1.94	0.48
1:A:96:ILE:HB	1:A:229:TYR:O	2.13	0.47
2:E:158:VAL:HG12	2:E:186:LEU:HD21	1.95	0.47
3:F:170:SER:HB2	3:F:171:LYS:NZ	2.28	0.47
3:F:206:VAL:HB	3:F:207:LYS:HZ2	1.79	0.47
1:G:163:LYS:HA	2:H:56:ARG:HH22	1.79	0.47
3:I:183:LEU:HB2	3:I:186:TYR:HB2	1.95	0.47
2:K:158:VAL:HG13	2:K:208:HIS:CD2	2.49	0.47
3:L:31:TYR:C	3:L:33:ILE:HG12	2.38	0.47
2:H:171:VAL:HG23	3:I:175:TYR:CD2	2.41	0.47
3:I:31:TYR:OH	3:I:71:GLY:N	2.47	0.47
2:K:60:ARG:HD2	2:K:61:ASP:H	1.79	0.47
2:K:96:ALA:HA	2:K:110:TYR:O	2.14	0.47
1:A:91:TYR:CD2	1:A:227:MET:HG3	2.50	0.47
3:C:51:ILE:HD11	3:C:57:LYS:HE3	1.95	0.47
1:D:116:ILE:HG23	1:D:117:PHE:CD2	2.49	0.47
3:F:181:LEU:HG	3:F:182:THR:N	2.29	0.47
1:J:76:TRP:CE2	1:J:108:VAL:HG11	2.49	0.47
3:L:61:VAL:HG13	3:L:62:PRO:HD2	1.96	0.47
3:L:209:PHE:HD1	3:L:209:PHE:N	2.12	0.47
1:A:116:ILE:HG21	1:A:251:PRO:HB2	1.95	0.47
1:A:203:SER:HB3	1:A:206:TYR:O	2.14	0.47
2:E:162:TRP:HD1	2:E:167:LEU:CD1	2.27	0.47
3:F:86:THR:HA	3:F:107:LEU:HD23	1.97	0.47
1:A:103:GLU:O	1:A:106:SER:OG	2.24	0.47
3:C:97:VAL:HG22	3:C:98:PRO:HD2	1.97	0.47
1:G:116:ILE:HD11	1:G:165:TYR:CG	2.48	0.47
3:I:62:PRO:HB2	3:I:64:ARG:HG3	1.96	0.47
3:L:78:ILE:HG13	3:L:79:ASN:O	2.15	0.47
3:C:142:PHE:CD1	3:C:142:PHE:N	2.83	0.47
2:K:60:ARG:NE	3:L:98:PRO:HB2	2.27	0.47
2:K:106:TYR:CZ	3:L:37:ASN:OD1	2.67	0.47
3:L:184:ASP:HB3	3:L:186:TYR:CD1	2.49	0.47
1:A:89:THR:O	1:A:145:TYR:OH	2.33	0.47
2:B:120:SER:OG	2:B:121:SER:N	2.46	0.47
1:D:134:ALA:HA	1:D:142:LYS:HD2	1.95	0.47
1:D:182:PRO:CB	1:D:187:ASP:HB3	2.44	0.47
2:E:177:VAL:HG22	2:E:184:TYR:CD2	2.50	0.47
3:F:11:ALA:HA	3:F:108:GLU:O	2.15	0.47
1:G:163:LYS:O	1:G:242:PHE:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:179:ILE:HG13	1:G:210:PHE:CD2	2.50	0.47
2:H:28:PHE:CE1	2:H:33:MET:HG3	2.50	0.47
2:H:106:TYR:CD1	2:H:107:ALA:HB3	2.50	0.47
2:H:173:THR:C	2:H:174:PHE:CG	2.90	0.47
2:H:177:VAL:HG13	2:H:184:TYR:CZ	2.50	0.47
1:J:67:CYS:O	1:J:69:SER:OG	2.25	0.47
1:J:123:TRP:CE3	1:J:163:LYS:HD2	2.50	0.47
1:J:146:LYS:NZ	1:J:252:ARG:HH22	2.13	0.47
3:L:38:TRP:HA	3:L:92:GLN:OE1	2.15	0.47
3:L:64:ARG:HB2	3:L:78:ILE:HD12	1.95	0.47
2:B:203:ILE:HG22	2:B:216:ASP:HB2	1.96	0.47
2:E:4:GLN:HE22	2:E:97:ARG:HD2	1.80	0.47
1:G:91:TYR:N	1:G:145:TYR:OH	2.48	0.47
2:H:203:ILE:HD12	2:H:203:ILE:H	1.79	0.47
1:J:70:LEU:HD13	1:J:71:SER:H	1.79	0.47
1:A:84:SER:HB2	1:A:87:ASN:CG	2.40	0.47
3:C:145:LYS:HG2	3:C:146:ILE:N	2.30	0.47
1:D:115:GLU:OE1	3:F:96:GLU:HB3	2.15	0.47
2:E:152:ASP:O	2:E:183:LEU:HD22	2.15	0.47
3:F:163:ASN:HB3	3:F:179:SER:O	2.15	0.47
1:J:208:LYS:HG2	1:J:210:PHE:CZ	2.50	0.47
2:K:2:LYS:NZ	2:K:25:GLY:HA3	2.29	0.47
1:A:119:LYS:HB2	1:A:149:ILE:HG12	1.97	0.47
2:B:19:LEU:HD11	2:B:117:VAL:HG21	1.97	0.47
2:B:127:PRO:CA	2:B:153:TYR:HB3	2.45	0.47
1:D:227:MET:SD	1:D:249:VAL:HG21	2.54	0.47
3:F:37:ASN:HB2	3:F:92:GLN:HG2	1.96	0.47
2:H:143:THR:HG23	2:H:192:VAL:O	2.14	0.47
2:H:203:ILE:HA	2:H:218:LYS:HA	1.97	0.47
3:L:36:ILE:HD11	3:L:91:CYS:SG	2.54	0.47
1:A:174:LEU:HD22	1:A:232:THR:O	2.15	0.46
2:B:153:TYR:O	2:B:183:LEU:HA	2.15	0.46
2:E:51:LEU:HD13	2:E:52:GLY:H	1.80	0.46
1:G:50:LEU:HD22	1:G:76:TRP:CG	2.49	0.46
1:G:60:TRP:N	1:G:67:CYS:SG	2.88	0.46
2:H:33:MET:HE1	2:H:97:ARG:HB3	1.97	0.46
3:I:26:GLU:O	3:I:72:THR:HG22	2.15	0.46
1:A:118:PRO:O	1:A:122:SER:OG	2.20	0.46
1:A:153:LYS:HE2	1:A:154:LYS:N	2.26	0.46
1:A:215:ALA:O	1:A:217:ARG:NH1	2.44	0.46
3:C:184:ASP:HB3	3:C:185:GLU:H	1.54	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:144:PHE:CE2	1:D:150:TRP:HB2	2.50	0.46
2:E:60:ARG:HD3	2:E:61:ASP:H	1.80	0.46
3:F:42:LYS:C	3:F:44:GLY:H	2.21	0.46
1:G:164:SER:N	2:H:56:ARG:HH12	2.14	0.46
2:H:6:SER:HA	2:H:20:SER:O	2.15	0.46
1:J:232:THR:OG1	1:J:233:LEU:N	2.47	0.46
3:L:124:SER:OG	3:L:126:GLU:HG2	2.15	0.46
1:A:192:TYR:CD1	1:A:192:TYR:N	2.83	0.46
3:C:172:ASP:CG	3:C:173:SER:N	2.70	0.46
2:H:11:VAL:HG12	2:H:12:GLN:O	2.14	0.46
2:H:36:ILE:HD13	3:I:101:PHE:CZ	2.50	0.46
1:J:257:MET:HE2	1:J:257:MET:HB2	1.75	0.46
2:K:101:PRO:C	2:K:103:TYR:N	2.72	0.46
1:A:123:TRP:CZ2	1:A:250:VAL:HG21	2.51	0.46
3:C:206:VAL:HG12	3:C:207:LYS:HE2	1.97	0.46
1:D:91:TYR:HD2	1:D:227:MET:HE2	1.80	0.46
3:I:57:LYS:NZ	3:I:62:PRO:O	2.41	0.46
1:J:133:THR:HG23	1:J:135:ALA:N	2.30	0.46
1:A:248:LEU:HG	1:A:250:VAL:HG12	1.96	0.46
2:B:162:TRP:NE1	2:B:170:SER:HG	2.11	0.46
1:D:107:SER:HB3	1:D:262:GLY:O	2.15	0.46
2:E:178:LEU:C	2:E:180:SER:N	2.74	0.46
1:A:56[B]:ASN:OD1	1:A:84:SER:OG	2.28	0.46
1:A:112:GLU:OE1	2:B:103:TYR:HB2	2.16	0.46
3:C:35:PHE:CD2	3:C:95:LYS:HG2	2.51	0.46
3:C:35:PHE:CG	3:C:95:LYS:HA	2.50	0.46
1:D:158:TYR:CD1	1:D:158:TYR:C	2.94	0.46
3:I:157:ARG:HG3	3:I:159:ASN:N	2.30	0.46
2:K:67:PHE:CD1	2:K:82:MET:HA	2.50	0.46
2:K:209:LYS:N	2:K:210:PRO:HD2	2.31	0.46
3:C:133:ALA:O	3:C:181:LEU:HD12	2.15	0.46
2:E:37:ARG:HA	2:E:92:VAL:O	2.15	0.46
2:E:203:ILE:O	2:E:204:CYS:SG	2.73	0.46
3:F:208:SER:O	3:F:209:PHE:HD1	1.99	0.46
1:G:172:GLU:HG2	1:G:235:GLU:OE1	2.16	0.46
2:H:46:TRP:O	2:H:60:ARG:NH2	2.48	0.46
3:L:1:ILE:O	3:L:2:GLN:HG3	2.15	0.46
3:L:28:VAL:HG12	3:L:35:PHE:HB2	1.97	0.46
2:B:150:VAL:HB	2:B:186:LEU:HD12	1.97	0.46
3:F:92:GLN:O	3:F:94:THR:N	2.42	0.46
2:H:187:SER:OG	3:I:177:MET:SD	2.73	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:142:PHE:H	3:I:142:PHE:HD1	1.64	0.46
3:I:151:LYS:CB	3:I:193:THR:HB	2.36	0.46
3:L:12:VAL:HG11	3:L:18:ALA:HB2	1.98	0.46
3:L:23:ARG:HA	3:L:72:THR:O	2.15	0.46
1:A:263:SER:OG	1:A:264:GLY:N	2.45	0.46
3:C:40:GLN:HB2	3:C:89:TYR:CD2	2.51	0.46
1:D:152:VAL:HG23	1:D:153:LYS:H	1.81	0.46
2:E:146:LEU:HD22	2:E:202:TYR:HE2	1.81	0.46
3:F:31:TYR:C	3:F:33:ILE:N	2.73	0.46
3:I:53:THR:O	3:I:55:SER:N	2.40	0.46
3:I:142:PHE:CE2	3:I:146:ILE:HB	2.50	0.46
1:J:132:VAL:HB	1:J:142:LYS:C	2.41	0.46
2:H:113:GLN:OE1	3:I:45:GLN:HB3	2.16	0.46
2:H:207:ASN:OD1	2:H:214:LYS:HA	2.15	0.46
1:J:77:SER:O	1:J:106:SER:HA	2.16	0.46
1:J:133:THR:CG2	1:J:136:CYS:H	2.28	0.46
2:K:11:VAL:HG21	2:K:85:LEU:HD13	1.98	0.46
1:A:90:CYS:O	1:A:221:ARG:NH1	2.49	0.45
1:A:187:ASP:O	1:A:191:LEU:HD13	2.16	0.45
3:C:92:GLN:C	3:C:94:THR:N	2.73	0.45
3:C:142:PHE:O	3:C:173:SER:HB3	2.16	0.45
2:E:173:THR:OG1	2:E:186:LEU:HD13	2.17	0.45
2:E:206:VAL:N	2:E:215:VAL:O	2.48	0.45
3:F:12:VAL:HG22	3:F:81:VAL:HG11	1.98	0.45
2:H:10:VAL:HB	2:H:118:THR:HG23	1.98	0.45
2:H:174:PHE:CD1	3:I:165:TRP:HB3	2.51	0.45
1:J:108:VAL:HG23	1:J:110:SER:O	2.16	0.45
2:K:37:ARG:HD3	2:K:93:TYR:CE2	2.51	0.45
2:B:106:TYR:CD1	2:B:107:ALA:HB3	2.51	0.45
2:B:189:VAL:HB	3:C:138:PHE:CE2	2.52	0.45
2:B:205:ASN:OD1	2:B:205:ASN:N	2.49	0.45
3:C:207:LYS:H	3:C:207:LYS:HG3	1.32	0.45
1:D:72:THR:O	1:D:72:THR:OG1	2.28	0.45
1:D:180:HIS:CD2	1:D:182:PRO:HG3	2.52	0.45
3:I:185:GLU:C	3:I:187:GLU:H	2.23	0.45
2:K:194:SER:C	2:K:196:SER:H	2.23	0.45
1:A:178:GLY:O	1:A:179:ILE:HD12	2.17	0.45
1:D:144:PHE:CG	1:D:145:TYR:N	2.84	0.45
3:F:163:ASN:ND2	3:F:179:SER:O	2.50	0.45
1:G:166:ILE:HD11	1:G:239:LYS:HD3	1.99	0.45
3:I:81:VAL:HG13	3:I:85:ASP:OD2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:56[A]:ASN:ND2	1:J:58:ALA:HB3	2.31	0.45
3:L:9:SER:HB3	3:L:106:LYS:H	1.80	0.45
1:J:245:THR:HG22	1:J:245:THR:O	2.15	0.45
2:K:100:SER:HA	2:K:105:LEU:H	1.81	0.45
2:K:186:LEU:HG	2:K:187:SER:H	1.80	0.45
2:B:130:PHE:HD2	2:B:149:LEU:HD23	1.80	0.45
1:D:126:HIS:CD2	1:D:159:PRO:HD2	2.52	0.45
1:D:234:VAL:HG23	1:D:238:ASP:OD1	2.17	0.45
2:E:29:SER:OG	2:E:73:ASN:ND2	2.50	0.45
1:G:173:VAL:HB	1:G:234:VAL:HG13	1.99	0.45
3:I:52:TYR:O	3:I:56:ASN:HB2	2.16	0.45
2:K:38:GLN:O	2:K:91:ALA:HB1	2.17	0.45
2:K:158:VAL:HA	2:K:207:ASN:O	2.17	0.45
1:A:174:LEU:CD2	1:A:233:LEU:HD22	2.46	0.45
2:E:75:ARG:H	2:E:75:ARG:HG2	1.53	0.45
2:E:173:THR:HG23	3:F:175:TYR:OH	2.16	0.45
3:F:49:LEU:HD11	3:F:52:TYR:HB3	1.99	0.45
3:F:126:GLU:CD	3:F:126:GLU:N	2.72	0.45
3:I:17:ARG:HA	3:I:79:ASN:HA	1.99	0.45
3:I:184:ASP:CG	3:I:185:GLU:H	2.24	0.45
1:J:57:ILE:HG12	1:J:79:ILE:HG21	1.99	0.45
1:J:177:TRP:CE2	1:J:230:TYR:HB2	2.51	0.45
1:A:91:TYR:HE2	1:A:180:HIS:CD2	2.35	0.45
2:B:35:TRP:NE1	2:B:78:LEU:HD11	2.31	0.45
2:B:199:THR:HG23	2:B:200:GLN:H	1.82	0.45
3:C:17:ARG:HH22	3:C:19:THR:CG2	2.25	0.45
1:G:95:PHE:HD1	1:G:98:TYR:HB2	1.82	0.45
2:H:142:ALA:O	2:H:194:SER:HB3	2.17	0.45
2:H:143:THR:CG2	2:H:191:THR:HG22	2.46	0.45
3:I:202:THR:OG1	3:I:204:PRO:HD3	2.16	0.45
1:J:61:ILE:HD13	1:J:61:ILE:O	2.16	0.45
2:B:154:PHE:HA	2:B:155:PRO:HA	1.68	0.45
3:C:39:PHE:HD2	3:C:92:GLN:CG	2.29	0.45
1:D:93:GLY:HA3	1:D:227:MET:O	2.17	0.45
1:D:158:TYR:C	1:D:158:TYR:HD1	2.25	0.45
2:E:18:ARG:HG3	2:E:81:GLN:HA	1.97	0.45
2:E:67:PHE:CE1	2:E:82:MET:HG2	2.52	0.45
1:G:112:GLU:OE1	2:H:103:TYR:HD1	2.00	0.45
1:J:73:ALA:O	1:J:74:SER:HB3	2.17	0.45
3:L:111:ARG:HD2	3:L:143:TYR:CG	2.52	0.45
1:A:174:LEU:HD22	1:A:174:LEU:HA	1.74	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:217:LYS:HZ2	2:E:217:LYS:N	2.12	0.45
1:G:170:GLY:HA2	1:G:236:PRO:HG3	1.98	0.45
2:H:80:LEU:C	2:H:80:LEU:HD13	2.41	0.45
3:I:115:ALA:HB1	3:I:116:PRO:CA	2.43	0.45
1:J:158:TYR:CE2	1:J:192:TYR:HD2	2.35	0.45
3:L:46:PRO:HA	3:L:47:PRO:HD3	1.50	0.45
3:C:69:GLY:O	3:C:74:PHE:HE1	2.00	0.45
3:F:207:LYS:HE3	3:F:207:LYS:HB3	1.56	0.45
2:K:37:ARG:HD3	2:K:93:TYR:CZ	2.52	0.45
3:L:39:PHE:H	3:L:92:GLN:NE2	2.14	0.45
3:L:161:VAL:HG11	3:L:180:THR:HA	1.99	0.45
3:C:57:LYS:HE2	3:C:65:PHE:HB2	1.99	0.44
1:D:89:THR:HG22	1:D:92:PRO:HA	1.99	0.44
2:E:146:LEU:CB	2:E:202:TYR:OH	2.64	0.44
3:F:205:ILE:HD12	3:F:205:ILE:N	2.32	0.44
1:G:54:LYS:HB3	1:G:55:CYS:SG	2.57	0.44
2:K:8:GLY:HA2	2:K:17:LEU:HD21	1.98	0.44
2:K:9:GLY:H	2:K:17:LEU:HD11	1.82	0.44
