



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:07 PM UTC

PDB ID : 1I9R / pdb_00001i9r
Title : STRUCTURE OF CD40L IN COMPLEX WITH THE FAB FRAGMENT OF HUMANIZED 5C8 ANTIBODY
Authors : Karpusas, M.; Lucci, J.; Ferrant, J.; Benjamin, C.; Hsu, Y.-M.
Deposited on : 2001-03-20
Resolution : 3.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

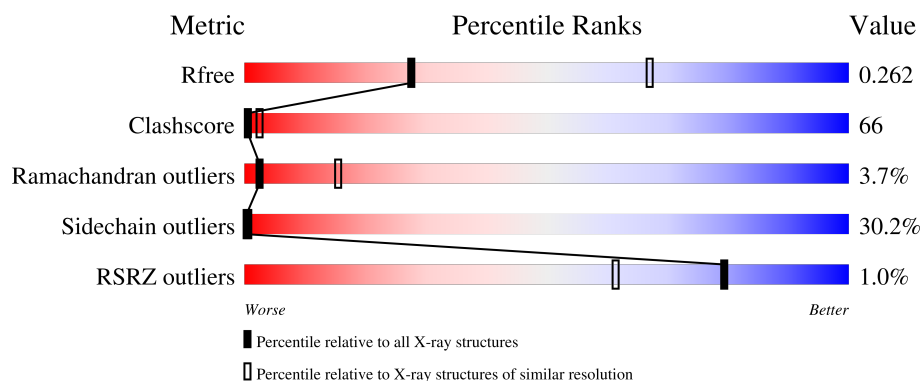
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	146	18% 53% 22% 5%
1	B	146	18% 49% 26%
1	C	146	18% 53% 21% 5%
2	H	219	21% 53% 22%
2	K	219	21% 57% 19%

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Mol	Chain	Length	Quality of chain
2	X	219	% 25%51%22%
3	L	218	26%46%25%
3	M	218	22%50%24%
3	Y	218	% 26%45%25%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13170 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 CD40 LIGAND.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	143	Total	C	N	O	S	8	0	0
			1092	690	191	207	4			
1	B	143	Total	C	N	O	S	8	0	0
			1092	690	191	207	4			
1	C	143	Total	C	N	O	S	8	0	0
			1092	690	191	207	4			

- Molecule 2 is a protein called IMMUNOGLOBULIN H.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	219	Total	C	N	O	S	15	0	0
			1637	1029	269	332	7			
2	K	219	Total	C	N	O	S	15	0	0
			1637	1029	269	332	7			
2	X	219	Total	C	N	O	S	15	0	0
			1637	1029	269	332	7			

- Molecule 3 is a protein called IMMUNOGLOBULIN L.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	215	Total	C	N	O	S	0	0	0
			1660	1043	278	334	5			
3	M	215	Total	C	N	O	S	0	0	0
			1660	1043	278	334	5			
3	Y	215	Total	C	N	O	S	0	0	0
			1660	1043	278	334	5			

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	1	Total	Zn	0	0
			1	1		

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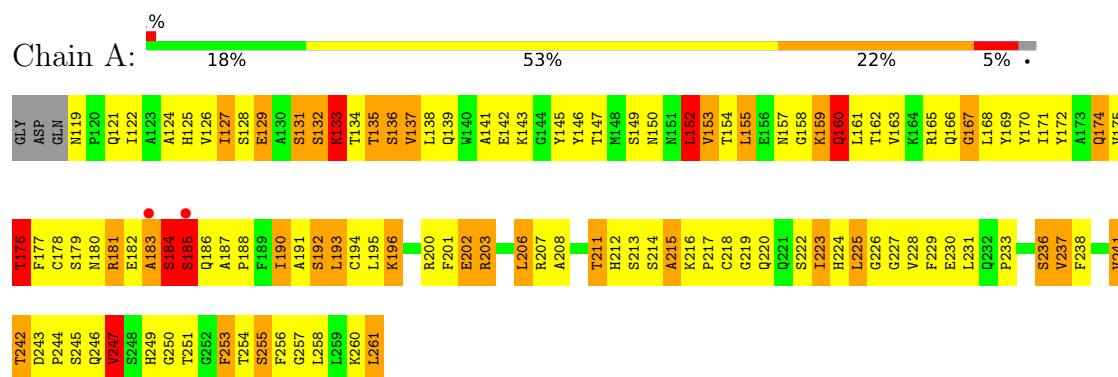
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	K	1	Total 1	Zn 1	0	0
4	X	1	Total 1	Zn 1	0	0

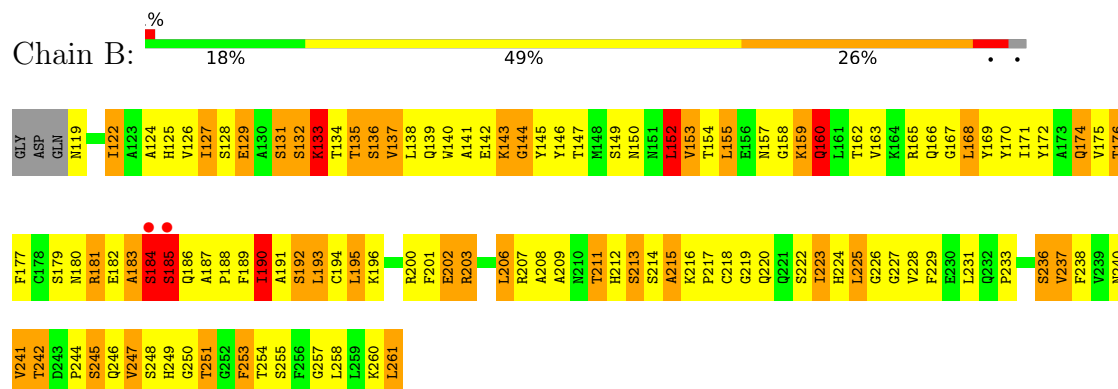
3 Residue-property plots [i](#)