3:L:38:TRP:CG	3:L:76:LEU:HD22	2.52	0.44
2:E:42:LYS:HE2	2:E:43:GLY:N	2.33	0.44
2:E:162:TRP:H	2:E:167:LEU:CD1	2.30	0.44
1:G:91:TYR:HH	1:G:180:HIS:CD2	2.31	0.44
2:H:30:ASP:OD1	2:H:30:ASP:C	2.59	0.44
3:L:172:ASP:OD1	3:L:173:SER:N	2.50	0.44
1:A:147:ASN:O	1:A:148:LEU:HD13	2.16	0.44
3:C:88:ASN:HA	3:C:105:THR:O	2.17	0.44
2:E:18:ARG:HH11	2:E:18:ARG:HB2	1.82	0.44
3:I:42:LYS:HD2	3:I:45:GLN:HB2	1.97	0.44
3:I:53:THR:O	3:I:53:THR:HG22	2.17	0.44
3:I:157:ARG:CG	3:I:159:ASN:H	2.29	0.44
3:L:202:THR:HG22	3:L:203:SER:N	2.33	0.44
1:D:215:ALA:O	1:D:217:ARG:HD2	2.18	0.44
3:F:157:ARG:HB3	3:F:159:ASN:N	2.25	0.44
1:J:52:LEU:HD23	1:J:52:LEU:H	1.81	0.44
1:J:98:TYR:O	1:J:102:ARG:HB3	2.18	0.44
2:K:19:LEU:HD12	2:K:19:LEU:N	2.32	0.44
2:K:63:VAL:CG2	2:K:66:ARG:HH22	2.29	0.44
2:K:163:ASN:HB3	2:K:164:SER:H	1.49	0.44
3:L:146:ILE:HD13	3:L:198:HIS:HB2	2.00	0.44
3:L:187:GLU:HB2	3:L:188:ARG:H	1.55	0.44
1:A:71:SER:O	3:C:31:TYR:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:ARG:HB3	1:A:218:PRO:HD2	1.99	0.44
2:B:39:ALA:H	2:B:43:GLY:HA2	1.82	0.44
2:B:50:ILE:HD13	2:B:51:LEU:O	2.16	0.44
3:C:138:PHE:CD1	3:C:175:TYR:HE1	2.35	0.44
3:C:207:LYS:HZ1	3:C:209:PHE:HE2	1.65	0.44
2:E:146:LEU:HD13	2:E:202:TYR:CZ	2.52	0.44
2:E:146:LEU:HB3	2:E:202:TYR:OH	2.17	0.44
3:F:96:GLU:C	3:F:97:VAL:HG22	2.41	0.44
3:F:145:LYS:HA	3:F:145:LYS:HZ3	1.83	0.44
3:F:185:GLU:O	3:F:186:TYR:HD1	2.00	0.44
1:G:56[A]:ASN:HA	1:G:81:GLU:HG2	2.00	0.44
2:H:174:PHE:HE2	3:I:167:ASP:HB3	1.72	0.44
3:I:33:ILE:O	3:I:53:THR:HG23	2.16	0.44
1:J:221:ARG:HH11	1:J:221:ARG:CB	2.25	0.44
2:K:130:PHE:HA	2:K:131:PRO:HD2	1.73	0.44
3:L:152:ILE:O	3:L:189:HIS:CE1	2.71	0.44
3:L:199:LYS:O	3:L:200:THR:HG23	2.18	0.44
1:D:95:PHE:HE1	1:D:231:TRP:CD1	2.36	0.44
2:E:63:VAL:HG13	2:E:67:PHE:HB2	1.98	0.44
1:G:200:PHE:HD1	1:G:201:VAL:N	2.15	0.44
3:I:45:GLN:CB	3:I:46:PRO:HD3	2.48	0.44
3:I:172:ASP:CG	3:I:173:SER:N	2.71	0.44
1:J:115:GLU:OE1	3:L:96:GLU:HG3	2.17	0.44
3:L:85:ASP:O	3:L:86:THR:C	2.61	0.44
2:B:36:ILE:HG13	2:B:46:TRP:HA	1.99	0.44
3:C:142:PHE:CE2	3:C:145:LYS:HA	2.53	0.44
1:D:119:LYS:HA	1:D:149:ILE:HD11	1.99	0.44
2:E:39:ALA:HB3	2:E:43:GLY:N	2.32	0.44
2:E:45:GLU:OE2	3:F:99:TYR:O	2.35	0.44
3:F:192:TYR:O	3:F:207:LYS:HA	2.18	0.44
1:G:50:LEU:HD23	1:G:50:LEU:H	1.83	0.44
3:I:123:PRO:HD3	3:I:135:VAL:HG22	1.98	0.44
2:K:11:VAL:N	2:K:118:THR:O	2.38	0.44
2:K:37:ARG:CD	2:K:93:TYR:CZ	3.01	0.44
1:A:50:LEU:H	1:A:76:TRP:HB2	1.82	0.44
3:C:13:SER:C	3:C:15:GLY:N	2.75	0.44
3:C:16:GLN:CG	3:C:17:ARG:H	2.28	0.44
1:D:183:SER:HA	1:D:215:ALA:O	2.18	0.44
2:E:60:ARG:HH21	3:F:98:PRO:C	2.25	0.44
2:E:146:LEU:HD22	2:E:202:TYR:CE2	2.52	0.44
2:E:170:SER:HA	2:E:189:VAL:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:35:PHE:HB3	3:F:95:LYS:HA	2.00	0.44
3:I:184:ASP:C	3:I:186:TYR:H	2.25	0.44
2:K:104:THR:HG22	2:K:106:TYR:HB2	1.98	0.44
1:D:153:LYS:HE2	1:D:157:SER:C	2.43	0.44
2:E:29:SER:HA	2:E:73:ASN:OD1	2.18	0.44
2:E:36:ILE:HG21	2:E:111:TRP:CZ3	2.52	0.44
3:F:151:LYS:O	3:F:193:THR:N	2.50	0.44
1:G:56[B]:ASN:HA	1:G:81:GLU:HG2	2.00	0.44
1:G:119:LYS:HG3	1:G:149:ILE:HG21	1.99	0.44
2:H:29:SER:HA	2:H:73:ASN:ND2	2.32	0.44
2:H:100:SER:O	2:H:102:GLY:N	2.51	0.44
3:I:64:ARG:HH21	3:I:85:ASP:HB3	1.83	0.44
1:J:182:PRO:HD2	1:J:214:ILE:HG23	2.00	0.44
2:K:159:THR:HG22	2:K:207:ASN:HB3	2.00	0.44
2:B:161:SER:N	2:B:205:ASN:O	2.47	0.43
3:C:28:VAL:O	3:C:35:PHE:HD2	2.00	0.43
3:C:35:PHE:O	3:C:37:ASN:ND2	2.51	0.43
2:E:13:PRO:HG3	2:E:119:VAL:HG12	2.00	0.43
2:E:197:LEU:HG	2:E:198:GLY:H	1.78	0.43
3:F:202:THR:CG2	3:F:203:SER:N	2.81	0.43
1:G:57:ILE:HG21	1:G:105:LEU:HD12	2.00	0.43
1:G:110:SER:O	1:G:257:MET:HB2	2.17	0.43
3:I:134:SER:HB3	3:I:181:LEU:HD12	2.00	0.43
1:A:73:ALA:HA	3:C:31:TYR:O	2.18	0.43
2:B:190:VAL:HG22	2:B:191:THR:H	1.83	0.43
1:D:75:SER:HA	1:D:108:VAL:O	2.18	0.43
2:E:111:TRP:CD1	2:E:111:TRP:N	2.86	0.43
2:E:209:LYS:HB2	2:E:210:PRO:HD3	2.00	0.43
3:F:9:SER:HA	3:F:105:THR:HG23	1.99	0.43
3:F:114:ALA:HB3	3:F:142:PHE:C	2.42	0.43
3:F:159:ASN:C	3:F:161:VAL:N	2.76	0.43
2:H:104:THR:CG2	2:H:106:TYR:HB3	2.48	0.43
3:I:111:ARG:HB3	3:I:111:ARG:NH1	2.33	0.43
2:K:101:PRO:O	2:K:103:TYR:N	2.50	0.43
2:K:108:TRP:HD1	3:L:39:PHE:CZ	2.35	0.43
3:L:35:PHE:HD1	3:L:35:PHE:HA	1.72	0.43
3:L:86:THR:HG23	3:L:86:THR:O	2.18	0.43
3:L:96:GLU:HA	3:L:99:TYR:CE1	2.52	0.43
2:B:75:ARG:H	2:B:75:ARG:HG2	1.54	0.43
3:F:203:SER:HA	3:F:204:PRO:HD3	1.61	0.43
1:G:116:ILE:HD11	1:G:165:TYR:CD2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:34:SER:HB2	2:H:48:SER:C	2.43	0.43
3:I:92:GLN:C	3:I:94:THR:H	2.22	0.43
1:A:217:ARG:HG3	1:G:94:ASP:HB3	1.99	0.43
2:B:36:ILE:HG12	3:C:101:PHE:HZ	1.83	0.43
3:C:163:ASN:OD1	3:C:163:ASN:N	2.50	0.43
1:D:95:PHE:HZ	1:D:176:LEU:HD23	1.83	0.43
2:E:26:PHE:CD1	2:E:76:LYS:HE2	2.53	0.43
2:E:175:PRO:HB3	2:E:186:LEU:HD23	2.01	0.43
2:H:37:ARG:HD2	2:H:93:TYR:CE1	2.52	0.43
3:I:112:ALA:O	3:I:113:ASP:HB2	2.18	0.43
3:I:183:LEU:O	3:I:186:TYR:HB2	2.18	0.43
1:J:201:VAL:HG22	1:J:242:PHE:CD1	2.54	0.43
3:F:58:GLY:O	3:F:61:VAL:HB	2.19	0.43
1:G:90:CYS:O	1:G:221:ARG:NH1	2.51	0.43
3:I:92:GLN:NE2	3:I:101:PHE:CG	2.86	0.43
3:C:152:ILE:HG22	3:C:192:TYR:HD1	1.84	0.43
3:F:106:LYS:NZ	3:F:108:GLU:OE1	2.36	0.43
3:I:24:ALA:N	3:I:72:THR:O	2.49	0.43
3:I:136:VAL:HG12	3:I:179:SER:CB	2.48	0.43
2:K:132:LEU:HB2	3:L:121:PHE:HB3	1.99	0.43
2:K:163:ASN:HD22	2:K:203:ILE:HG12	1.82	0.43
1:A:179:ILE:N	1:A:228:ASN:O	2.50	0.43
1:A:416:ASP:C	1:A:418:PHE:H	2.27	0.43
2:E:139:THR:O	2:E:140:SER:HB2	2.19	0.43
2:H:163:ASN:HB2	2:H:203:ILE:CD1	2.43	0.43
2:H:203:ILE:HG22	2:H:217:LYS:O	2.19	0.43
1:J:136:CYS:O	1:J:143:SER:OG	2.28	0.43
2:K:28:PHE:CD2	2:K:76:LYS:HA	2.54	0.43
1:A:165:TYR:CE1	1:A:167:ASN:HA	2.42	0.43
2:B:36:ILE:HG23	2:B:45:GLU:C	2.44	0.43
2:B:174:PHE:HE1	3:C:167:ASP:HB3	1.84	0.43
1:D:146:LYS:O	1:D:148:LEU:N	2.52	0.43
1:D:172:GLU:HG2	1:D:233:LEU:HD11	2.00	0.43
2:E:87:ALA:O	2:E:90:THR:HG23	2.18	0.43
3:F:2:GLN:HB3	3:F:94:THR:HG21	2.01	0.43
3:F:38:TRP:CZ3	3:F:76:LEU:HB2	2.54	0.43
3:I:117:THR:O	3:I:117:THR:HG22	2.18	0.43
1:J:114:PHE:CE1	1:J:254:ALA:HB3	2.53	0.43
2:K:148:CYS:HB2	2:K:162:TRP:CZ2	2.54	0.43
1:A:140:GLY:O	1:A:142:LYS:NZ	2.47	0.43
1:A:166:ILE:CG1	2:B:54:SER:HB2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:37:ARG:HA	2:B:92:VAL:O	2.18	0.43
3:C:13:SER:HA	3:C:110:LYS:HB3	2.01	0.43
1:D:72:THR:HA	3:F:31:TYR:HB3	2.00	0.43
1:D:263:SER:OG	1:D:264:GLY:N	2.50	0.43
2:E:180:SER:C	2:E:182:GLY:N	2.76	0.43
1:G:72:THR:HG22	3:I:31:TYR:CD2	2.54	0.43
2:H:5:GLN:O	2:H:21:CYS:HA	2.19	0.43
2:H:174:PHE:HE1	3:I:165:TRP:HB3	1.80	0.43
3:I:72:THR:OG1	3:I:73:ASP:OD1	2.25	0.43
1:J:180:HIS:HA	1:J:227:MET:HG2	2.00	0.43
2:K:16:SER:OG	2:K:81:GLN:NE2	2.45	0.43
1:A:54:LYS:HG2	1:A:66:GLU:HG2	2.00	0.43
3:C:128:LEU:HD23	3:C:132:GLY:O	2.19	0.43
1:D:69:SER:O	1:D:70:LEU:HD22	2.19	0.43
3:F:92:GLN:C	3:F:94:THR:H	2.25	0.43
3:F:156:GLU:H	3:F:156:GLU:HG3	1.56	0.43
2:H:124:THR:HG22	2:H:155:PRO:HD3	2.00	0.43
3:I:29:SER:HB3	3:I:34:ASN:HA	2.00	0.43
3:I:76:LEU:HD22	3:I:76:LEU:HA	1.70	0.43
1:J:166:ILE:HA	1:J:239:LYS:HA	2.01	0.43
1:A:116:ILE:HG22	1:A:252:ARG:O	2.18	0.42
3:C:169:ASP:HB3	3:C:172:ASP:H	1.83	0.42
2:E:60:ARG:HH22	3:F:100:THR:HG22	1.84	0.42
3:F:2:GLN:OE1	3:F:2:GLN:HA	2.19	0.42
1:G:178:GLY:HA2	1:G:228:ASN:O	2.18	0.42
3:I:109:ILE:HA	3:I:109:ILE:HD12	1.63	0.42
1:J:64:ASN:HA	1:J:65:PRO:HD3	1.80	0.42
2:K:146:LEU:H	2:K:146:LEU:CD2	2.26	0.42
2:B:203:ILE:O	2:B:204:CYS:HB3	2.18	0.42
3:C:12:VAL:HG11	3:C:81:VAL:HG21	1.99	0.42
1:D:150:TRP:CD1	1:D:150:TRP:C	2.97	0.42
3:F:106:LYS:O	3:F:107:LEU:HB3	2.19	0.42
2:H:19:LEU:HD12	2:H:80:LEU:HD12	2.01	0.42
2:H:163:ASN:O	2:H:164:SER:HB3	2.19	0.42
3:I:138:PHE:C	3:I:139:LEU:HD12	2.44	0.42
3:I:171:LYS:HB2	3:I:171:LYS:NZ	2.34	0.42
1:J:77:SER:OG	1:J:78:TYR:N	2.52	0.42
1:J:90:CYS:HB3	1:J:91:TYR:H	1.53	0.42
3:L:113:ASP:OD1	3:L:113:ASP:N	2.48	0.42
2:B:204:CYS:HB3	2:B:217:LYS:HZ1	1.83	0.42
3:C:42:LYS:O	3:C:45:GLN:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:125:ASN:O	1:D:154:LYS:HD2	2.19	0.42
1:G:118:PRO:HG2	2:H:58:TYR:CD1	2.54	0.42
1:G:182:PRO:HB3	1:G:187:ASP:HB3	2.01	0.42
1:G:194:ASN:OD1	1:G:194:ASN:N	2.34	0.42
2:H:173:THR:OG1	2:H:187:SER:O	2.26	0.42
3:L:27:SER:HA	3:L:72:THR:HG22	2.01	0.42
3:L:62:PRO:HG2	3:L:65:PHE:CE2	2.54	0.42
1:A:74:SER:O	1:A:110:SER:HA	2.20	0.42
3:C:92:GLN:NE2	3:C:101:PHE:CG	2.86	0.42
3:C:191:SER:HA	3:C:207:LYS:CD	2.49	0.42
1:D:179:ILE:HD13	1:D:179:ILE:HA	1.88	0.42
2:E:4:GLN:HB3	2:E:112:GLY:HA3	2.00	0.42
2:E:174:PHE:HD2	3:F:166:THR:O	2.02	0.42
3:F:168:GLN:NE2	3:F:172:ASP:O	2.52	0.42
2:K:47:VAL:CG1	2:K:63:VAL:HG11	2.49	0.42
2:K:112:GLY:C	2:K:114:GLY:H	2.28	0.42
2:K:155:PRO:HD2	2:K:210:PRO:HB3	2.01	0.42
1:A:210:PHE:CD1	1:A:210:PHE:N	2.87	0.42
1:A:221:ARG:HB2	1:A:221:ARG:CZ	2.46	0.42
3:C:115:ALA:HB1	3:C:116:PRO:CA	2.49	0.42
1:D:153:LYS:HB2	1:D:191:LEU:O	2.20	0.42
3:F:31:TYR:C	3:F:33:ILE:H	2.28	0.42
1:G:171:LYS:HD2	1:G:171:LYS:HA	1.51	0.42
2:H:26:PHE:HB3	2:H:27:THR:H	1.75	0.42
2:H:34:SER:HB2	2:H:49:GLY:N	2.34	0.42
2:H:151:LYS:HE2	3:I:181:LEU:HD13	2.00	0.42
2:H:202:TYR:CD1	2:H:203:ILE:HD12	2.54	0.42
2:B:4:GLN:HG3	2:B:95:CYS:SG	2.59	0.42
2:B:207:ASN:OD1	2:B:214:LYS:HB3	2.19	0.42
2:E:86:ARG:HG2	2:E:89:ASP:OD2	2.20	0.42
2:E:197:LEU:HD13	2:E:202:TYR:CD2	2.55	0.42
1:G:252:ARG:HH22	3:I:97:VAL:HA	1.83	0.42
2:H:176:ALA:HA	3:I:165:TRP:HE1	1.84	0.42
3:I:46:PRO:HA	3:I:47:PRO:HD3	1.81	0.42
1:J:187:ASP:O	1:J:191:LEU:HB2	2.20	0.42
2:K:163:ASN:HB2	2:K:203:ILE:CD1	2.40	0.42