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

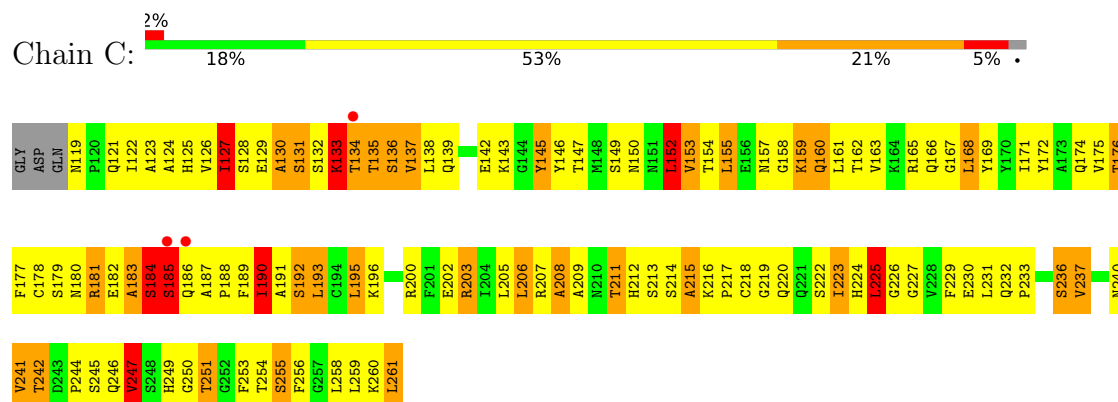
• Molecule 1: CD40 LIGAND



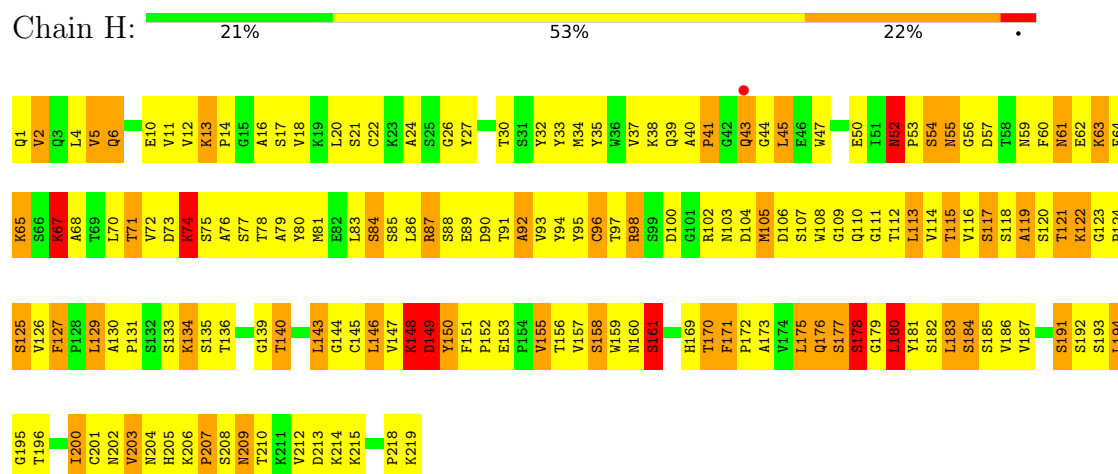
• Molecule 1: CD40 LIGAND



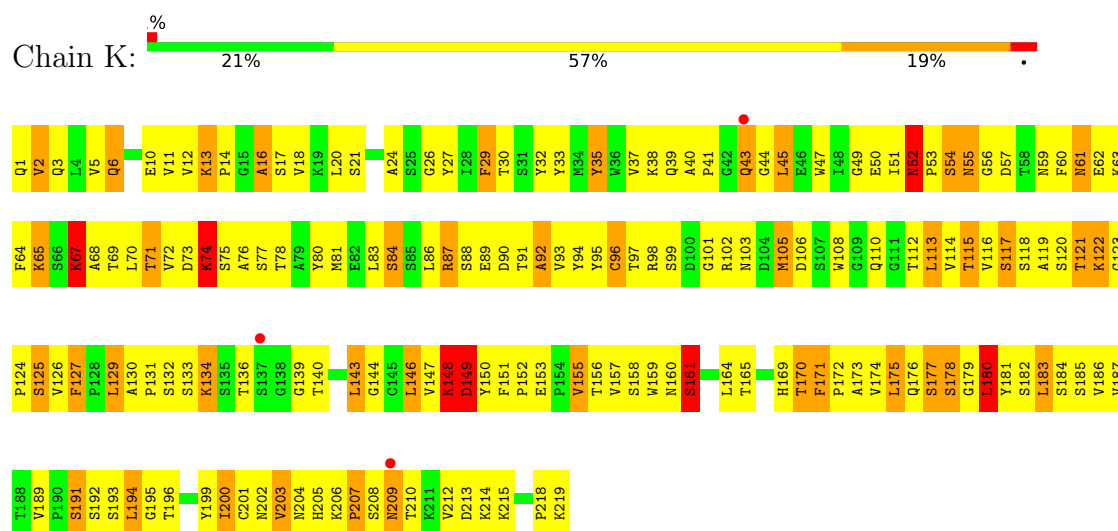
• Molecule 1: CD40 LIGAND



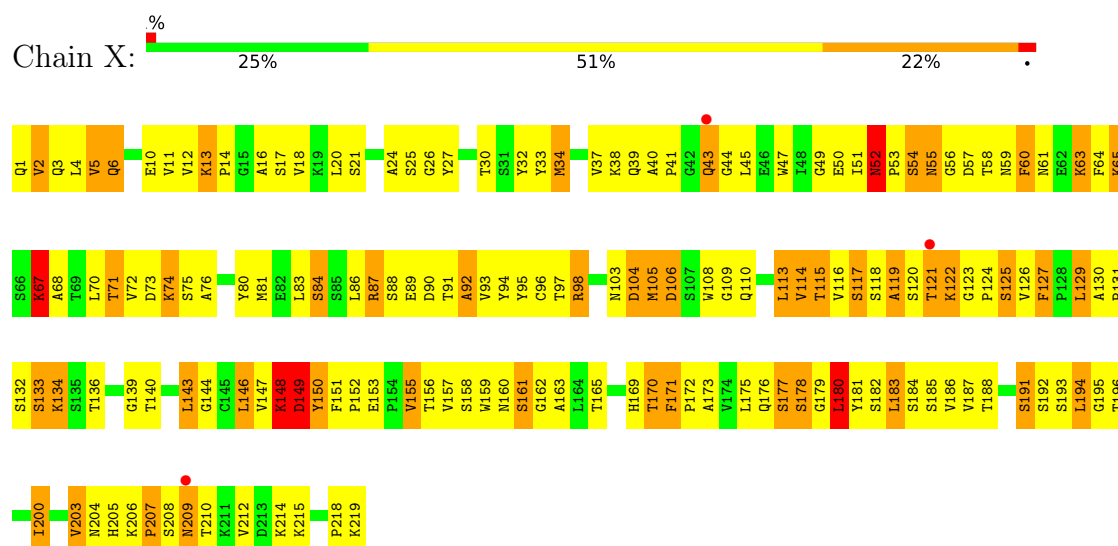
• Molecule 2: IMMUNOGLOBULIN H



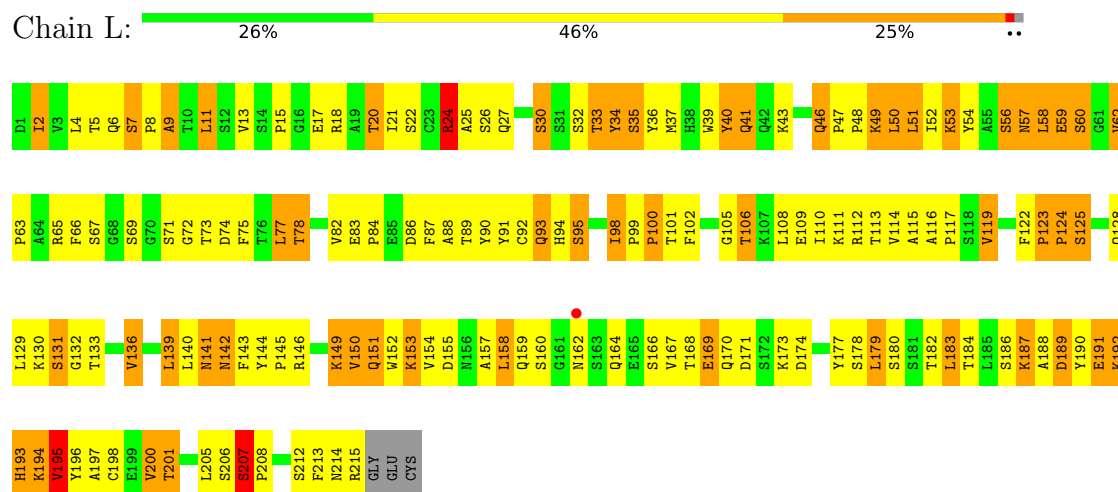
• Molecule 2: IMMUNOGLOBULIN H



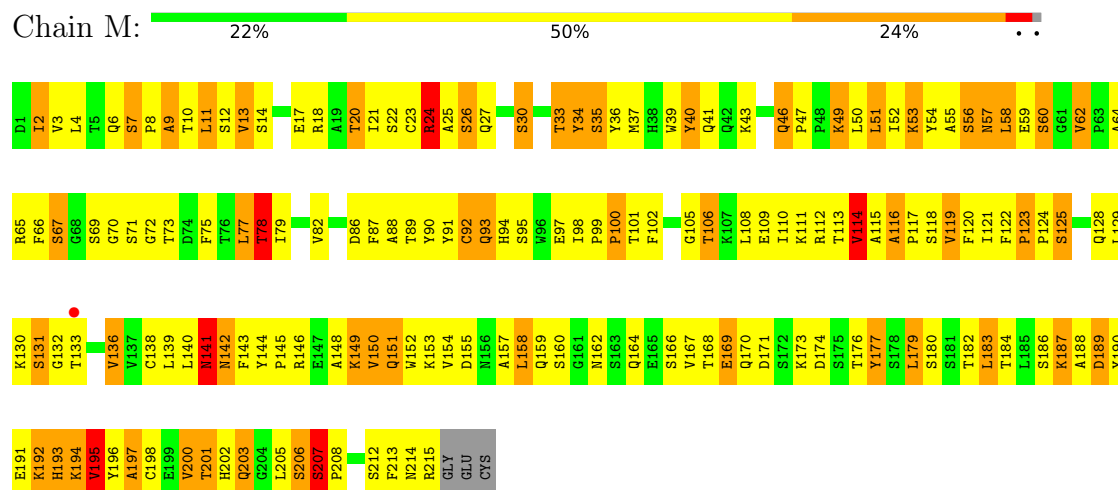
• Molecule 2: IMMUNOGLOBULIN H



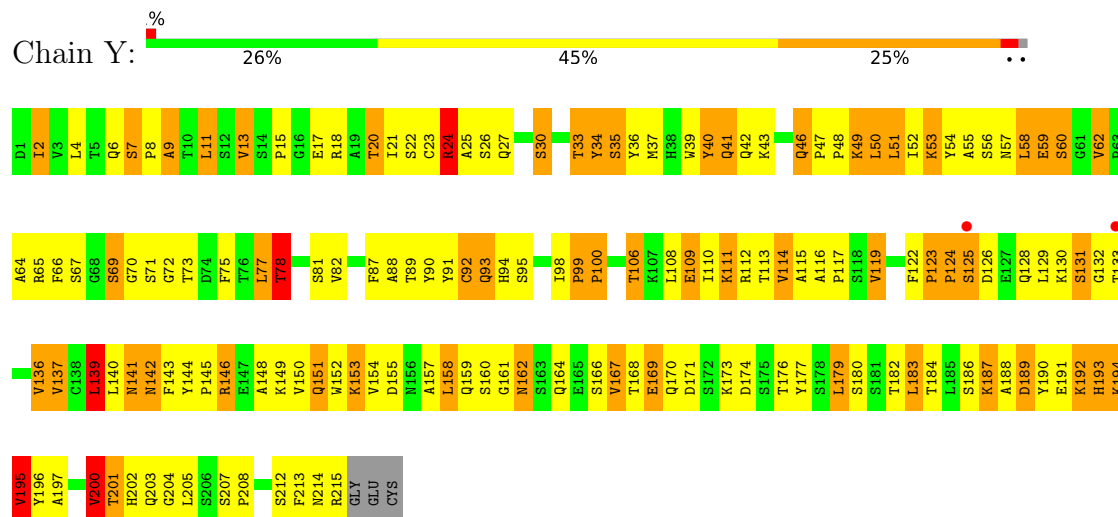
● Molecule 3: IMMUNOGLOBULIN L



● Molecule 3: IMMUNOGLOBULIN L



● Molecule 3: IMMUNOGLOBULIN L



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	224.48Å 129.91Å 96.49Å 90.00° 109.60° 90.00°	Depositor
Resolution (Å)	35.00 – 3.10 35.00 – 3.10	Depositor EDS
% Data completeness (in resolution range)	(Not available) (35.00-3.10) 96.5 (35.00-3.10)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.21 (at 2.64Å)	Xtriage
Refinement program	X-PLOR 98.0	Depositor
R, R_{free}	0.233 , 0.285 0.212 , 0.262	Depositor DCC
R_{free} test set	4671 reflections (10.04%)	wwPDB-VP
Wilson B-factor (Å ²)	41.6	Xtriage
Anisotropy	0.448	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 72.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	13170	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.29% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	1.07	0/1115	1.33	12/1510 (0.8%)
1	B	1.18	3/1115 (0.3%)	1.31	8/1510 (0.5%)
1	C	1.11	4/1115 (0.4%)	1.32	9/1510 (0.6%)
2	H	0.86	0/1674	1.35	24/2277 (1.1%)
2	K	0.95	0/1674	1.35	22/2277 (1.0%)
2	X	0.97	2/1674 (0.1%)	1.37	23/2277 (1.0%)
3	L	0.98	1/1701 (0.1%)	1.32	22/2314 (1.0%)
3	M	1.07	2/1701 (0.1%)	1.38	28/2314 (1.2%)
3	Y	1.04	1/1701 (0.1%)	1.36	25/2314 (1.1%)
All	All	1.02	13/13470 (0.1%)	1.35	173/18303 (0.9%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
2	H	0	1
2	K	0	2
3	M	0	1
All	All	0	5

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	X	5	VAL	CA-CB	-7.21	1.45	1.53
1	C	237	VAL	CA-CB	-6.65	1.44	1.54
3	M	114	VAL	CA-CB	-6.41	1.45	1.54
2	X	34	MET	SD-CE	6.22	1.95	1.79
1	B	228	VAL	CA-CB	-6.07	1.46	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	64	ALA	CA-CB	-6.00	1.42	1.53
1	B	190	ILE	CA-CB	5.77	1.61	1.54
1	C	190	ILE	CA-CB	5.59	1.62	1.54
3	Y	137	VAL	CA-CB	-5.55	1.47	1.54
1	C	130	ALA	CA-CB	-5.41	1.44	1.53
3	L	98	ILE	CA-CB	-5.40	1.47	1.54
1	B	122	ILE	C-O	-5.33	1.18	1.24
1	C	208	ALA	CA-C	-5.07	1.46	1.52