3:C:21:THR:HA	3:C:75:THR:HA	2.01	0.42
1:D:210:PHE:O	1:D:211:LYS:HG2	2.20	0.42
2:E:36:ILE:HG12	2:E:46:TRP:HA	2.01	0.42
3:F:10:LEU:O	3:F:107:LEU:HA	2.19	0.42
3:F:76:LEU:HD22	3:F:76:LEU:HA	1.86	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:125:ASN:HB3	1:G:159:PRO:HG2	2.00	0.42
1:G:164:SER:H	2:H:56:ARG:NH1	2.18	0.42
2:H:207:ASN:ND2	2:H:214:LYS:HB3	2.35	0.42
3:I:92:GLN:O	3:I:94:THR:N	2.43	0.42
3:L:111:ARG:H	3:L:111:ARG:HG3	1.68	0.42
1:A:114:PHE:O	1:A:253:TYR:HD1	2.02	0.42
1:A:156:ASN:HB2	1:A:193:GLN:HE22	1.85	0.42
2:B:97:ARG:NH2	2:B:109:ASP:OD2	2.39	0.42
1:G:138:HIS:O	1:G:138:HIS:CG	2.71	0.42
2:H:151:LYS:HA	2:H:185:SER:OG	2.20	0.42
2:H:177:VAL:HG13	2:H:184:TYR:CE2	2.55	0.42
1:J:150:TRP:C	1:J:150:TRP:HD1	2.24	0.42
2:K:152:ASP:OD2	2:K:178:LEU:HG	2.19	0.42
1:A:91:TYR:HA	1:A:92:PRO:HD2	1.78	0.42
2:B:174:PHE:N	2:B:174:PHE:CD1	2.85	0.42
3:C:93:GLN:HA	3:C:100:THR:H	1.85	0.42
3:C:111:ARG:NE	3:C:171:LYS:O	2.53	0.42
1:D:91:TYR:HE2	1:D:227:MET:HB2	1.83	0.42
2:E:35:TRP:CD1	2:E:80:LEU:HD13	2.53	0.42
3:F:175:TYR:CE1	3:F:177:MET:HB3	2.55	0.42
3:I:171:LYS:HA	3:I:171:LYS:HD3	1.80	0.42
1:J:109:SER:N	1:J:258:GLU:O	2.46	0.42
2:K:36:ILE:HD11	3:L:101:PHE:CE2	2.52	0.42
3:L:39:PHE:CE1	3:L:92:GLN:HG2	2.55	0.42
3:L:116:PRO:O	3:L:117:THR:C	2.62	0.42
3:L:188:ARG:HD2	3:L:188:ARG:C	2.45	0.42
3:C:116:PRO:HG3	3:C:146:ILE:HD11	2.01	0.42
3:C:198:HIS:CG	3:C:199:LYS:H	2.38	0.42
1:D:147:ASN:CB	1:D:253:TYR:HB2	2.49	0.42
1:D:183:SER:OG	1:D:184:THR:N	2.52	0.42
2:E:78:LEU:O	2:E:79:TYR:HD1	2.02	0.42
2:E:194:SER:C	2:E:196:SER:N	2.78	0.42
1:G:61:ILE:HD12	1:G:61:ILE:HA	1.89	0.42
2:H:70:SER:O	2:H:78:LEU:HD12	2.20	0.42
3:I:62:PRO:HG2	3:I:65:PHE:HE1	1.83	0.42
3:I:187:GLU:HA	3:I:188:ARG:HD2	2.02	0.42
1:J:174:LEU:HD12	1:J:174:LEU:C	2.45	0.42
3:L:128:LEU:C	3:L:131:GLY:H	2.28	0.42
3:L:151:LYS:HE2	3:L:193:THR:OG1	2.20	0.42
2:B:34:SER:CB	2:B:98:HIS:HE1	2.32	0.41
2:B:162:TRP:H	2:B:167:LEU:HD12	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:42:LYS:HA	3:C:87:ALA:CB	2.50	0.41
1:D:76:TRP:HH2	1:D:111:PHE:CD2	2.38	0.41
1:D:89:THR:HB	1:D:221:ARG:HH12	1.86	0.41
1:D:110:SER:O	1:D:258:GLU:N	2.47	0.41
3:I:92:GLN:NE2	3:I:101:PHE:CD1	2.84	0.41
3:L:9:SER:CB	3:L:106:LYS:H	2.33	0.41
3:L:143:TYR:O	3:L:198:HIS:HE1	2.03	0.41
1:A:176:LEU:O	1:A:251:PRO:HB3	2.19	0.41
2:E:60:ARG:NE	3:F:98:PRO:HB2	2.35	0.41
3:I:185:GLU:C	3:I:187:GLU:N	2.78	0.41
1:J:111:PHE:CE1	1:J:255:PHE:HB3	2.55	0.41
1:J:192:TYR:O	1:J:193:GLN:HB3	2.20	0.41
1:J:240:ILE:HG12	1:J:241:THR:N	2.36	0.41
3:L:195:GLU:HG3	3:L:202:THR:HG21	2.02	0.41
2:B:163:ASN:CG	2:B:203:ILE:HD13	2.45	0.41
3:C:187:GLU:C	3:C:188:ARG:HD2	2.45	0.41
1:D:112:GLU:N	1:D:256:ALA:O	2.49	0.41
3:F:51:ILE:HD11	3:F:57:LYS:HZ3	1.85	0.41
3:F:127:GLN:HG2	3:F:132:GLY:O	2.21	0.41
1:J:212:PRO:HG3	1:J:247:ASN:OD1	2.21	0.41
1:J:250:VAL:CG2	1:J:251:PRO:HD2	2.50	0.41
2:K:155:PRO:HD2	2:K:210:PRO:CB	2.50	0.41
1:A:73:ALA:HB1	1:A:74:SER:H	1.66	0.41
1:A:219:LYS:HZ1	1:A:222:ASP:HA	1.85	0.41
1:A:222:ASP:OD1	1:A:222:ASP:N	2.52	0.41
2:B:12:GLN:HA	2:B:120:SER:O	2.21	0.41
3:C:152:ILE:HG23	3:C:159:ASN:HD21	1.84	0.41
2:E:104:THR:HG23	3:F:35:PHE:CZ	2.55	0.41
3:F:111:ARG:HG2	3:F:143:TYR:CD2	2.55	0.41
3:F:171:LYS:HB3	3:F:171:LYS:HE3	1.74	0.41
3:F:189:HIS:HB2	3:F:191:SER:H	1.84	0.41
1:G:101:LEU:O	1:G:104:GLN:HB3	2.20	0.41
3:F:141:ASN:OD1	3:F:141:ASN:N	2.51	0.41
1:G:62:LEU:O	1:G:147:ASN:HB2	2.20	0.41
1:G:189:GLN:NE2	1:G:193:GLN:O	2.53	0.41
2:H:42:LYS:HB3	2:H:42:LYS:HE2	1.58	0.41
2:K:45:GLU:OE2	2:K:46:TRP:HE3	2.03	0.41
1:A:63:GLY:O	1:A:145:TYR:HA	2.20	0.41
1:A:119:LYS:CB	1:A:252:ARG:HH11	2.29	0.41
3:C:142:PHE:O	3:C:143:TYR:HB2	2.21	0.41
3:C:172:ASP:OD1	3:C:174:THR:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:26:PHE:HB3	2:E:27:THR:H	1.71	0.41
2:E:36:ILE:HG21	2:E:111:TRP:HZ3	1.85	0.41
3:F:142:PHE:CD1	3:F:142:PHE:N	2.89	0.41
1:J:93:GLY:HA3	1:J:227:MET:O	2.20	0.41
2:K:112:GLY:O	2:K:114:GLY:N	2.54	0.41
3:L:123:PRO:HG3	3:L:134:SER:O	2.19	0.41
1:A:153:LYS:N	1:A:191:LEU:O	2.53	0.41
2:B:33:MET:HE3	2:B:33:MET:HB3	1.77	0.41
2:B:80:LEU:HD23	2:B:82:MET:SD	2.61	0.41
2:B:189:VAL:HG11	3:C:175:TYR:CE1	2.56	0.41
3:C:1:ILE:HG23	3:C:3:MET:HB3	2.01	0.41
1:D:50:LEU:HD21	1:D:79:ILE:CG1	2.50	0.41
3:F:146:ILE:HG12	3:F:147:ASN:N	2.28	0.41
1:G:64:ASN:O	1:G:67:CYS:N	2.53	0.41
1:G:119:LYS:H	1:G:252:ARG:HH11	1.58	0.41
1:G:215:ALA:HB3	1:G:217:ARG:NH1	2.35	0.41
2:H:94:TYR:HB3	2:H:111:TRP:HE3	1.84	0.41
3:I:165:TRP:HA	3:I:165:TRP:CE3	2.55	0.41
1:J:53:GLY:HA2	1:J:82:THR:OG1	2.21	0.41
1:J:149:ILE:HD11	1:J:252:ARG:HG3	2.02	0.41
1:J:183:SER:HA	1:J:215:ALA:O	2.20	0.41
3:L:7:PRO:HD2	3:L:21:THR:O	2.21	0.41
3:L:182:THR:HG21	3:L:187:GLU:HG2	2.02	0.41
3:C:144:PRO:HD2	3:C:198:HIS:CE1	2.55	0.41
1:D:133:THR:OG1	1:D:134:ALA:N	2.53	0.41
2:E:188:SER:OG	2:E:189:VAL:N	2.54	0.41
1:G:51:HIS:HA	1:G:80:VAL:HB	2.03	0.41
3:I:126:GLU:CD	3:I:126:GLU:H	2.28	0.41
3:I:157:ARG:HG3	3:I:159:ASN:HA	2.03	0.41
2:K:46:TRP:CD1	2:K:48:SER:O	2.74	0.41
2:K:156:GLU:H	2:K:156:GLU:HG2	1.67	0.41
3:L:187:GLU:OE1	3:L:192:TYR:OH	2.33	0.41
1:A:116:ILE:HG22	1:A:252:ARG:C	2.46	0.41
1:A:165:TYR:HD1	1:A:166:ILE:N	2.19	0.41
2:B:34:SER:HB2	2:B:98:HIS:CE1	2.55	0.41
2:B:163:ASN:HA	2:B:205:ASN:ND2	2.30	0.41
2:B:180:SER:C	2:B:182:GLY:N	2.75	0.41
3:C:151:LYS:HB2	3:C:193:THR:HB	2.03	0.41
1:D:108:VAL:HG12	1:D:259:ARG:HB3	2.02	0.41
1:D:127:ASP:CG	1:D:130:LYS:HG3	2.45	0.41
1:D:163:LYS:NZ	2:E:56:ARG:HG3	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:37:ARG:HD3	2:E:47:VAL:HG21	2.03	0.41
2:E:50:ILE:O	2:E:50:ILE:HG23	2.21	0.41
2:E:82:MET:HB3	2:E:85:LEU:HD21	2.03	0.41
2:E:162:TRP:HB2	2:E:166:ALA:O	2.21	0.41
3:F:183:LEU:N	3:F:183:LEU:HD23	2.36	0.41
3:F:190:ASN:HB3	3:F:209:PHE:O	2.20	0.41
1:G:64:ASN:OD1	1:G:66:GLU:HG2	2.21	0.41
1:G:91:TYR:HE2	1:G:180:HIS:CD2	2.36	0.41
1:G:178:GLY:O	1:G:179:ILE:HD13	2.21	0.41
2:H:42:LYS:HG2	2:H:43:GLY:HA3	2.02	0.41
2:H:63:VAL:CG1	2:H:67:PHE:HB2	2.51	0.41
2:H:92:VAL:HB	2:H:116:MET:HG2	2.03	0.41
3:I:64:ARG:H	3:I:64:ARG:HG2	1.56	0.41
1:J:101:LEU:HD22	1:J:101:LEU:HA	1.87	0.41
2:K:45:GLU:HA	3:L:101:PHE:CD2	2.56	0.41
3:L:92:GLN:HB3	3:L:93:GLN:H	1.63	0.41
3:L:184:ASP:HB3	3:L:186:TYR:HE1	1.81	0.41
1:A:52:LEU:O	1:A:82:THR:HG23	2.21	0.41
1:A:114:PHE:CE1	1:A:165:TYR:HE2	2.39	0.41
1:A:171:LYS:HE2	1:A:257:MET:C	2.46	0.41
2:B:35:TRP:HB2	2:B:47:VAL:HG22	2.03	0.41
3:C:54:ALA:O	3:C:67:GLY:C	2.64	0.41
3:C:139:LEU:HD12	3:C:139:LEU:HA	1.79	0.41
1:D:73:ALA:C	1:D:75:SER:H	2.27	0.41
2:E:147:GLY:HA2	2:E:189:VAL:HA	2.02	0.41
2:E:172:HIS:O	2:E:173:THR:OG1	2.33	0.41
1:G:77:SER:O	1:G:106:SER:O	2.38	0.41
1:G:198:TYR:C	1:G:198:TYR:CD1	2.99	0.41
2:H:215:VAL:HG13	2:H:216:ASP:N	2.36	0.41
1:J:62:LEU:HD22	1:J:62:LEU:HA	1.93	0.41
2:K:132:LEU:HD21	2:K:149:LEU:HB2	2.02	0.41
2:K:170:SER:HA	2:K:189:VAL:O	2.21	0.41
1:A:130:LYS:HB2	1:A:152:VAL:HG21	2.03	0.40
2:B:40:PRO:O	2:B:42:LYS:N	2.46	0.40
1:G:99:GLU:HG3	1:G:102:ARG:HH21	1.86	0.40
1:G:118:PRO:HG2	2:H:58:TYR:CE1	2.56	0.40
2:H:36:ILE:HG12	2:H:111:TRP:CZ3	2.56	0.40
3:I:43:PRO:HD3	3:I:87:ALA:CB	2.51	0.40
3:I:65:PHE:CZ	3:I:78:ILE:HD12	2.55	0.40
3:C:183:LEU:O	3:C:186:TYR:HD2	2.05	0.40
1:D:172:GLU:HG2	1:D:172:GLU:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:177:TRP:CZ3	1:D:232:THR:HG22	2.56	0.40
2:E:161:SER:O	2:E:205:ASN:N	2.53	0.40
1:G:84:SER:OG	1:G:87:ASN:HB2	2.21	0.40
1:G:252:ARG:HH21	3:I:97:VAL:HA	1.80	0.40
2:H:130:PHE:HA	2:H:131:PRO:HD3	1.77	0.40
1:J:171:LYS:HG3	1:J:172:GLU:N	2.36	0.40
1:A:135:ALA:HB2	1:A:223:GLN:HG3	2.02	0.40
3:C:16:GLN:HA	3:C:79:ASN:O	2.22	0.40
3:C:52:TYR:C	3:C:53:THR:HG1	2.29	0.40
3:C:150:TRP:HB2	3:C:159:ASN:HD22	1.87	0.40
1:D:96:ILE:HA	1:J:216:ILE:O	2.21	0.40
3:F:163:ASN:CB	3:F:179:SER:H	2.33	0.40
1:G:103:GLU:O	1:G:103:GLU:HG3	2.19	0.40
2:H:27:THR:O	2:H:31:TYR:HD2	2.04	0.40
2:H:48:SER:OG	2:H:49:GLY:N	2.53	0.40
2:H:100:SER:OG	2:H:105:LEU:HG	2.21	0.40
2:H:193:PRO:C	2:H:195:SER:N	2.79	0.40
2:E:21:CYS:HB3	2:E:78:LEU:HB3	2.03	0.40
1:G:158:TYR:CZ	1:G:246:GLY:HA2	2.56	0.40
1:G:220:VAL:C	1:G:222:ASP:N	2.75	0.40
3:I:191:SER:HA	3:I:207:LYS:HE2	2.03	0.40
2:K:17:LEU:O	2:K:82:MET:N	2.55	0.40
2:K:143:THR:HG23	2:K:193:PRO:HA	2.02	0.40
2:B:19:LEU:HD13	2:B:82:MET:HG3	2.04	0.40
2:B:19:LEU:HD21	2:B:93:TYR:CG	2.57	0.40
2:B:34:SER:CB	2:B:108:TRP:HZ3	2.34	0.40
3:C:40:GLN:HB2	3:C:50:LEU:HD11	2.03	0.40
1:D:135:ALA:O	1:D:137:PRO:HD3	2.21	0.40
1:D:184:THR:OG1	1:D:185:SER:N	2.54	0.40
3:F:88:ASN:HA	3:F:105:THR:O	2.21	0.40
1:G:199:VAL:HB	1:G:210:PHE:HB2	2.04	0.40
2:H:10:VAL:CG2	2:H:155:PRO:HG3	2.50	0.40
2:H:100:SER:N	2:H:101:PRO:HD3	2.36	0.40
3:I:29:SER:CB	3:I:34:ASN:HA	2.52	0.40
2:K:38:GLN:HG3	2:K:43:GLY:HA3	2.04	0.40
3:L:127:GLN:O	3:L:131:GLY:N	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	233/518 (45%)	191 (82%)	40 (17%)	2 (1%)	14	41
1	D	221/518 (43%)	183 (83%)	38 (17%)	0	100	100
1	G	221/518 (43%)	189 (86%)	30 (14%)	2 (1%)	14	41
1	J	221/518 (43%)	187 (85%)	32 (14%)	2 (1%)	14	41
2	B	214/222 (96%)	180 (84%)	29 (14%)	5 (2%)	5	18
2	E	214/222 (96%)	176 (82%)	35 (16%)	3 (1%)	9	30
2	H	214/222 (96%)	173 (81%)	35 (16%)	6 (3%)	4	14
2	K	214/222 (96%)	164 (77%)	47 (22%)	3 (1%)	9	30
3	C	208/211 (99%)	147 (71%)	50 (24%)	11 (5%)	1	5
3	F	208/211 (99%)	150 (72%)	47 (23%)	11 (5%)	1	5
3	I	208/211 (99%)	157 (76%)	41 (20%)	10 (5%)	2	6
3	L	205/211 (97%)	152 (74%)	44 (22%)	9 (4%)	2	7
All	All	2581/3804 (68%)	2049 (79%)	468 (18%)	64 (2%)	4	16

All (64) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	F	34	ASN
2	K	48	SER
3	L	5	GLN
3	L	45	GLN
3	L	79	ASN
3	L	80	PRO
3	L	191	SER
2	B	27	THR
3	C	34	ASN
3	C	115	ALA
2	E	27	THR
3	F	8	ALA

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Mol	Chain	Res	Type
3	F	93	GLN
3	I	30	ASN
2	K	26	PHE
3	L	115	ALA
3	L	192	TYR
2	B	155	PRO
3	C	93	GLN
3	C	157	ARG
3	C	186	TYR
2	E	110	TYR
3	F	31	TYR
3	F	140	ASN
2	H	27	THR
2	H	101	PRO
3	I	45	GLN
3	I	158	GLN
1	J	67	CYS
2	E	26	PHE
3	F	45	GLN
3	F	115	ALA
3	F	209	PHE
1	G	120	THR
2	H	44	LEU
2	H	49	GLY
2	H	163	ASN
3	I	8	ALA
3	I	88	ASN
3	I	93	GLN
3	I	115	ALA
3	L	156	GLU
3	L	190	ASN
1	A	205	ARG
1	A	422	TRP
2	B	105	LEU
2	B	181	SER
3	C	85	ASP
3	C	88	ASN
3	C	97	VAL
3	F	85	ASP
1	J	86	ASP
2	K	64	LYS
2	B	164	SER