All (173) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	56	GLY	N-CA-C	-13.12	99.54	113.58
2	K	56	GLY	N-CA-C	-11.57	100.71	114.48
2	X	106	ASP	N-CA-C	11.08	126.90	113.16
1	C	247	VAL	N-CA-C	-10.74	98.35	110.05
2	H	106	ASP	N-CA-C	10.58	126.00	113.20
2	K	106	ASP	N-CA-C	10.46	125.85	113.20
1	A	247	VAL	N-CA-C	-10.39	98.47	110.21
2	X	56	GLY	N-CA-C	-9.80	102.02	114.37
2	K	52	ASN	N-CA-C	-9.62	97.70	109.72
2	H	52	ASN	N-CA-C	-8.95	96.80	109.24
2	X	55	ASN	N-CA-C	8.32	121.98	111.24
1	B	136	SER	N-CA-C	-8.18	102.86	113.17
2	H	55	ASN	N-CA-C	8.15	121.75	111.24
3	M	92	CYS	N-CA-C	-8.14	97.00	109.95
2	X	129	LEU	N-CA-C	-8.06	92.40	107.71
1	C	136	SER	N-CA-C	-8.05	102.51	113.30
2	X	61	ASN	N-CA-C	-7.94	97.10	109.25
2	K	52	ASN	CA-C-N	-7.93	111.63	119.64
2	K	52	ASN	C-N-CA	-7.93	111.63	119.64
3	L	41	GLN	N-CA-C	-7.75	97.63	109.95
3	L	24	ARG	N-CA-C	7.71	121.38	108.13
1	A	184	SER	N-CA-C	-7.70	102.52	112.23
3	L	162	ASN	N-CA-C	7.68	120.94	108.34
1	C	184	SER	N-CA-C	-7.68	102.55	112.23
3	M	24	ARG	N-CA-C	7.61	121.22	108.13
1	A	136	SER	N-CA-C	-7.54	104.10	113.38
2	X	52	ASN	CA-C-N	-7.49	111.99	119.56
2	X	52	ASN	C-N-CA	-7.49	111.99	119.56
1	B	184	SER	N-CA-C	-7.49	102.80	112.23
2	H	129	LEU	N-CA-C	-7.48	93.50	107.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	X	96	CYS	N-CA-C	-7.41	97.67	109.59
3	M	123	PRO	CA-C-N	7.40	129.09	119.84
3	M	123	PRO	C-N-CA	7.40	129.09	119.84
2	K	129	LEU	N-CA-C	-7.39	93.67	107.71
2	K	55	ASN	N-CA-C	7.33	120.70	111.24
3	Y	24	ARG	N-CA-C	7.25	120.60	108.13
2	K	125	SER	N-CA-C	-7.17	98.25	109.72
2	H	130	ALA	N-CA-C	7.09	118.84	109.83
3	Y	92	CYS	N-CA-C	-7.05	98.75	109.95
3	M	162	ASN	N-CA-C	7.02	120.62	108.76
2	X	52	ASN	N-CA-C	-7.01	99.49	109.24
1	B	237	VAL	N-CA-C	6.96	119.47	108.89
2	H	52	ASN	CA-C-N	-6.93	112.64	119.64
2	H	52	ASN	C-N-CA	-6.93	112.64	119.64
1	A	167	GLY	N-CA-C	6.92	119.97	110.56
2	K	130	ALA	N-CA-C	6.84	118.52	109.83
3	Y	111	LYS	N-CA-C	-6.81	101.51	110.43
2	X	87	ARG	N-CA-C	-6.80	99.32	109.86
2	H	61	ASN	N-CA-C	-6.77	98.20	108.96
3	L	193	HIS	N-CA-C	6.76	119.68	109.41
3	M	207	SER	N-CA-C	6.75	114.20	108.13
1	A	152	LEU	N-CA-C	-6.73	105.04	113.18
2	H	67	LYS	N-CA-C	6.68	119.57	111.82
2	K	61	ASN	N-CA-C	-6.65	98.38	108.96
3	Y	15	PRO	N-CA-C	-6.60	100.71	111.21
2	H	127	PHE	CA-C-N	-6.60	113.19	119.85
2	H	127	PHE	C-N-CA	-6.60	113.19	119.85
3	M	100	PRO	N-CA-C	-6.59	100.89	111.38
2	X	125	SER	N-CA-C	-6.58	99.19	109.72
2	X	148	LYS	N-CA-C	6.53	120.71	110.32
2	K	171	PHE	N-CA-C	6.53	119.48	110.01
3	Y	62	VAL	CA-C-N	6.51	126.43	119.85
3	Y	62	VAL	C-N-CA	6.51	126.43	119.85
2	H	96	CYS	N-CA-C	-6.51	99.11	109.59
2	H	171	PHE	N-CA-C	6.50	119.44	110.01
2	H	148	LYS	N-CA-C	6.48	120.62	110.32
2	K	87	ARG	N-CA-C	-6.45	100.36	110.36
3	Y	90	TYR	N-CA-C	6.44	119.96	109.59
2	X	5	VAL	N-CA-C	6.41	115.95	106.85
3	Y	162	ASN	N-CA-C	6.41	119.59	108.76
3	L	123	PRO	CA-C-N	6.39	127.83	119.84
3	L	123	PRO	C-N-CA	6.39	127.83	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	15	PRO	N-CA-C	-6.32	101.16	111.21
3	M	64	ALA	N-CA-C	6.30	120.06	112.38
3	Y	59	GLU	N-CA-C	-6.21	102.77	110.41
3	M	116	ALA	CA-C-N	-6.20	113.90	120.66
3	M	116	ALA	C-N-CA	-6.20	113.90	120.66
3	M	97	GLU	CA-C-N	-6.14	117.39	123.04
3	M	97	GLU	C-N-CA	-6.14	117.39	123.04
2	H	87	ARG	N-CA-C	-6.14	100.85	110.36
2	H	180	LEU	N-CA-C	6.13	119.60	110.52
2	K	96	CYS	N-CA-C	-6.12	99.74	109.59
2	X	68	ALA	N-CA-C	6.12	119.62	110.14
2	K	67	LYS	N-CA-C	6.06	118.85	111.82
2	X	171	PHE	N-CA-C	6.05	118.78	110.01
3	Y	193	HIS	N-CA-C	6.01	119.00	109.81
2	K	68	ALA	N-CA-C	5.95	119.37	110.14
2	H	176	GLN	N-CA-C	-5.95	103.10	110.41
2	H	5	VAL	N-CA-C	5.92	115.26	106.85
3	Y	195	VAL	N-CA-C	5.92	116.38	107.80
3	M	62	VAL	CA-C-N	5.91	125.82	119.85
3	M	62	VAL	C-N-CA	5.91	125.82	119.85
3	Y	167	VAL	N-CA-C	5.89	117.33	108.96
3	L	32	SER	N-CA-C	5.89	120.08	113.01
2	H	68	ALA	N-CA-C	5.89	119.27	110.14
1	B	152	LEU	N-CA-C	-5.86	105.62	112.89
3	M	195	VAL	N-CA-C	5.86	116.30	107.80
2	H	125	SER	N-CA-C	-5.83	99.89	109.40
3	Y	99	PRO	CA-C-N	-5.83	113.97	119.85
3	Y	99	PRO	C-N-CA	-5.83	113.97	119.85
2	K	127	PHE	CA-C-N	-5.79	114.00	119.85
2	K	127	PHE	C-N-CA	-5.79	114.00	119.85
1	A	170	TYR	N-CA-C	-5.77	99.33	108.73
3	M	148	ALA	N-CA-C	5.75	116.98	107.20
3	Y	9	ALA	N-CA-C	-5.75	104.62	111.69
3	M	193	HIS	N-CA-C	5.75	118.14	109.41
2	X	127	PHE	CA-C-N	-5.74	114.02	119.76
2	X	127	PHE	C-N-CA	-5.74	114.02	119.76
2	K	101	GLY	N-CA-C	-5.73	106.25	115.08
1	B	253	PHE	N-CA-C	5.73	118.63	111.24
3	M	51	LEU	CA-C-N	-5.72	114.99	122.94
3	M	51	LEU	C-N-CA	-5.72	114.99	122.94
3	L	9	ALA	N-CA-C	-5.71	104.67	111.69
3	L	195	VAL	N-CA-C	5.69	116.14	108.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Y	123	PRO	CA-C-N	5.67	126.93	119.84
3	Y	123	PRO	C-N-CA	5.67	126.93	119.84
3	L	100	PRO	N-CA-C	-5.66	102.38	111.38
2	X	104	ASP	N-CA-C	-5.66	101.91	110.28
3	Y	148	ALA	N-CA-C	5.62	116.61	107.23
3	Y	35	SER	N-CA-C	-5.61	99.26	108.41
1	A	174	GLN	N-CA-C	-5.60	100.06	109.07
1	C	127	ILE	N-CA-C	5.58	117.36	108.87
1	A	237	VAL	N-CA-C	5.56	117.41	108.85
1	B	160	GLN	N-CA-C	5.55	117.06	109.18
2	X	3	GLN	N-CA-C	5.53	118.23	109.50
2	K	3	GLN	N-CA-C	5.50	118.19	109.50
1	C	225	LEU	N-CA-C	5.49	117.38	108.26
2	H	178	SER	N-CA-C	-5.48	99.12	110.80
3	L	182	THR	N-CA-C	5.48	118.47	107.41
1	B	167	GLY	N-CA-C	5.45	117.97	110.56
3	Y	100	PRO	N-CA-C	-5.43	102.74	111.38
3	L	207	SER	N-CA-C	5.38	112.97	108.13
2	H	140	THR	N-CA-C	5.37	118.81	110.17
3	Y	200	VAL	N-CA-C	5.37	116.31	108.53
3	M	9	ALA	N-CA-C	-5.36	105.52	111.36
1	C	152	LEU	N-CA-C	-5.36	106.58	113.01
3	L	59	GLU	N-CA-C	-5.36	103.46	110.53
2	X	180	LEU	N-CA-C	5.35	118.43	110.52
1	A	253	PHE	N-CA-C	5.34	118.14	111.24
3	M	182	THR	N-CA-C	5.33	118.17	107.41
1	A	257	GLY	N-CA-C	5.33	118.49	110.18
3	L	141	ASN	N-CA-C	5.33	118.79	110.32
3	L	24	ARG	CG-CD-NE	-5.28	100.39	112.00
3	M	35	SER	N-CA-C	-5.26	99.83	108.41
3	M	206	SER	N-CA-C	-5.24	105.99	112.38
3	Y	64	ALA	N-CA-C	5.23	118.77	112.38
3	L	86	ASP	N-CA-C	5.22	117.72	111.71
3	Y	41	GLN	N-CA-C	-5.22	101.65	109.95
3	M	141	ASN	N-CA-C	5.20	118.17	110.48
1	A	176	THR	N-CA-C	-5.18	101.43	109.72
1	C	232	GLN	CA-C-N	-5.16	114.25	119.83
1	C	232	GLN	C-N-CA	-5.16	114.25	119.83
2	K	148	LYS	N-CA-C	5.16	118.48	110.17
2	X	60	PHE	N-CA-C	5.16	118.14	110.14
3	L	62	VAL	CA-C-N	5.15	125.06	119.85
3	L	62	VAL	C-N-CA	5.15	125.06	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	197	ALA	N-CA-C	5.14	117.73	108.48
2	K	29	PHE	N-CA-C	5.13	117.27	111.11
2	X	130	ALA	N-CA-C	5.13	117.73	110.24
3	M	99	PRO	CA-C-N	-5.11	114.69	119.85
3	M	99	PRO	C-N-CA	-5.11	114.69	119.85
2	X	67	LYS	N-CA-C	5.10	117.74	111.82
1	C	237	VAL	N-CA-C	5.07	117.05	109.20
3	L	26	SER	N-CA-C	-5.05	106.94	113.01
3	L	35	SER	N-CA-C	-5.05	100.17	108.41
1	B	174	GLN	N-CA-C	-5.05	101.00	109.24
3	Y	78	THR	N-CA-C	5.05	117.63	108.69
3	Y	139	LEU	N-CA-C	5.05	116.64	108.26
1	A	160	GLN	N-CA-C	5.04	117.07	109.41
3	L	24	ARG	NE-CZ-NH2	-5.03	114.67	119.20
2	K	180	LEU	N-CA-C	5.02	117.95	110.52
3	M	78	THR	N-CA-C	5.01	117.56	108.69
2	H	145	CYS	N-CA-C	5.01	117.66	109.59

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	145	TYR	Sidechain
2	H	35	TYR	Sidechain
2	K	32	TYR	Sidechain
2	K	35	TYR	Sidechain
3	M	177	TYR	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1092	0	1085	155	0
1	B	1092	0	1085	176	0
1	C	1092	0	1085	164	0
2	H	1637	0	1606	214	0
2	K	1637	0	1606	193	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	X	1637	0	1606	223	0
3	L	1660	0	1610	220	3
3	M	1660	0	1610	215	1
3	Y	1660	0	1610	235	3
4	H	1	0	0	0	0
4	K	1	0	0	0	0
4	X	1	0	0	0	0
All	All	13170	0	12903	1698	4

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 66.