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Mol	Chain	Res	Type
3	C	31	TYR
1	G	67	CYS
3	F	97	VAL
3	C	161	VAL
3	I	123	PRO
3	F	123	PRO
2	H	215	VAL
3	I	161	VAL
3	C	116	PRO
3	I	144	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	193/451 (43%)	141 (73%)	52 (27%)	0	1
1	D	193/451 (43%)	145 (75%)	48 (25%)	0	2
1	G	193/451 (43%)	148 (77%)	45 (23%)	1	3
1	J	193/451 (43%)	139 (72%)	54 (28%)	0	1
2	B	180/184 (98%)	124 (69%)	56 (31%)	0	1
2	E	180/184 (98%)	125 (69%)	55 (31%)	0	1
2	H	180/184 (98%)	115 (64%)	65 (36%)	0	0
2	K	180/184 (98%)	129 (72%)	51 (28%)	0	1
3	C	182/183 (100%)	134 (74%)	48 (26%)	0	2
3	F	182/183 (100%)	130 (71%)	52 (29%)	0	1
3	I	182/183 (100%)	133 (73%)	49 (27%)	0	1
3	L	181/183 (99%)	126 (70%)	55 (30%)	0	1
All	All	2219/3272 (68%)	1589 (72%)	630 (28%)	0	1