All (1698) 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)
3:Y:13:VAL:HG22	3:Y:17:GLU:HB3	1.25	1.10
3:L:13:VAL:HG22	3:L:17:GLU:HB3	1.30	1.09
2:K:91:THR:HG23	2:K:115:THR:HA	1.29	1.08
2:H:91:THR:HG23	2:H:115:THR:HA	1.32	1.08
2:H:124:PRO:HD2	2:H:210:THR:HG21	1.31	1.08
2:K:124:PRO:HD2	2:K:210:THR:HG21	1.30	1.07
3:M:13:VAL:HG22	3:M:17:GLU:HB3	1.20	1.07
1:C:181:ARG:HG3	1:C:182:GLU:H	1.19	1.05
2:X:91:THR:HG23	2:X:115:THR:HA	1.37	1.04
1:C:166:GLN:HB3	1:C:233:PRO:HD3	1.39	1.03
2:X:124:PRO:HD2	2:X:210:THR:HG21	1.34	1.03
1:B:181:ARG:HG3	1:B:182:GLU:H	1.22	1.01
3:Y:146:ARG:HH12	3:Y:167:VAL:HG21	1.25	1.01
3:L:117:PRO:HB3	3:L:143:PHE:HB3	1.43	1.00
1:B:187:ALA:HB1	1:B:188:PRO:HD2	1.44	0.99
1:A:181:ARG:HG3	1:A:182:GLU:H	1.24	0.97
3:Y:117:PRO:HD2	3:Y:205:LEU:HD13	1.47	0.96
3:Y:117:PRO:HD2	3:Y:205:LEU:CD1	1.96	0.95
3:M:13:VAL:HG11	3:M:82:VAL:HG21	1.47	0.95
1:C:261:LEU:N	1:C:261:LEU:HD23	1.82	0.95
3:Y:179:LEU:HD23	3:Y:180:SER:N	1.82	0.95
1:A:186:GLN:HE21	1:A:212:HIS:HE1	1.12	0.94
3:Y:50:LEU:HD12	3:Y:51:LEU:N	1.82	0.94
3:Y:117:PRO:HB3	3:Y:143:PHE:HB3	1.48	0.94
2:H:6:GLN:N	2:H:110:GLN:HE22	1.64	0.93
1:A:187:ALA:HB1	1:A:188:PRO:HD2	1.50	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:166:GLN:HB3	1:B:233:PRO:HD3	1.49	0.93
3:M:41:GLN:HB3	3:M:51:LEU:HD11	1.46	0.93
1:A:196:LYS:HE2	1:A:200:ARG:O	1.67	0.93
1:B:150:ASN:OD1	1:B:152:LEU:HB2	1.69	0.92
1:B:186:GLN:HE21	1:B:212:HIS:HE1	1.18	0.92
3:L:33:THR:HB	3:L:34:TYR:CD1	2.04	0.92
3:M:117:PRO:HD2	3:M:205:LEU:HD13	1.50	0.91
1:C:187:ALA:HB1	1:C:188:PRO:HD2	1.53	0.91
2:K:176:GLN:HA	3:M:164:GLN:HE22	1.34	0.91
1:C:186:GLN:HE21	1:C:212:HIS:HE1	1.19	0.91
2:K:205:HIS:HB3	2:K:210:THR:HB	1.51	0.90
3:M:117:PRO:HD2	3:M:205:LEU:CD1	2.01	0.89
3:L:146:ARG:HH12	3:L:167:VAL:HG21	1.36	0.89
3:L:110:ILE:H	3:L:170:GLN:HE22	1.15	0.89
3:M:17:GLU:OE2	3:M:111:LYS:NZ	2.05	0.89
3:M:58:LEU:HD23	3:M:62:VAL:HB	1.53	0.89
3:M:123:PRO:HB3	3:M:213:PHE:CZ	2.07	0.89
3:L:201:THR:HG23	3:L:208:PRO:HG3	1.54	0.88
2:X:6:GLN:N	2:X:110:GLN:HE22	1.71	0.88
3:Y:58:LEU:HD23	3:Y:62:VAL:HB	1.53	0.88
3:M:179:LEU:HD23	3:M:180:SER:N	1.87	0.88
1:A:181:ARG:O	1:A:185:SER:HA	1.74	0.88
3:Y:110:ILE:H	3:Y:170:GLN:HE22	1.14	0.88
3:L:41:GLN:HB3	3:L:51:LEU:HD11	1.56	0.88
3:Y:13:VAL:HG11	3:Y:82:VAL:HG21	1.55	0.88
2:X:176:GLN:HA	3:Y:164:GLN:HE22	1.39	0.88
3:Y:123:PRO:HB3	3:Y:213:PHE:CZ	2.09	0.88
1:C:190:ILE:H	1:C:242:THR:HG21	1.38	0.87
2:K:131:PRO:HD3	2:K:143:LEU:HB2	1.57	0.87
3:Y:33:THR:HB	3:Y:34:TYR:CD1	2.10	0.87
1:A:190:ILE:H	1:A:242:THR:HG21	1.39	0.87
3:M:117:PRO:HB3	3:M:143:PHE:HB3	1.56	0.87
3:M:197:ALA:HB2	3:M:212:SER:HB3	1.56	0.87
2:H:176:GLN:HA	3:L:164:GLN:HE22	1.36	0.87
3:M:33:THR:HB	3:M:34:TYR:CD1	2.10	0.86
3:M:13:VAL:HG22	3:M:17:GLU:CB	2.05	0.86
3:L:30:SER:HB3	3:L:72:GLY:H	1.41	0.86
3:Y:30:SER:HB3	3:Y:72:GLY:H	1.40	0.85
2:K:6:GLN:N	2:K:110:GLN:HE22	1.74	0.85
1:B:190:ILE:H	1:B:242:THR:HG21	1.41	0.85
1:C:181:ARG:HG3	1:C:182:GLU:N	1.91	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:146:ARG:HH12	3:M:167:VAL:HG21	1.42	0.85
3:L:123:PRO:HB3	3:L:213:PHE:CZ	2.12	0.84
3:L:4:LEU:HD13	3:L:37:MET:HE1	1.60	0.84
1:B:181:ARG:O	1:B:185:SER:HA	1.78	0.83
3:L:58:LEU:HD23	3:L:62:VAL:HB	1.59	0.83
3:M:110:ILE:H	3:M:170:GLN:HE22	1.20	0.83
3:L:117:PRO:HD2	3:L:205:LEU:CD1	2.08	0.83
2:X:87:ARG:O	2:X:116:VAL:HG21	1.78	0.83
3:Y:146:ARG:NH1	3:Y:167:VAL:HG21	1.92	0.83
2:X:205:HIS:HB3	2:X:210:THR:HB	1.61	0.82
1:C:181:ARG:O	1:C:185:SER:HA	1.79	0.82
1:C:135:THR:HB	1:C:137:VAL:HG12	1.61	0.82
1:C:160:GLN:HB2	1:C:237:VAL:O	1.80	0.82
3:L:33:THR:HB	3:L:34:TYR:HD1	1.41	0.82
2:H:6:GLN:N	2:H:110:GLN:NE2	2.27	0.82
3:L:50:LEU:HD12	3:L:51:LEU:N	1.94	0.82
3:Y:159:GLN:HE21	3:Y:183:LEU:HD11	1.44	0.82
1:A:261:LEU:N	1:A:261:LEU:HD23	1.91	0.81
1:A:182:GLU:O	1:A:185:SER:HB2	1.81	0.81
2:K:87:ARG:O	2:K:116:VAL:HG21	1.80	0.81
3:M:30:SER:HB3	3:M:72:GLY:H	1.44	0.81
3:Y:201:THR:HG23	3:Y:208:PRO:HG3	1.62	0.81
1:A:203:ARG:HE	1:C:145:TYR:HB2	1.46	0.81
2:H:6:GLN:H	2:H:110:GLN:NE2	1.77	0.81
1:B:181:ARG:HG3	1:B:182:GLU:N	1.92	0.81
2:H:205:HIS:HB3	2:H:210:THR:HB	1.61	0.81
1:A:181:ARG:HG3	1:A:182:GLU:N	1.95	0.81
3:L:117:PRO:HD2	3:L:205:LEU:HD13	1.62	0.80
2:H:170:THR:HB	2:H:185:SER:OG	1.81	0.80
3:Y:33:THR:HB	3:Y:34:TYR:HD1	1.44	0.80
1:B:135:THR:HB	1:B:137:VAL:HG12	1.61	0.80
3:Y:197:ALA:HB2	3:Y:212:SER:HB3	1.62	0.80
1:C:171:ILE:CG2	1:C:193:LEU:HD11	2.11	0.80
2:K:146:LEU:C	2:K:146:LEU:HD12	2.06	0.80
1:B:145:TYR:HB2	1:C:203:ARG:HE	1.47	0.80
3:M:51:LEU:HA	3:M:62:VAL:HG21	1.64	0.80
2:K:170:THR:HB	2:K:185:SER:OG	1.81	0.80
3:Y:13:VAL:HG22	3:Y:17:GLU:CB	2.11	0.80
3:Y:41:GLN:HB3	3:Y:51:LEU:HD11	1.61	0.80
2:H:131:PRO:HD3	2:H:143:LEU:HB2	1.61	0.79
1:C:196:LYS:HE2	1:C:200:ARG:O	1.83	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:179:LEU:HD23	3:L:180:SER:N	1.97	0.79
3:L:13:VAL:HG11	3:L:82:VAL:HG21	1.63	0.79
2:X:37:VAL:HG21	2:X:105:MET:HE1	1.65	0.78
2:X:40:ALA:HB3	2:X:43:GLN:HB3	1.65	0.78
1:A:139:GLN:HE22	1:A:159:LYS:HD3	1.47	0.78
2:K:123:GLY:HA2	2:K:205:HIS:HD2	1.48	0.78
3:M:33:THR:HB	3:M:34:TYR:HD1	1.46	0.78
1:A:176:THR:HG21	1:A:253:PHE:HD1	1.47	0.78
3:L:197:ALA:HB2	3:L:212:SER:HB3	1.66	0.78
3:M:41:GLN:HB3	3:M:51:LEU:CD1	2.14	0.78
3:M:159:GLN:HE21	3:M:183:LEU:HD11	1.49	0.77
3:M:4:LEU:HA	3:M:24:ARG:O	1.84	0.77
2:X:146:LEU:C	2:X:146:LEU:HD12	2.09	0.77
2:K:93:VAL:HG22	2:K:113:LEU:HD23	1.67	0.77
2:H:50:GLU:HG2	2:H:59:ASN:HB2	1.66	0.77
2:K:55:ASN:HB3	2:K:57:ASP:H	1.49	0.77
2:X:6:GLN:N	2:X:110:GLN:NE2	2.32	0.77
1:B:169:TYR:CZ	1:B:260:LYS:HD2	2.20	0.77
2:X:131:PRO:HD3	2:X:143:LEU:HB2	1.67	0.76
1:C:136:SER:HB2	1:C:241:VAL:O	1.86	0.76
1:C:176:THR:HB	1:C:222:SER:OG	1.84	0.76
1:A:157:ASN:HB3	1:A:159:LYS:CG	2.16	0.76
1:A:142:GLU:HG2	1:A:146:TYR:CE2	2.20	0.76
1:A:145:TYR:HB2	1:B:203:ARG:HE	1.50	0.76
1:B:139:GLN:HE22	1:B:159:LYS:HD3	1.50	0.76
1:B:169:TYR:CE2	1:B:260:LYS:HB2	2.21	0.76
2:K:147:VAL:HG11	2:K:155:VAL:HG21	1.67	0.76
3:L:136:VAL:HG22	3:L:152:TRP:HH2	1.51	0.75
3:M:119:VAL:HG11	3:M:200:VAL:HG11	1.67	0.75
3:L:4:LEU:HA	3:L:24:ARG:O	1.87	0.75
1:C:182:GLU:O	1:C:185:SER:HB2	1.85	0.75
3:L:17:GLU:OE2	3:L:111:LYS:NZ	2.16	0.75
2:K:6:GLN:N	2:K:110:GLN:NE2	2.35	0.75
1:A:135:THR:HB	1:A:137:VAL:HG12	1.67	0.75
1:B:143:LYS:NZ	2:K:103:ASN:HD21	1.84	0.75
2:H:93:VAL:HG22	2:H:113:LEU:HD23	1.69	0.75
3:Y:112:ARG:HD2	3:Y:144:TYR:CG	2.20	0.75
1:A:171:ILE:O	1:A:226:GLY:HA2	1.87	0.74
2:H:87:ARG:O	2:H:116:VAL:HG21	1.87	0.74
3:Y:17:GLU:OE2	3:Y:111:LYS:NZ	2.18	0.74
3:Y:136:VAL:HG13	3:Y:183:LEU:HB3	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Y:151:GLN:HG2	3:Y:158:LEU:HD21	1.69	0.74
1:B:182:GLU:O	1:B:185:SER:HB2	1.87	0.74
3:M:116:ALA:HB1	3:M:205:LEU:CD1	2.17	0.74