All (630) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	HIS
1	A	52	LEU
1	A	54	LYS
1	A	69	SER
1	A	70	LEU
1	A	83	SER
1	A	87	ASN
1	A	89	THR
1	A	101	LEU
1	A	102	ARG
1	A	104	GLN
1	A	110	SER
1	A	112	GLU
1	A	113	ARG
1	A	117	PHE
1	A	119	LYS
1	A	121	SER
1	A	125	ASN
1	A	127	ASP
1	A	128	SER
1	A	142	LYS
1	A	148	LEU
1	A	153	LYS
1	A	160	LYS
1	A	164	SER
1	A	165	TYR
1	A	168	ASP
1	A	169	LYS
1	A	173	VAL
1	A	174	LEU
1	A	175	VAL
1	A	179	ILE
1	A	183	SER
1	A	189	GLN
1	A	192	TYR
1	A	196	ASP
1	A	204	SER
1	A	209	LYS
1	A	214	ILE
1	A	221	ARG
1	A	233	LEU
1	A	234	VAL
1	A	239	LYS

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Mol	Chain	Res	Type
1	A	240	ILE
1	A	245	THR
1	A	248	LEU
1	A	252	ARG
1	A	260	ASN
1	A	265	ILE
1	A	266	ILE
1	A	269	ASP
1	A	270	THR
2	B	4	GLN
2	B	6	SER
2	B	12	GLN
2	B	18	ARG
2	B	20	SER
2	B	29	SER
2	B	32	ASP
2	B	42	LYS
2	B	45	GLU
2	B	50	ILE
2	B	54	SER
2	B	55	GLU
2	B	61	ASP
2	B	63	VAL
2	B	64	LYS
2	B	69	ILE
2	B	71	ARG
2	B	74	SER
2	B	75	ARG
2	B	78	LEU
2	B	81	GLN
2	B	85	LEU
2	B	86	ARG
2	B	88	GLU
2	B	90	THR
2	B	95	CYS
2	B	97	ARG
2	B	103	TYR
2	B	104	THR
2	B	108	TRP
2	B	109	ASP
2	B	111	TRP
2	B	116	MET