1:C:180:ASN:HB3	1:C:183:ALA:CB	2.18	0.74
3:M:17:GLU:OE1	3:M:111:LYS:HE3	1.87	0.74
1:A:171:ILE:CG2	1:A:193:LEU:HD11	2.18	0.74
3:L:159:GLN:HE21	3:L:183:LEU:HD11	1.52	0.74
1:C:157:ASN:HB3	1:C:159:LYS:CG	2.18	0.74
2:K:95:TYR:CE1	3:M:47:PRO:HB3	2.23	0.74
2:X:169:HIS:CD2	3:Y:141:ASN:HD21	2.06	0.74
3:L:51:LEU:HD23	3:L:62:VAL:HG13	1.70	0.73
3:M:116:ALA:HB1	3:M:205:LEU:HD12	1.69	0.73
3:M:136:VAL:HG13	3:M:183:LEU:HB3	1.70	0.73
3:M:146:ARG:HB2	3:M:177:TYR:CE2	2.23	0.73
1:B:135:THR:HB	1:B:137:VAL:CG1	2.18	0.73
1:B:244:PRO:O	1:B:246:GLN:N	2.21	0.73
2:H:147:VAL:HG11	2:H:155:VAL:HG21	1.68	0.73
1:C:171:ILE:HG21	1:C:193:LEU:HD11	1.70	0.73
3:L:146:ARG:NH1	3:L:167:VAL:HG21	2.04	0.73
2:X:50:GLU:HG2	2:X:59:ASN:HB2	1.71	0.73
3:Y:192:LYS:HE3	3:Y:193:HIS:CD2	2.23	0.73
1:B:206:LEU:HD21	1:B:226:GLY:O	1.88	0.73
1:A:172:TYR:CZ	1:B:227:GLY:HA2	2.23	0.72
3:L:13:VAL:HG22	3:L:17:GLU:CB	2.16	0.72
3:L:195:VAL:HG12	3:L:214:ASN:ND2	2.04	0.72
3:Y:30:SER:HA	3:Y:35:SER:HA	1.71	0.72
2:H:116:VAL:HG23	2:H:116:VAL:O	1.88	0.72
3:M:4:LEU:HD13	3:M:37:MET:HE1	1.70	0.72
1:B:153:VAL:HG23	1:B:163:VAL:HG12	1.70	0.72
3:Y:21:ILE:HG22	3:Y:22:SER:N	2.03	0.72
2:H:183:LEU:HD12	2:H:183:LEU:C	2.15	0.72
2:H:43:GLN:NE2	2:H:44:GLY:H	1.87	0.72
2:X:129:LEU:HD21	2:X:146:LEU:HB2	1.72	0.72
1:B:136:SER:HB2	1:B:241:VAL:O	1.89	0.71
1:A:172:TYR:HA	1:A:225:LEU:O	1.90	0.71
2:H:155:VAL:HG13	2:H:155:VAL:O	1.90	0.71
3:M:201:THR:HG23	3:M:208:PRO:HG3	1.71	0.71
1:A:157:ASN:HB3	1:A:159:LYS:HG2	1.72	0.71
1:A:180:ASN:HB3	1:A:183:ALA:CB	2.20	0.71
3:L:136:VAL:HG13	3:L:183:LEU:HB3	1.72	0.71
3:M:58:LEU:HD23	3:M:62:VAL:CB	2.21	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:129:GLU:OE1	1:B:143:LYS:HE3	1.90	0.71
2:K:146:LEU:HD12	2:K:147:VAL:N	2.05	0.71
2:H:40:ALA:HB3	2:H:43:GLN:HB3	1.72	0.71
2:K:37:VAL:HG21	2:K:105:MET:HE1	1.73	0.71
2:K:43:GLN:NE2	2:K:44:GLY:H	1.88	0.70
2:H:176:GLN:HA	3:L:164:GLN:NE2	2.07	0.70
2:K:191:SER:O	2:K:194:LEU:HD12	1.91	0.70
3:M:159:GLN:HG3	3:M:183:LEU:CD1	2.21	0.70
2:X:93:VAL:HG22	2:X:113:LEU:HD23	1.73	0.70
1:A:127:ILE:CD1	1:A:127:ILE:N	2.54	0.70
2:K:89:GLU:H	2:K:89:GLU:CD	1.99	0.70
3:Y:116:ALA:HB1	3:Y:205:LEU:HD12	1.74	0.70
2:X:127:PHE:HB3	3:Y:125:SER:OG	1.92	0.70
1:A:208:ALA:HB2	1:A:225:LEU:HD23	1.73	0.70
1:B:196:LYS:HE2	1:B:200:ARG:O	1.91	0.70
1:C:153:VAL:HG21	1:C:258:LEU:HD11	1.74	0.70
3:L:159:GLN:HG3	3:L:183:LEU:CD1	2.21	0.70
3:M:114:VAL:HG12	3:M:115:ALA:N	2.05	0.70
1:C:135:THR:HB	1:C:137:VAL:CG1	2.21	0.69
3:L:119:VAL:HG11	3:L:200:VAL:HG11	1.73	0.69
1:B:157:ASN:HB3	1:B:159:LYS:CG	2.22	0.69
1:B:261:LEU:N	1:B:261:LEU:HD23	2.07	0.69
3:M:151:GLN:HG2	3:M:158:LEU:HD21	1.71	0.69
3:L:171:ASP:HB3	3:L:174:ASP:OD1	1.92	0.69
2:K:40:ALA:HB3	2:K:43:GLN:HB3	1.72	0.69
2:K:200:ILE:HG23	2:K:215:LYS:HA	1.74	0.69
2:X:33:TYR:CZ	2:X:52:ASN:HB2	2.27	0.69
2:K:169:HIS:CD2	3:M:141:ASN:HD21	2.10	0.69
1:C:143:LYS:NZ	2:X:103:ASN:HD21	1.91	0.69
3:L:37:MET:HG3	3:L:75:PHE:CD1	2.28	0.69
3:Y:119:VAL:HG11	3:Y:200:VAL:HG11	1.72	0.69
1:B:172:TYR:CZ	1:C:227:GLY:HA2	2.27	0.69
3:L:151:GLN:HG2	3:L:158:LEU:HD21	1.75	0.69
2:K:143:LEU:C	2:K:143:LEU:CD2	2.66	0.69
2:X:183:LEU:HD12	2:X:183:LEU:C	2.17	0.69
1:B:206:LEU:CD1	1:B:229:PHE:HZ	2.06	0.69
2:X:126:VAL:HG21	2:X:212:VAL:HG11	1.75	0.69
3:Y:146:ARG:HB2	3:Y:177:TYR:CE2	2.28	0.69
3:Y:179:LEU:HD23	3:Y:179:LEU:C	2.18	0.69
1:C:150:ASN:OD1	1:C:152:LEU:HB2	1.93	0.69
1:C:190:ILE:HD12	1:C:191:ALA:N	2.07	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:206:LYS:HB2	2:K:207:PRO:HD3	1.73	0.69
1:B:193:LEU:HD12	1:B:206:LEU:HD22	1.75	0.68
1:C:166:GLN:CB	1:C:233:PRO:HD3	2.20	0.68
1:B:190:ILE:HD11	1:B:207:ARG:HE	1.57	0.68
1:B:244:PRO:C	1:B:246:GLN:H	2.01	0.68
1:C:171:ILE:O	1:C:226:GLY:HA2	1.93	0.68
2:H:12:VAL:CG1	2:H:116:VAL:HG12	2.22	0.68
2:X:143:LEU:C	2:X:143:LEU:CD2	2.67	0.68
3:Y:51:LEU:HD23	3:Y:62:VAL:HG13	1.74	0.68
3:L:192:LYS:HE3	3:L:193:HIS:CD2	2.29	0.68
3:M:51:LEU:HD23	3:M:62:VAL:HG13	1.73	0.68
1:A:176:THR:HB	1:A:222:SER:OG	1.93	0.68
3:L:110:ILE:H	3:L:170:GLN:NE2	1.90	0.68
1:A:227:GLY:HA2	1:C:172:TYR:CZ	2.29	0.68
1:B:180:ASN:HB3	1:B:183:ALA:CB	2.24	0.68
2:X:176:GLN:HA	3:Y:164:GLN:NE2	2.08	0.68
1:A:190:ILE:H	1:A:242:THR:CG2	2.07	0.68
3:Y:159:GLN:HG3	3:Y:183:LEU:CD1	2.24	0.68
1:A:150:ASN:OD1	1:A:152:LEU:HB2	1.93	0.68
1:B:206:LEU:HD11	1:B:229:PHE:HZ	1.58	0.68
1:C:171:ILE:HD11	1:C:231:LEU:HD11	1.76	0.68
2:X:43:GLN:NE2	2:X:44:GLY:H	1.92	0.68
3:Y:167:VAL:HG12	3:Y:168:THR:N	2.09	0.68
3:Y:58:LEU:HD23	3:Y:62:VAL:CB	2.23	0.68
2:X:6:GLN:H	2:X:110:GLN:NE2	1.89	0.67
3:L:52:ILE:HD12	3:L:77:LEU:HD23	1.77	0.67
2:X:89:GLU:CD	2:X:89:GLU:H	2.01	0.67
3:L:17:GLU:OE1	3:L:111:LYS:HE3	1.93	0.67
3:L:116:ALA:HB1	3:L:205:LEU:HD12	1.75	0.67
2:K:6:GLN:HE22	2:K:95:TYR:HA	1.60	0.67
3:Y:117:PRO:HD2	3:Y:205:LEU:HD11	1.76	0.67
2:H:206:LYS:HB2	2:H:207:PRO:HD3	1.77	0.67
3:M:192:LYS:HE3	3:M:193:HIS:CD2	2.30	0.67
3:Y:27:GLN:C	3:Y:73:THR:HG22	2.20	0.67
3:Y:189:ASP:O	3:Y:192:LYS:HG2	1.93	0.67
2:X:147:VAL:HG11	2:X:155:VAL:HG21	1.76	0.67
1:C:169:TYR:CE2	1:C:260:LYS:HB2	2.30	0.67
1:C:190:ILE:H	1:C:242:THR:CG2	2.08	0.67
3:L:41:GLN:HB3	3:L:51:LEU:CD1	2.23	0.67
2:X:191:SER:O	2:X:194:LEU:HD12	1.93	0.67
1:C:139:GLN:HE22	1:C:159:LYS:HD3	1.58	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:12:VAL:CG2	2:H:16:ALA:HB3	2.25	0.66
2:H:127:PHE:HB3	3:L:125:SER:OG	1.95	0.66
2:K:50:GLU:CG	2:K:59:ASN:HB2	2.25	0.66
3:M:13:VAL:CG2	3:M:17:GLU:HB3	2.12	0.66
1:B:258:LEU:HD12	1:B:258:LEU:O	1.95	0.66
3:L:117:PRO:CB	3:L:143:PHE:HB3	2.23	0.66
2:K:193:SER:O	2:K:195:GLY:N	2.29	0.66
3:Y:13:VAL:CG2	3:Y:17:GLU:HB3	2.17	0.66
3:Y:195:VAL:HG12	3:Y:214:ASN:ND2	2.11	0.66
1:C:157:ASN:HB3	1:C:159:LYS:HG2	1.75	0.66
3:L:159:GLN:HG3	3:L:183:LEU:HD11	1.77	0.66
2:K:6:GLN:HE22	2:K:95:TYR:CA	2.08	0.66
2:X:12:VAL:CG1	2:X:116:VAL:HG12	2.25	0.66
1:A:181:ARG:O	1:A:185:SER:CA	2.44	0.66
3:L:51:LEU:HD23	3:L:62:VAL:CG1	2.25	0.66
1:A:136:SER:HB2	1:A:241:VAL:O	1.96	0.66
1:C:186:GLN:HE21	1:C:212:HIS:CE1	2.10	0.66
3:M:112:ARG:HD2	3:M:144:TYR:CG	2.30	0.66
1:C:143:LYS:HZ3	2:X:103:ASN:HD21	1.42	0.66
1:C:181:ARG:CZ	1:C:182:GLU:HB2	2.26	0.66
3:L:167:VAL:HG12	3:L:168:THR:N	2.10	0.66
3:M:159:GLN:HG3	3:M:183:LEU:HD11	1.78	0.65
1:C:244:PRO:C	1:C:246:GLN:H	2.03	0.65
3:L:33:THR:HB	3:L:34:TYR:CE1	2.32	0.65
3:L:189:ASP:O	3:L:192:LYS:HG2	1.96	0.65
3:M:114:VAL:CG1	3:M:115:ALA:N	2.59	0.65
3:L:33:THR:C	3:L:34:TYR:CD1	2.74	0.65
2:K:155:VAL:HG13	2:K:155:VAL:O	1.95	0.65
3:M:87:PHE:HD2	3:M:108:LEU:O	1.79	0.65
2:X:12:VAL:O	2:X:116:VAL:HA	1.97	0.65
1:A:190:ILE:HD12	1:A:191:ALA:N	2.11	0.65
2:H:32:TYR:CG	2:H:98:ARG:HD3	2.31	0.65
3:M:146:ARG:NH1	3:M:167:VAL:HG21	2.10	0.65
2:X:6:GLN:HE22	2:X:95:TYR:HA	1.61	0.65
3:Y:4:LEU:HA	3:Y:24:ARG:O	1.96	0.65
1:B:139:GLN:HA	1:B:158:GLY:O	1.96	0.65
1:A:206:LEU:CD1	1:A:229:PHE:HZ	2.09	0.65
3:M:144:TYR:CD2	3:M:145:PRO:N	2.65	0.65
2:X:12:VAL:HG23	2:X:13:LYS:HE2	1.78	0.65
2:X:153:GLU:OE1	2:X:173:ALA:HB3	1.96	0.65
1:A:176:THR:HG21	1:A:253:PHE:CD1	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:20:THR:HB	3:M:78:THR:HB	1.79	0.65
1:A:180:ASN:HB3	1:A:183:ALA:HB2	1.78	0.65
3:L:33:THR:C	3:L:34:TYR:HD1	2.05	0.65
3:Y:171:ASP:HB3	3:Y:174:ASP:OD1	1.96	0.65
1:A:135:THR:HB	1:A:137:VAL:CG1	2.26	0.65
1:A:185:SER:C	1:A:186:GLN:HG3	2.22	0.65
3:M:33:THR:C	3:M:34:TYR:CD1	2.75	0.65
1:A:186:GLN:HE21	1:A:212:HIS:CE1	2.05	0.65
1:B:190:ILE:HD12	1:B:191:ALA:N	2.12	0.65
1:C:180:ASN:HB3	1:C:183:ALA:HB2	1.77	0.65
2:K:105:MET:HE2	2:K:108:TRP:CZ2	2.32	0.65
2:X:175:LEU:HD13	2:X:181:TYR:CE1	2.32	0.65
1:C:139:GLN:HA	1:C:158:GLY:O	1.98	0.64
2:K:126:VAL:HG21	2:K:212:VAL:HG11	1.79	0.64
3:Y:2:ILE:HG13	3:Y:94:HIS:HE1	1.62	0.64
1:A:190:ILE:N	1:A:242:THR:HG21	2.10	0.64
1:B:171:ILE:HD11	1:B:231:LEU:HD11	1.79	0.64
2:X:193:SER:O	2:X:195:GLY:N	2.29	0.64
3:L:117:PRO:HB3	3:L:143:PHE:CB	2.21	0.64
3:L:110:ILE:N	3:L:170:GLN:HE22	1.93	0.64
2:X:176:GLN:HE22	2:X:182:SER:HB2	1.62	0.64
3:Y:59:GLU:HG3	3:Y:60:SER:N	2.12	0.64
3:L:20:THR:HB	3:L:78:THR:HB	1.78	0.64
2:K:127:PHE:CD1	3:M:128:GLN:HB2	2.32	0.64
2:X:13:LYS:H	2:X:13:LYS:CD	2.09	0.64
2:X:123:GLY:HA2	2:X:205:HIS:HD2	1.63	0.64
3:Y:33:THR:C	3:Y:34:TYR:HD1	2.05	0.64
3:Y:112:ARG:NH1	3:Y:113:THR:O	2.27	0.64
2:H:13:LYS:H	2:H:13:LYS:CD	2.08	0.64
3:L:116:ALA:HB1	3:L:205:LEU:CD1	2.26	0.64
2:X:200:ILE:HG23	2:X:215:LYS:HA	1.79	0.64
3:Y:51:LEU:HD22	3:Y:66:PHE:CD1	2.32	0.64
3:M:21:ILE:HG22	3:M:22:SER:N	2.11	0.64
1:A:153:VAL:HG23	1:A:163:VAL:HG12	1.80	0.64
1:B:127:ILE:N	1:B:127:ILE:CD1	2.60	0.64
1:C:190:ILE:HD11	1:C:192:SER:OG	1.97	0.64
3:L:51:LEU:HA	3:L:62:VAL:HG21	1.80	0.64
3:M:33:THR:C	3:M:34:TYR:HD1	2.05	0.64
2:X:40:ALA:HB3	2:X:43:GLN:CB	2.27	0.64
1:B:187:ALA:HB1	1:B:188:PRO:CD	2.22	0.64
1:B:190:ILE:H	1:B:242:THR:CG2	2.10	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:190:ILE:O	1:B:242:THR:HG22	1.98	0.64
2:K:13:LYS:H	2:K:13:LYS:CD	2.09	0.64
2:K:144:GLY:HA2	2:K:159:TRP:CH2	2.32	0.64
1:B:157:ASN:HB3	1:B:159:LYS:HG2	1.80	0.64
1:C:190:ILE:O	1:C:242:THR:HG22	1.98	0.64
2:H:122:LYS:NZ	2:H:123:GLY:O	2.24	0.64
2:X:39:GLN:O	2:X:92:ALA:HB1	1.98	0.64
2:X:122:LYS:HG3	2:X:123:GLY:O	1.98	0.64
3:Y:33:THR:C	3:Y:34:TYR:CD1	2.75	0.64
3:Y:110:ILE:H	3:Y:170:GLN:NE2	1.92	0.64
2:H:124:PRO:CD	2:H:210:THR:HG21	2.21	0.63
1:C:261:LEU:N	1:C:261:LEU:CD2	2.52	0.63
3:M:179:LEU:HD23	3:M:179:LEU:C	2.22	0.63
2:X:95:TYR:CE1	3:Y:47:PRO:HB3	2.33	0.63
2:X:105:MET:HE2	2:X:108:TRP:CZ2	2.34	0.63
2:H:12:VAL:HG23	2:H:13:LYS:HE2	1.80	0.63
2:H:37:VAL:HG21	2:H:105:MET:HE1	1.80	0.63
2:H:186:VAL:HG11	3:L:139:LEU:HD22	1.81	0.63
2:X:47:TRP:HZ2	2:X:50:GLU:HB3	1.63	0.63
2:X:155:VAL:HG13	2:X:155:VAL:O	1.98	0.63
1:A:171:ILE:HG21	1:A:193:LEU:HD11	1.79	0.63
1:C:171:ILE:HG22	1:C:193:LEU:HD11	1.80	0.63
3:L:136:VAL:HG22	3:L:152:TRP:CH2	2.32	0.63
1:B:244:PRO:C	1:B:246:GLN:N	2.53	0.63
2:K:6:GLN:H	2:K:110:GLN:NE2	1.96	0.63
2:H:55:ASN:HB3	2:H:57:ASP:H	1.63	0.63
2:H:148:LYS:HD2	2:H:149:ASP:OD1	1.98	0.63
3:M:195:VAL:HG12	3:M:214:ASN:ND2	2.13	0.63
1:B:171:ILE:HG21	1:B:193:LEU:HD11	1.81	0.63
2:H:89:GLU:H	2:H:89:GLU:CD	2.06	0.63
2:H:191:SER:O	2:H:194:LEU:HD12	1.99	0.63
3:M:146:ARG:HH22	3:M:167:VAL:CG2	2.12	0.63
3:M:159:GLN:OE1	3:M:159:GLN:HA	1.99	0.63
3:Y:146:ARG:HH22	3:Y:167:VAL:CG2	2.11	0.63
1:A:166:GLN:HB3	1:A:233:PRO:HD3	1.81	0.63
3:L:21:ILE:HG22	3:L:22:SER:N	2.14	0.63
1:B:142:GLU:HG2	1:B:146:TYR:CE2	2.34	0.62
1:A:185:SER:O	1:A:186:GLN:HG3	1.98	0.62
3:M:30:SER:HA	3:M:35:SER:HA	1.80	0.62
1:C:185:SER:C	1:C:186:GLN:HG3	2.24	0.62
3:L:167:VAL:HG22	3:L:179:LEU:HB2	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:189:ASP:OD2	3:M:192:LYS:HE2	1.98	0.62
1:A:182:GLU:HA	1:A:185:SER:OG	1.99	0.62
2:K:50:GLU:HG2	2:K:59:ASN:HB2	1.82	0.62
3:M:189:ASP:CG	3:M:192:LYS:HE2	2.24	0.62
2:H:178:SER:OG	2:H:180:LEU:HD12	1.99	0.62
3:L:189:ASP:OD2	3:L:192:LYS:HE2	1.99	0.62
2:K:93:VAL:CG2	2:K:113:LEU:HD23	2.28	0.62
3:M:37:MET:HG3	3:M:75:PHE:CD1	2.34	0.62
3:M:154:VAL:O	3:M:157:ALA:HB3	1.99	0.62
1:A:172:TYR:CE2	1:B:227:GLY:HA2	2.34	0.62
1:B:190:ILE:N	1:B:242:THR:HG21	2.12	0.62
2:H:6:GLN:HE22	2:H:95:TYR:CA	2.13	0.62
3:M:167:VAL:HG12	3:M:168:THR:N	2.15	0.62
1:C:181:ARG:O	1:C:185:SER:CA	2.48	0.62
2:H:193:SER:O	2:H:195:GLY:N	2.31	0.62
1:B:153:VAL:HG21	1:B:258:LEU:HD11	1.81	0.62
2:X:176:GLN:HG2	2:X:180:LEU:O	1.99	0.62
3:Y:117:PRO:HB3	3:Y:143:PHE:CB	2.27	0.62
1:A:162:THR:OG1	1:A:236:SER:HB2	1.99	0.62
1:A:190:ILE:HD11	1:A:207:ARG:HE	1.65	0.62
2:H:12:VAL:O	2:H:116:VAL:HA	1.99	0.62
3:L:50:LEU:HG	3:L:59:GLU:HB2	1.82	0.62
2:K:78:THR:HG22	2:K:80:TYR:CE2	2.35	0.62
3:Y:30:SER:CB	3:Y:72:GLY:H	2.13	0.62
3:Y:51:LEU:HA	3:Y:62:VAL:HG21	1.80	0.62
1:B:133:LYS:HA	1:B:133:LYS:CE	2.29	0.62
3:L:30:SER:HA	3:L:35:SER:HA	1.80	0.62
2:K:33:TYR:CZ	2:K:52:ASN:HB2	2.35	0.62
2:X:170:THR:HB	2:X:185:SER:OG	2.00	0.62
1:B:175:VAL:HG22	1:B:254:THR:HG23	1.81	0.61
1:B:185:SER:C	1:B:186:GLN:HG3	2.25	0.61
1:C:190:ILE:N	1:C:242:THR:HG21	2.11	0.61
2:K:178:SER:OG	2:K:180:LEU:HD12	2.00	0.61
2:X:177:SER:OG	2:X:178:SER:N	2.33	0.61
2:H:129:LEU:HD21	2:H:146:LEU:HB2	1.81	0.61
3:L:51:LEU:HD22	3:L:66:PHE:CD1	2.35	0.61
3:M:189:ASP:O	3:M:192:LYS:HG2	1.99	0.61
3:M:4:LEU:HD23	3:M:25:ALA:HA	1.82	0.61
1:B:181:ARG:O	1:B:185:SER:CA	2.48	0.61
1:C:193:LEU:HD12	1:C:206:LEU:HD22	1.82	0.61
2:X:47:TRP:CD2	3:Y:100:PRO:HD2	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Y:43:LYS:HD3	3:Y:88:ALA:HB2	1.82	0.61
1:C:153:VAL:HG23	1:C:163:VAL:HG12	1.82	0.61
1:C:244:PRO:O	1:C:246:GLN:N	2.33	0.61
3:M:117:PRO:HD2	3:M:205:LEU:HD11	1.82	0.61
3:M:129:LEU:C	3:M:131:SER:H	2.07	0.61
2:H:200:ILE:HG23	2:H:215:LYS:HA	1.81	0.61
1:B:215:ALA:HB3	1:B:219:GLY:HA3	1.81	0.61
2:H:169:HIS:CD2	3:L:141:ASN:HD21	2.18	0.61
2:X:6:GLN:HE22	2:X:95:TYR:CA	2.14	0.61
2:X:108:TRP:CE3	3:Y:48:PRO:HD2	2.36	0.61
1:B:181:ARG:CZ	1:B:182:GLU:HB2	2.31	0.61
3:M:13:VAL:CG1	3:M:82:VAL:HG21	2.24	0.61
2:H:127:PHE:CD1	3:L:128:GLN:HB2	2.36	0.61
2:K:12:VAL:CG1	2:K:116:VAL:HG12	2.30	0.61
3:Y:116:ALA:HB1	3:Y:205:LEU:CD1	2.30	0.61
1:B:162:THR:OG1	1:B:236:SER:HB2	2.00	0.61
1:C:128:SER:HB3	1:C:254:THR:O	2.00	0.61
1:C:172:TYR:HA	1:C:225:LEU:O	2.01	0.61
3:M:17:GLU:O	3:M:82:VAL:HG23	2.01	0.61
2:X:120:SER:O	2:X:121:THR:C	2.44	0.60
3:Y:50:LEU:HD12	3:Y:50:LEU:C	2.25	0.60
2:K:129:LEU:HD21	2:K:146:LEU:HB2	1.83	0.60
2:K:175:LEU:HD22	2:K:181:TYR:CE1	2.36	0.60
3:M:141:ASN:ND2	3:M:142:ASN:H	1.99	0.60
3:Y:20:THR:HB	3:Y:78:THR:HB	1.81	0.60
3:Y:41:GLN:HB3	3:Y:51:LEU:CD1	2.30	0.60