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Mol	Chain	Res	Type
2	B	117	VAL
2	B	118	THR
2	B	124	THR
2	B	125	LYS
2	B	140	SER
2	B	143	THR
2	B	151	LYS
2	B	158	VAL
2	B	167	LEU
2	B	169	SER
2	B	177	VAL
2	B	189	VAL
2	B	191	THR
2	B	194	SER
2	B	199	THR
2	B	200	GLN
2	B	205	ASN
2	B	206	VAL
2	B	209	LYS
2	B	214	LYS
2	B	215	VAL
2	B	216	ASP
2	B	217	LYS
3	C	3	MET
3	C	4	THR
3	C	5	GLN
3	C	13	SER
3	C	16	GLN
3	C	17	ARG
3	C	22	CYS
3	C	25	SER
3	C	45	GLN
3	C	48	LYS
3	C	50	LEU
3	C	53	THR
3	C	55	SER
3	C	73	ASP
3	C	76	LEU
3	C	81	VAL
3	C	82	GLU
3	C	96	GLU
3	C	97	VAL

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Mol	Chain	Res	Type
3	C	105	THR
3	C	117	THR
3	C	139	LEU
3	C	140	ASN
3	C	142	PHE
3	C	147	ASN
3	C	149	LYS
3	C	151	LYS
3	C	157	ARG
3	C	163	ASN
3	C	164	SER
3	C	165	TRP
3	C	166	THR
3	C	167	ASP
3	C	171	LYS
3	C	179	SER
3	C	183	LEU
3	C	184	ASP
3	C	187	GLU
3	C	188	ARG
3	C	189	HIS
3	C	192	TYR
3	C	195	GLU
3	C	201	SER
3	C	206	VAL
3	C	207	LYS
3	C	208	SER
3	C	209	PHE
3	C	210	ASN
1	D	54	LYS
1	D	62	LEU
1	D	66	GLU
1	D	70	LEU
1	D	72	THR
1	D	75	SER
1	D	79	ILE
1	D	94	ASP
1	D	101	LEU
1	D	102	ARG
1	D	109	SER
1	D	110	SER
1	D	112	GLU

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Mol	Chain	Res	Type
1	D	120	THR
1	D	121	SER
1	D	130	LYS
1	D	132	VAL
1	D	148	LEU
1	D	149	ILE
1	D	150	TRP
1	D	151	LEU
1	D	153	LYS
1	D	154	LYS
1	D	158	TYR
1	D	160	LYS
1	D	164	SER
1	D	168	ASP
1	D	169	LYS
1	D	174	LEU
1	D	175	VAL
1	D	184	THR
1	D	190	SER
1	D	191	LEU
1	D	198	TYR
1	D	199	VAL
1	D	204	SER
1	D	209	LYS
1	D	214	ILE
1	D	217	ARG
1	D	234	VAL
1	D	235	GLU
1	D	239	LYS
1	D	240	ILE
1	D	243	GLU
1	D	245	THR
1	D	250	VAL
1	D	258	GLU
1	D	263	SER
2	E	3	LEU
2	E	4	GLN
2	E	11	VAL
2	E	18	ARG
2	E	27	THR
2	E	32	ASP
2	E	36	ILE

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Mol	Chain	Res	Type
2	E	38	GLN
2	E	42	LYS
2	E	44	LEU
2	E	45	GLU
2	E	47	VAL
2	E	51	LEU
2	E	56	ARG
2	E	57	SER
2	E	60	ARG
2	E	64	LYS
2	E	68	THR
2	E	73	ASN
2	E	75	ARG
2	E	76	LYS
2	E	80	LEU
2	E	83	ASN
2	E	86	ARG
2	E	90	THR
2	E	98	HIS
2	E	108	TRP
2	E	109	ASP
2	E	110	TYR
2	E	111	TRP
2	E	113	GLN
2	E	117	VAL
2	E	139	THR
2	E	148	CYS
2	E	150	VAL
2	E	151	LYS
2	E	158	VAL
2	E	168	THR
2	E	170	SER
2	E	171	VAL
2	E	172	HIS
2	E	173	THR
2	E	178	LEU
2	E	189	VAL
2	E	199	THR
2	E	201	THR
2	E	202	TYR
2	E	203	ILE
2	E	205	ASN

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Mol	Chain	Res	Type
2	E	207	ASN
2	E	209	LYS
2	E	214	LYS
2	E	215	VAL
2	E	216	ASP
2	E	217	LYS
3	F	2	GLN
3	F	3	MET
3	F	10	LEU
3	F	12	VAL
3	F	13	SER
3	F	23	ARG
3	F	36	ILE
3	F	37	ASN
3	F	41	GLN
3	F	53	THR
3	F	55	SER
3	F	68	SER
3	F	73	ASP
3	F	76	LEU
3	F	78	ILE
3	F	81	VAL
3	F	85	ASP
3	F	95	LYS
3	F	97	VAL
3	F	106	LYS
3	F	108	GLU
3	F	118	VAL
3	F	119	SER
3	F	120	ILE
3	F	125	SER
3	F	126	GLU
3	F	135	VAL
3	F	139	LEU
3	F	141	ASN
3	F	145	LYS
3	F	148	VAL
3	F	152	ILE
3	F	156	GLU
3	F	161	VAL
3	F	162	LEU
3	F	163	ASN

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Mol	Chain	Res	Type
3	F	171	LYS
3	F	177	MET
3	F	183	LEU
3	F	184	ASP
3	F	185	GLU
3	F	188	ARG
3	F	190	ASN
3	F	191	SER
3	F	194	CYS
3	F	197	THR
3	F	200	THR
3	F	202	THR
3	F	207	LYS
3	F	208	SER
3	F	209	PHE
3	F	210	ASN
1	G	51	HIS
1	G	52	LEU
1	G	55	CYS
1	G	67	CYS
1	G	69	SER
1	G	74	SER
1	G	81	GLU
1	G	85	SER
1	G	86	ASP
1	G	87	ASN
1	G	89	THR
1	G	96	ILE
1	G	99	GLU
1	G	101	LEU
1	G	103	GLU
1	G	108	VAL
1	G	111	PHE
1	G	115	GLU
1	G	122	SER
1	G	128	SER
1	G	129	ASN
1	G	133	THR
1	G	136	CYS
1	G	138	HIS
1	G	142	LYS
1	G	146	LYS

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Mol	Chain	Res	Type
1	G	149	ILE
1	G	153	LYS
1	G	154	LYS
1	G	156	ASN
1	G	161	LEU
1	G	166	ILE
1	G	167	ASN
1	G	171	LYS
1	G	174	LEU
1	G	187	ASP
1	G	194	ASN
1	G	196	ASP
1	G	205	ARG
1	G	232	THR
1	G	233	LEU
1	G	234	VAL
1	G	245	THR
1	G	250	VAL
1	G	267	ILE
2	H	4	GLN
2	H	10	VAL
2	H	12	GLN
2	H	18	ARG
2	H	34	SER
2	H	36	ILE
2	H	44	LEU
2	H	46	TRP
2	H	47	VAL
2	H	51	LEU
2	H	55	GLU
2	H	60	ARG
2	H	63	VAL
2	H	66	ARG
2	H	68	THR
2	H	69	ILE
2	H	73	ASN
2	H	75	ARG
2	H	78	LEU
2	H	80	LEU
2	H	82	MET
2	H	84	SER
2	H	88	GLU

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Mol	Chain	Res	Type
2	H	90	THR
2	H	95	CYS
2	H	97	ARG
2	H	98	HIS
2	H	100	SER
2	H	104	THR
2	H	110	TYR
2	H	111	TRP
2	H	116	MET
2	H	118	THR
2	H	121	SER
2	H	129	VAL
2	H	132	LEU
2	H	139	THR
2	H	140	SER
2	H	143	THR
2	H	146	LEU
2	H	148	CYS
2	H	149	LEU
2	H	150	VAL
2	H	158	VAL
2	H	161	SER
2	H	169	SER
2	H	171	VAL
2	H	174	PHE
2	H	177	VAL
2	H	186	LEU
2	H	189	VAL
2	H	190	VAL
2	H	193	PRO
2	H	194	SER
2	H	195	SER
2	H	199	THR
2	H	200	GLN
2	H	201	THR
2	H	202	TYR
2	H	203	ILE
2	H	206	VAL
2	H	207	ASN
2	H	209	LYS
2	H	213	THR
2	H	215	VAL

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Mol	Chain	Res	Type
3	I	1	ILE
3	I	10	LEU
3	I	16	GLN
3	I	17	ARG
3	I	22	CYS
3	I	28	VAL
3	I	31	TYR
3	I	33	ILE
3	I	36	ILE
3	I	42	LYS
3	I	48	LYS
3	I	49	LEU
3	I	59	THR
3	I	64	ARG
3	I	66	SER
3	I	70	SER
3	I	73	ASP
3	I	75	THR
3	I	76	LEU
3	I	78	ILE
3	I	82	GLU
3	I	97	VAL
3	I	105	THR
3	I	107	LEU
3	I	109	ILE
3	I	110	LYS
3	I	117	THR
3	I	126	GLU
3	I	128	LEU
3	I	134	SER
3	I	141	ASN
3	I	145	LYS
3	I	149	LYS
3	I	152	ILE
3	I	166	THR
3	I	170	SER
3	I	171	LYS
3	I	177	MET
3	I	183	LEU
3	I	188	ARG
3	I	189	HIS
3	I	195	GLU

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Mol	Chain	Res	Type
3	I	199	LYS
3	I	200	THR
3	I	205	ILE
3	I	207	LYS
3	I	208	SER
3	I	209	PHE
3	I	210	ASN
1	J	51	HIS
1	J	52	LEU
1	J	54	LYS
1	J	61	ILE
1	J	62	LEU
1	J	64	ASN
1	J	68	GLU
1	J	70	LEU
1	J	74	SER
1	J	82	THR
1	J	86	ASP
1	J	94	ASP
1	J	95	PHE
1	J	96	ILE
1	J	99	GLU
1	J	101	LEU
1	J	102	ARG
1	J	103	GLU
1	J	108	VAL
1	J	111	PHE
1	J	115	GLU
1	J	120	THR
1	J	123	TRP
1	J	133	THR
1	J	149	ILE
1	J	153	LYS
1	J	154	LYS
1	J	163	LYS
1	J	171	LYS
1	J	172	GLU
1	J	173	VAL
1	J	174	LEU
1	J	175	VAL
1	J	176	LEU
1	J	179	ILE