2:H:40:ALA:O	2:H:43:GLN:N	2.34	0.60
2:K:12:VAL:O	2:K:116:VAL:HA	2.02	0.60
3:M:197:ALA:CB	3:M:212:SER:HB3	2.30	0.60
1:B:180:ASN:HB3	1:B:183:ALA:HB2	1.84	0.60
2:H:126:VAL:HG21	2:H:212:VAL:HG11	1.82	0.60
2:H:153:GLU:OE1	2:H:173:ALA:HB3	2.01	0.60
2:K:131:PRO:HG2	2:K:218:PRO:HB3	1.82	0.60
3:M:136:VAL:HG22	3:M:152:TRP:HH2	1.64	0.60
3:Y:184:THR:HG23	3:Y:184:THR:O	2.01	0.60
1:C:129:GLU:OE1	1:C:143:LYS:HE3	2.01	0.60
2:H:172:PRO:HG2	3:L:166:SER:OG	2.00	0.60
3:L:39:TRP:CE2	3:L:77:LEU:HB2	2.36	0.60
2:K:177:SER:OG	2:K:178:SER:N	2.32	0.60
1:A:215:ALA:HB3	1:A:219:GLY:HA3	1.81	0.60
1:A:244:PRO:C	1:A:246:GLN:H	2.09	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:190:ILE:HD12	1:B:190:ILE:C	2.26	0.60
1:B:171:ILE:CG2	1:B:193:LEU:HD11	2.32	0.60
2:X:50:GLU:CG	2:X:59:ASN:HB2	2.31	0.60
2:X:206:LYS:C	2:X:208:SER:H	2.08	0.60
1:B:215:ALA:HB2	1:C:211:THR:HG21	1.84	0.60
1:C:258:LEU:HD12	1:C:258:LEU:O	2.02	0.60
2:X:178:SER:OG	2:X:180:LEU:HD12	2.02	0.60
3:Y:93:GLN:HG2	3:Y:94:HIS:N	2.16	0.60
3:Y:123:PRO:HB3	3:Y:213:PHE:CE2	2.37	0.60
1:A:153:VAL:HG21	1:A:258:LEU:HD11	1.83	0.60
2:K:206:LYS:C	2:K:208:SER:H	2.10	0.60
1:C:185:SER:O	1:C:186:GLN:HG3	2.02	0.60
2:H:50:GLU:CG	2:H:59:ASN:HB2	2.32	0.60
3:L:129:LEU:C	3:L:131:SER:H	2.10	0.60
3:Y:40:TYR:CD2	3:Y:40:TYR:N	2.69	0.60
1:A:129:GLU:OE1	1:A:143:LYS:HE3	2.01	0.59
2:K:67:LYS:O	2:K:83:LEU:HA	2.02	0.59
3:M:77:LEU:HD22	3:M:78:THR:N	2.17	0.59
2:X:147:VAL:HG22	2:X:203:VAL:HG21	1.84	0.59
3:Y:190:TYR:HA	3:Y:196:TYR:OH	2.00	0.59
1:A:138:LEU:HD22	1:A:247:VAL:HG11	1.82	0.59
1:A:160:GLN:HB2	1:A:237:VAL:O	2.02	0.59
1:C:169:TYR:CZ	1:C:260:LYS:HD2	2.37	0.59
1:C:182:GLU:HA	1:C:185:SER:OG	2.02	0.59
2:H:67:LYS:O	2:H:83:LEU:HA	2.02	0.59
2:X:30:THR:HA	2:X:53:PRO:HG2	1.83	0.59
1:A:206:LEU:HD11	1:A:229:PHE:HZ	1.67	0.59
1:C:133:LYS:HA	1:C:133:LYS:CE	2.31	0.59
1:C:244:PRO:C	1:C:246:GLN:N	2.58	0.59
1:A:124:ALA:HB2	1:A:153:VAL:HG11	1.85	0.59
1:B:182:GLU:HA	1:B:185:SER:OG	2.03	0.59
2:K:12:VAL:HG23	2:K:13:LYS:HE2	1.83	0.59
3:M:144:TYR:CD2	3:M:144:TYR:C	2.81	0.59
3:M:146:ARG:HH22	3:M:167:VAL:HG21	1.68	0.59
1:C:206:LEU:HD11	1:C:229:PHE:HZ	1.68	0.59
2:X:120:SER:O	2:X:121:THR:O	2.20	0.59
3:L:52:ILE:CD1	3:L:77:LEU:HD23	2.32	0.59
3:Y:21:ILE:CG2	3:Y:22:SER:N	2.65	0.59
3:Y:17:GLU:OE1	3:Y:111:LYS:HE3	2.02	0.59
1:B:180:ASN:O	1:B:212:HIS:HB3	2.03	0.59
2:X:175:LEU:HD22	2:X:181:TYR:CE1	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:146:LEU:HD12	2:X:147:VAL:N	2.18	0.59
3:Y:117:PRO:CB	3:Y:143:PHE:HB3	2.29	0.59
2:K:175:LEU:HD13	2:K:181:TYR:CE1	2.38	0.58
1:B:208:ALA:HB2	1:B:225:LEU:HD23	1.85	0.58
2:H:6:GLN:HE22	2:H:95:TYR:HA	1.68	0.58
3:L:114:VAL:CG1	3:L:115:ALA:N	2.66	0.58
3:M:33:THR:HB	3:M:34:TYR:CE1	2.36	0.58
2:X:127:PHE:CD1	3:Y:128:GLN:HB2	2.38	0.58
3:Y:30:SER:HB3	3:Y:72:GLY:N	2.16	0.58
3:Y:33:THR:HB	3:Y:34:TYR:CE1	2.39	0.58
1:A:139:GLN:NE2	1:A:159:LYS:HD3	2.18	0.58
1:C:190:ILE:HD12	1:C:190:ILE:C	2.29	0.58
1:C:208:ALA:HB2	1:C:225:LEU:HD23	1.86	0.58
2:H:32:TYR:CD1	2:H:98:ARG:HD3	2.38	0.58
3:L:117:PRO:HD2	3:L:205:LEU:HD11	1.82	0.58
2:K:176:GLN:HA	3:M:164:GLN:NE2	2.10	0.58
1:C:206:LEU:HD21	1:C:226:GLY:O	2.02	0.58
1:C:215:ALA:HB3	1:C:219:GLY:HA3	1.84	0.58
2:H:176:GLN:C	2:H:177:SER:O	2.42	0.58
3:L:30:SER:CB	3:L:72:GLY:H	2.16	0.58
3:L:112:ARG:HD2	3:L:144:TYR:CG	2.38	0.58
3:M:146:ARG:NH2	3:M:167:VAL:HB	2.18	0.58
1:A:190:ILE:HD12	1:A:190:ILE:C	2.28	0.58
2:X:144:GLY:HA2	2:X:159:TRP:CH2	2.39	0.58
1:C:175:VAL:HG22	1:C:254:THR:HG23	1.84	0.58
1:C:187:ALA:HB1	1:C:188:PRO:CD	2.31	0.58
2:H:108:TRP:CE3	3:L:48:PRO:HD2	2.39	0.58
3:Y:50:LEU:HG	3:Y:59:GLU:HB2	1.86	0.58
1:A:157:ASN:O	1:A:159:LYS:HG2	2.03	0.58
1:B:176:THR:HB	1:B:222:SER:OG	2.03	0.58
3:L:34:TYR:CD1	3:L:34:TYR:N	2.69	0.58
2:K:127:PHE:HB3	3:M:125:SER:OG	2.02	0.58
3:L:146:ARG:HG2	3:L:146:ARG:HH11	1.68	0.58
2:K:183:LEU:C	2:K:183:LEU:HD12	2.28	0.58
1:A:157:ASN:C	1:A:159:LYS:HG2	2.29	0.57
1:B:170:TYR:HE1	1:B:227:GLY:H	1.49	0.57
1:B:190:ILE:CD1	1:B:207:ARG:HE	2.16	0.57
3:Y:34:TYR:CD1	3:Y:34:TYR:N	2.72	0.57
3:L:189:ASP:CG	3:L:192:LYS:HE2	2.29	0.57
3:Y:136:VAL:HG22	3:Y:152:TRP:HH2	1.68	0.57
3:Y:146:ARG:HG2	3:Y:146:ARG:HH11	1.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:ILE:N	1:A:127:ILE:HD12	2.18	0.57
1:A:176:THR:HA	1:A:222:SER:HA	1.86	0.57
1:B:143:LYS:O	1:B:146:TYR:HB3	2.05	0.57
3:M:158:LEU:HD13	3:M:158:LEU:O	2.04	0.57
1:A:190:ILE:N	1:A:242:THR:CG2	2.67	0.57
1:A:215:ALA:HB2	1:B:211:THR:HG21	1.85	0.57
1:B:128:SER:HB3	1:B:254:THR:O	2.05	0.57
2:H:52:ASN:C	2:H:52:ASN:OD1	2.47	0.57
2:H:177:SER:OG	2:H:178:SER:N	2.38	0.57
2:K:208:SER:O	2:K:209:ASN:HB3	2.03	0.57
2:X:30:THR:HB	2:X:54:SER:HB2	1.85	0.57
3:M:123:PRO:HB3	3:M:213:PHE:CE2	2.39	0.57
2:X:12:VAL:CG2	2:X:16:ALA:HB3	2.34	0.57
2:X:149:ASP:HB3	2:X:180:LEU:HD22	1.86	0.57
3:Y:87:PHE:HD2	3:Y:108:LEU:O	1.87	0.57
1:C:180:ASN:HB3	1:C:183:ALA:HB3	1.85	0.57
2:H:160:ASN:O	2:H:161:SER:C	2.46	0.57
3:M:21:ILE:HG12	3:M:106:THR:HG21	1.87	0.57
2:H:151:PHE:C	2:H:151:PHE:CD1	2.83	0.57
3:L:87:PHE:HD2	3:L:108:LEU:O	1.88	0.57
3:M:50:LEU:HG	3:M:59:GLU:HB2	1.87	0.57
2:X:67:LYS:O	2:X:83:LEU:HA	2.05	0.57
1:A:193:LEU:HD12	1:A:206:LEU:HD22	1.85	0.57
2:H:176:GLN:O	2:H:177:SER:O	2.23	0.57
2:X:124:PRO:CA	2:X:150:TYR:HB3	2.35	0.57
2:H:206:LYS:C	2:H:208:SER:H	2.13	0.57
2:X:40:ALA:O	2:X:43:GLN:N	2.37	0.57
2:X:63:LYS:HG3	2:X:64:PHE:CD1	2.40	0.57
1:B:124:ALA:HB2	1:B:153:VAL:HG11	1.87	0.56
1:B:169:TYR:CE2	1:B:260:LYS:HD2	2.39	0.56
1:B:177:PHE:O	1:B:220:GLN:HA	2.04	0.56
2:H:39:GLN:O	2:H:92:ALA:HB1	2.04	0.56
2:K:139:GLY:O	2:K:191:SER:HB2	2.05	0.56
3:Y:119:VAL:HG11	3:Y:200:VAL:CG1	2.34	0.56
3:Y:146:ARG:NH2	3:Y:167:VAL:HB	2.20	0.56
1:A:190:ILE:HD11	1:A:192:SER:OG	2.05	0.56
1:A:244:PRO:C	1:A:246:GLN:N	2.62	0.56
1:B:182:GLU:O	1:B:183:ALA:C	2.46	0.56
2:H:33:TYR:CZ	2:H:52:ASN:HB2	2.40	0.56
2:X:176:GLN:C	2:X:177:SER:O	2.45	0.56
1:A:190:ILE:O	1:A:242:THR:HG22	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:142:GLU:HG2	1:C:146:TYR:CE2	2.39	0.56
2:H:123:GLY:HA2	2:H:205:HIS:HD2	1.70	0.56
3:L:114:VAL:HG12	3:L:115:ALA:N	2.20	0.56
3:L:119:VAL:HA	3:L:139:LEU:O	2.05	0.56
3:L:132:GLY:C	3:L:187:LYS:HB2	2.30	0.56
2:X:97:THR:HG21	2:X:105:MET:HE3	1.86	0.56
3:Y:77:LEU:HD22	3:Y:78:THR:N	2.20	0.56
3:Y:110:ILE:HG13	3:Y:170:GLN:NE2	2.20	0.56
1:A:227:GLY:HA2	1:C:172:TYR:CE2	2.40	0.56
2:K:60:PHE:CZ	2:K:70:LEU:HG	2.41	0.56
1:A:187:ALA:HB1	1:A:188:PRO:CD	2.29	0.56
1:B:185:SER:O	1:B:186:GLN:HG3	2.05	0.56
2:H:119:ALA:HB3	2:H:151:PHE:CE2	2.40	0.56
3:L:190:TYR:HA	3:L:196:TYR:OH	2.04	0.56
2:K:6:GLN:NE2	2:K:94:TYR:O	2.39	0.56
2:K:17:SER:OG	2:K:84:SER:HA	2.05	0.56
2:K:159:TRP:O	2:K:160:ASN:C	2.49	0.56
3:Y:110:ILE:N	3:Y:170:GLN:HE22	1.95	0.56