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Mol	Chain	Res	Type
1	J	196	ASP
1	J	203	SER
1	J	214	ILE
1	J	216	ILE
1	J	221	ARG
1	J	222	ASP
1	J	223	GLN
1	J	224	GLU
1	J	227	MET
1	J	234	VAL
1	J	239	LYS
1	J	240	ILE
1	J	252	ARG
1	J	257	MET
1	J	260	ASN
1	J	266	ILE
1	J	268	SER
1	J	269	ASP
1	J	270	THR
2	K	5	GLN
2	K	10	VAL
2	K	12	GLN
2	K	18	ARG
2	K	19	LEU
2	K	24	SER
2	K	30	ASP
2	K	34	SER
2	K	37	ARG
2	K	44	LEU
2	K	46	TRP
2	K	48	SER
2	K	51	LEU
2	K	60	ARG
2	K	63	VAL
2	K	68	THR
2	K	77	THR
2	K	78	LEU
2	K	80	LEU
2	K	89	ASP
2	K	108	TRP
2	K	110	TYR
2	K	111	TRP

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Mol	Chain	Res	Type
2	K	116	MET
2	K	124	THR
2	K	125	LYS
2	K	132	LEU
2	K	146	LEU
2	K	148	CYS
2	K	150	VAL
2	K	151	LYS
2	K	158	VAL
2	K	167	LEU
2	K	168	THR
2	K	169	SER
2	K	171	VAL
2	K	172	HIS
2	K	177	VAL
2	K	178	LEU
2	K	180	SER
2	K	183	LEU
2	K	186	LEU
2	K	187	SER
2	K	188	SER
2	K	189	VAL
2	K	196	SER
2	K	203	ILE
2	K	204	CYS
2	K	215	VAL
2	K	217	LYS
2	K	218	LYS
3	L	1	ILE
3	L	3	MET
3	L	5	GLN
3	L	6	SER
3	L	12	VAL
3	L	17	ARG
3	L	21	THR
3	L	28	VAL
3	L	29	SER
3	L	31	TYR
3	L	35	PHE
3	L	36	ILE
3	L	40	GLN
3	L	42	LYS

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Mol	Chain	Res	Type
3	L	49	LEU
3	L	56	ASN
3	L	57	LYS
3	L	59	THR
3	L	61	VAL
3	L	75	THR
3	L	78	ILE
3	L	81	VAL
3	L	86	THR
3	L	88	ASN
3	L	91	CYS
3	L	97	VAL
3	L	106	LYS
3	L	110	LYS
3	L	111	ARG
3	L	113	ASP
3	L	118	VAL
3	L	126	GLU
3	L	141	ASN
3	L	148	VAL
3	L	163	ASN
3	L	165	TRP
3	L	166	THR
3	L	167	ASP
3	L	169	ASP
3	L	171	LYS
3	L	172	ASP
3	L	173	SER
3	L	179	SER
3	L	180	THR
3	L	182	THR
3	L	183	LEU
3	L	187	GLU
3	L	188	ARG
3	L	193	THR
3	L	200	THR
3	L	205	ILE
3	L	206	VAL
3	L	207	LYS
3	L	208	SER
3	L	209	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	193	GLN
2	B	4	GLN
2	B	73	ASN
2	B	98	HIS
2	B	163	ASN
2	B	205	ASN
3	C	40	GLN
3	C	93	GLN
3	C	141	ASN
3	C	158	GLN
3	C	159	ASN
1	D	126	HIS
1	D	193	GLN
2	E	4	GLN
2	E	5	GLN
2	E	38	GLN
2	E	81	GLN
2	E	98	HIS
2	E	163	ASN
3	F	5	GLN
3	F	40	GLN
1	G	64	ASN
1	G	104	GLN
1	G	189	GLN
2	H	83	ASN
3	I	37	ASN
3	I	79	ASN
3	I	140	ASN
3	I	198	HIS
1	J	87	ASN
1	J	194	ASN
1	J	223	GLN
2	K	12	GLN
2	K	200	GLN
2	K	205	ASN
3	L	45	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	236/518 (45%)	0.18	14 (5%) 28 21	6, 15, 85, 123	1 (0%)
1	D	222/518 (42%)	0.15	9 (4%) 41 33	8, 18, 41, 108	1 (0%)
1	G	222/518 (42%)	0.11	3 (1%) 73 64	7, 16, 47, 88	1 (0%)
1	J	222/518 (42%)	0.32	9 (4%) 41 33	6, 19, 50, 110	1 (0%)
2	B	218/222 (98%)	0.14	6 (2%) 55 45	8, 16, 30, 47	0
2	E	218/222 (98%)	0.32	11 (5%) 34 26	7, 17, 37, 50	0
2	H	218/222 (98%)	0.29	10 (4%) 37 29	6, 19, 37, 48	0
2	K	218/222 (98%)	0.48	15 (6%) 23 16	10, 23, 40, 64	0
3	C	210/211 (99%)	0.37	10 (4%) 35 28	10, 20, 47, 78	0
3	F	210/211 (99%)	0.33	4 (1%) 66 57	8, 21, 41, 56	0
3	I	210/211 (99%)	0.40	12 (5%) 29 22	11, 23, 49, 69	0
3	L	209/211 (99%)	0.37	10 (4%) 35 28	11, 24, 44, 82	0
All	All	2613/3804 (68%)	0.29	113 (4%) 40 31	6, 19, 44, 123	4 (0%)

All (113) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	427	GLU	6.4
1	D	262	GLY	5.5
1	A	425	ASN	5.5
2	E	107	ALA	5.4
2	K	202	TYR	5.3
1	A	417	GLY	4.7
3	I	184	ASP	4.5
1	A	420	ASP	4.3
1	D	270	THR	4.3
1	D	264	GLY	4.3
1	G	268	SER	4.3

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Mol	Chain	Res	Type	RSRZ
2	E	98	HIS	4.1
3	C	33	ILE	3.8
1	A	416	ASP	3.7
3	L	96	GLU	3.7
3	C	94	THR	3.7
2	B	98	HIS	3.6
2	H	181	SER	3.6
1	J	83	SER	3.5
1	A	426	ALA	3.5
1	J	265	ILE	3.4
2	H	98	HIS	3.4
2	E	103	TYR	3.4
3	L	35	PHE	3.3
3	L	182	THR	3.3
1	D	267	ILE	3.3
3	F	92	GLN	3.3
1	J	264	GLY	3.3
3	I	185	GLU	3.1
1	A	419	LEU	3.1
3	I	186	TYR	3.1
3	I	191	SER	3.1
3	L	155	SER	3.1
2	H	147	GLY	3.1
1	G	265	ILE	3.0
3	I	92	GLN	3.0
1	A	423	THR	3.0
2	K	98	HIS	3.0
3	L	184	ASP	2.9
2	K	104	THR	2.9
1	A	86	ASP	2.9
2	B	54	SER	2.9
3	C	184	ASP	2.9
2	K	53	GLY	2.9
3	I	210	ASN	2.8
1	A	178	GLY	2.8
1	D	263	SER	2.8
1	A	418	PHE	2.7
2	E	105	LEU	2.7
2	H	110	TYR	2.6
2	E	99	GLY	2.6
3	I	7	PRO	2.6
2	E	216	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
3	L	105	THR	2.6
1	G	269	ASP	2.6
3	F	79	ASN	2.6
1	A	422	TRP	2.6
1	D	265	ILE	2.6
1	D	266	ILE	2.5
2	B	180	SER	2.5
2	E	126	GLY	2.5
1	J	98	TYR	2.5
2	H	103	TYR	2.5
2	B	107	ALA	2.5
1	A	260	ASN	2.5
2	E	207	ASN	2.5
3	C	162	LEU	2.4
2	B	215	VAL	2.4
1	J	73	ALA	2.4
1	J	267	ILE	2.4
1	J	212	PRO	2.4
3	C	154	GLY	2.4
3	C	155	SER	2.4
2	K	133	ALA	2.3
2	E	164	SER	2.3
2	K	120	SER	2.3
1	J	266	ILE	2.3
2	H	49	GLY	2.3
3	I	33	ILE	2.3
2	H	48	SER	2.3
2	K	182	GLY	2.3
2	K	121	SER	2.3
3	F	130	SER	2.3
3	I	133	ALA	2.2
3	I	93	GLN	2.2
2	K	141	GLY	2.2
3	I	204	PRO	2.2
3	L	160	GLY	2.2
1	J	263	SER	2.2
3	L	32	GLY	2.2
3	L	209	PHE	2.2
2	K	3	LEU	2.2
1	D	269	ASP	2.2
2	K	101	PRO	2.2
2	K	216	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
3	C	29	SER	2.2
2	B	179	GLN	2.1
1	D	92	PRO	2.1
3	C	153	ASP	2.1
2	E	34	SER	2.1
2	H	180	SER	2.1
2	K	178	LEU	2.1
3	C	27	SER	2.1
3	L	206	VAL	2.1
2	E	101	PRO	2.1
3	C	30	ASN	2.1
2	H	217	LYS	2.0
2	K	183	LEU	2.0
3	F	56	ASN	2.0
3	I	183	LEU	2.0
2	H	173	THR	2.0
1	A	424	TYR	2.0
2	K	180	SER	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	CA	A	601	1/1	0.96	0.15	9,9,9,9	0
4	CA	D	601	1/1	0.96	0.10	7,7,7,7	0
4	CA	G	601	1/1	0.99	0.08	10,10,10,10	0
4	CA	J	601	1/1	0.99	0.09	3,3,3,3	0

6.5 Other polymers [i](#)

There are no such residues in this entry.