1:A:133:LYS:HA	1:A:133:LYS:CE	2.35	0.56
1:C:190:ILE:N	1:C:242:THR:CG2	2.69	0.56
1:C:206:LEU:CD1	1:C:229:PHE:HZ	2.18	0.56
2:H:120:SER:O	2:H:121:THR:O	2.24	0.56
3:L:34:TYR:HD1	3:L:34:TYR:N	2.02	0.56
3:M:124:PRO:HB2	3:M:129:LEU:HD11	1.86	0.56
1:B:206:LEU:HD23	1:B:225:LEU:HB2	1.88	0.56
2:K:160:ASN:O	2:K:161:SER:C	2.48	0.56
3:M:34:TYR:CD1	3:M:34:TYR:N	2.74	0.56
3:Y:186:SER:O	3:Y:187:LYS:C	2.48	0.56
3:Y:189:ASP:OD2	3:Y:192:LYS:HE2	2.05	0.56
3:L:184:THR:HG23	3:L:184:THR:O	2.05	0.56
3:M:146:ARG:HG2	3:M:146:ARG:HH11	1.69	0.56
2:X:151:PHE:CD1	2:X:151:PHE:C	2.84	0.56
3:L:4:LEU:CD1	3:L:37:MET:HE1	2.33	0.56
3:L:158:LEU:HD22	3:L:158:LEU:C	2.30	0.56
3:M:189:ASP:CB	3:M:192:LYS:HE2	2.36	0.56
2:X:206:LYS:HB2	2:X:207:PRO:HD3	1.87	0.56
3:Y:23:CYS:SG	3:Y:24:ARG:N	2.79	0.56
2:H:47:TRP:HZ2	2:H:50:GLU:HB3	1.71	0.56
2:H:103:ASN:ND2	3:L:95:SER:OG	2.30	0.56
2:H:116:VAL:O	2:H:116:VAL:CG2	2.54	0.56
3:M:171:ASP:HB3	3:M:174:ASP:OD1	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Y:129:LEU:C	3:Y:131:SER:H	2.13	0.55
3:L:5:THR:O	3:L:24:ARG:HB2	2.06	0.55
3:Y:154:VAL:O	3:Y:157:ALA:HB3	2.06	0.55
1:C:162:THR:OG1	1:C:236:SER:HB2	2.06	0.55
2:H:70:LEU:C	2:H:71:THR:HG22	2.31	0.55
2:H:73:ASP:O	2:H:74:LYS:C	2.48	0.55
2:K:18:VAL:HG12	2:K:86:LEU:HD11	1.88	0.55
2:K:45:LEU:HB3	3:M:102:PHE:CD1	2.42	0.55
3:M:21:ILE:CG2	3:M:22:SER:N	2.69	0.55
3:M:53:LYS:HG3	3:M:54:TYR:HD1	1.72	0.55
3:M:190:TYR:HA	3:M:196:TYR:OH	2.06	0.55
1:B:179:SER:N	1:B:218:CYS:HB2	2.22	0.55
2:H:146:LEU:C	2:H:146:LEU:HD12	2.31	0.55
2:H:169:HIS:NE2	3:L:141:ASN:ND2	2.50	0.55
2:K:105:MET:HG3	3:M:40:TYR:OH	2.05	0.55
2:X:186:VAL:CG1	2:X:187:VAL:N	2.69	0.55
2:X:206:LYS:O	2:X:208:SER:N	2.39	0.55
3:Y:59:GLU:HA	3:Y:59:GLU:OE2	2.06	0.55
1:A:138:LEU:CD2	1:A:247:VAL:HG11	2.37	0.55
1:A:180:ASN:ND2	1:A:216:LYS:HD3	2.21	0.55
1:B:143:LYS:HZ1	2:K:103:ASN:HD21	1.53	0.55
1:C:186:GLN:NE2	1:C:187:ALA:O	2.39	0.55
3:L:112:ARG:HD3	3:L:113:THR:O	2.06	0.55
2:X:124:PRO:CD	2:X:210:THR:HG21	2.23	0.55
1:A:181:ARG:N	1:A:213:SER:O	2.39	0.55
3:L:53:LYS:HG3	3:L:54:TYR:HD1	1.70	0.55
2:K:91:THR:O	2:K:92:ALA:HB2	2.06	0.55
3:Y:159:GLN:OE1	3:Y:159:GLN:HA	2.05	0.55
1:A:181:ARG:CZ	1:A:182:GLU:HB2	2.37	0.55
2:H:40:ALA:O	2:H:41:PRO:C	2.50	0.55
2:K:87:ARG:O	2:K:116:VAL:CG2	2.53	0.55
2:K:151:PHE:C	2:K:151:PHE:CD1	2.85	0.55
2:X:37:VAL:CG2	2:X:105:MET:HE1	2.36	0.55
2:X:143:LEU:C	2:X:143:LEU:HD23	2.31	0.55
2:X:186:VAL:HG11	3:Y:139:LEU:HD22	1.89	0.55
1:A:171:ILE:HD11	1:A:231:LEU:HD11	1.88	0.55
1:A:211:THR:HG21	1:C:215:ALA:HB2	1.89	0.55
1:C:182:GLU:O	1:C:183:ALA:C	2.49	0.55
1:C:244:PRO:HA	1:C:247:VAL:HG12	1.88	0.55
1:C:260:LYS:C	1:C:261:LEU:HD23	2.30	0.55
2:H:12:VAL:HG22	2:H:16:ALA:HB3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:12:VAL:HG12	2:H:116:VAL:HG12	1.89	0.55
3:Y:140:LEU:N	3:Y:140:LEU:HD12	2.21	0.55
1:B:166:GLN:CB	1:B:233:PRO:HD3	2.31	0.55
2:K:172:PRO:HD2	3:M:166:SER:OG	2.06	0.55
3:M:50:LEU:HD12	3:M:51:LEU:N	2.21	0.55
3:M:58:LEU:HD23	3:M:62:VAL:CG1	2.37	0.55
1:A:171:ILE:HG22	1:A:193:LEU:HD11	1.88	0.55
1:B:206:LEU:HD11	1:B:229:PHE:CZ	2.41	0.55
3:L:54:TYR:HB2	3:L:57:ASN:ND2	2.22	0.55
3:L:71:SER:N	3:L:75:PHE:CE2	2.75	0.55
2:X:176:GLN:O	2:X:177:SER:O	2.25	0.55
3:Y:114:VAL:CG1	3:Y:115:ALA:N	2.69	0.55
2:H:2:VAL:HA	2:H:26:GLY:HA3	1.89	0.54
2:H:93:VAL:CG2	2:H:113:LEU:HD23	2.36	0.54
2:H:143:LEU:C	2:H:143:LEU:CD2	2.81	0.54
3:L:50:LEU:HD12	3:L:50:LEU:C	2.32	0.54
3:M:23:CYS:SG	3:M:24:ARG:N	2.80	0.54
2:X:148:LYS:HD2	2:X:149:ASP:OD1	2.07	0.54
3:Y:6:GLN:OE1	3:Y:91:TYR:HA	2.07	0.54
1:A:131:SER:HB3	1:A:139:GLN:HG3	1.88	0.54
3:L:146:ARG:HH22	3:L:167:VAL:CG2	2.19	0.54
2:K:176:GLN:HG2	2:K:180:LEU:O	2.07	0.54
1:A:143:LYS:NZ	2:H:103:ASN:HD21	2.05	0.54
1:B:190:ILE:HB	1:B:209:ALA:HB2	1.89	0.54
3:L:2:ILE:HG13	3:L:94:HIS:HE1	1.72	0.54
3:L:27:GLN:C	3:L:73:THR:HG22	2.32	0.54
3:L:169:GLU:O	3:L:170:GLN:C	2.48	0.54
2:K:200:ILE:HG23	2:K:215:LYS:CA	2.37	0.54
3:M:2:ILE:HG13	3:M:94:HIS:HE1	1.72	0.54
3:M:36:TYR:O	3:M:94:HIS:HA	2.07	0.54
3:M:51:LEU:HD23	3:M:62:VAL:CG1	2.36	0.54
2:X:171:PHE:CZ	3:Y:180:SER:HB3	2.43	0.54
3:Y:141:ASN:ND2	3:Y:142:ASN:H	2.06	0.54
1:A:180:ASN:HB3	1:A:183:ALA:HB3	1.88	0.54
3:M:158:LEU:HD22	3:M:159:GLN:O	2.07	0.54
2:X:6:GLN:NE2	2:X:94:TYR:O	2.41	0.54
3:Y:159:GLN:HG3	3:Y:183:LEU:HD11	1.89	0.54
1:A:206:LEU:HD11	1:A:229:PHE:CZ	2.42	0.54
1:B:146:TYR:CD2	1:B:147:THR:N	2.76	0.54
1:B:155:LEU:C	1:B:155:LEU:CD2	2.80	0.54
1:B:214:SER:O	1:B:215:ALA:C	2.51	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:87:ARG:O	2:X:116:VAL:CG2	2.51	0.54
1:A:139:GLN:HA	1:A:158:GLY:O	2.06	0.54
1:A:214:SER:O	1:A:215:ALA:C	2.50	0.54
1:B:190:ILE:N	1:B:242:THR:CG2	2.69	0.54
3:M:112:ARG:NH1	3:M:113:THR:O	2.32	0.54
3:M:146:ARG:HH22	3:M:167:VAL:CB	2.21	0.54
2:X:155:VAL:HG13	2:X:183:LEU:HD21	1.90	0.54
3:Y:51:LEU:O	3:Y:62:VAL:HG21	2.08	0.54
1:A:184:SER:O	1:A:186:GLN:N	2.41	0.54
3:L:4:LEU:HD23	3:L:25:ALA:HA	1.88	0.54
3:L:13:VAL:HA	3:L:17:GLU:OE1	2.08	0.54
3:L:124:PRO:HB2	3:L:129:LEU:HD11	1.89	0.54
2:K:208:SER:C	2:K:210:THR:H	2.15	0.54
3:M:20:THR:CB	3:M:78:THR:HB	2.37	0.54
2:H:122:LYS:HG3	2:H:123:GLY:O	2.08	0.54
3:L:144:TYR:C	3:L:144:TYR:CD2	2.85	0.54
2:K:176:GLN:C	2:K:177:SER:O	2.44	0.54
3:M:186:SER:O	3:M:187:LYS:C	2.50	0.54
3:Y:34:TYR:HD1	3:Y:34:TYR:N	2.04	0.54
2:H:100:ASP:HB3	2:H:104:ASP:OD1	2.08	0.54
2:K:73:ASP:C	2:K:73:ASP:OD1	2.51	0.54
3:M:174:ASP:O	3:M:176:THR:HG23	2.07	0.54
3:Y:50:LEU:HD12	3:Y:51:LEU:H	1.70	0.54
2:K:148:LYS:HD2	2:K:149:ASP:OD1	2.08	0.54
3:Y:189:ASP:CG	3:Y:192:LYS:HE2	2.32	0.54
1:A:157:ASN:CB	1:A:159:LYS:HG2	2.37	0.53
1:B:258:LEU:HD12	1:B:258:LEU:C	2.32	0.53
1:C:146:TYR:CD2	1:C:147:THR:N	2.76	0.53
2:H:131:PRO:HG3	2:H:194:LEU:CD2	2.38	0.53
3:L:30:SER:HB3	3:L:72:GLY:N	2.16	0.53
2:K:116:VAL:HG23	2:K:116:VAL:O	2.08	0.53
3:M:206:SER:C	3:M:207:SER:OG	2.50	0.53
1:B:169:TYR:CD2	1:B:260:LYS:HB2	2.43	0.53
1:C:181:ARG:N	1:C:213:SER:O	2.42	0.53
2:H:144:GLY:HA2	2:H:159:TRP:CH2	2.44	0.53
2:K:175:LEU:HD11	2:K:179:GLY:O	2.08	0.53
3:Y:146:ARG:HH22	3:Y:167:VAL:HG21	1.74	0.53
1:B:180:ASN:HB3	1:B:183:ALA:HB3	1.90	0.53
1:C:176:THR:HA	1:C:222:SER:HA	1.90	0.53
2:H:124:PRO:CA	2:H:150:TYR:HB3	2.38	0.53
2:K:6:GLN:HE22	2:K:95:TYR:C	2.17	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:186:VAL:CG1	2:K:187:VAL:N	2.72	0.53
3:Y:81:SER:O	3:Y:81:SER:OG	2.26	0.53
1:A:186:GLN:NE2	1:A:212:HIS:HE1	1.93	0.53
1:B:139:GLN:NE2	1:B:159:LYS:HD3	2.20	0.53
1:B:176:THR:HG21	1:B:253:PHE:HD1	1.73	0.53
1:C:176:THR:HG21	1:C:253:PHE:HD1	1.74	0.53
3:L:94:HIS:CD2	3:L:101:THR:H	2.27	0.53
3:L:158:LEU:O	3:L:158:LEU:HD13	2.08	0.53
2:K:93:VAL:HA	2:K:112:THR:O	2.09	0.53
2:K:175:LEU:HD13	2:K:181:TYR:CD1	2.43	0.53
1:B:172:TYR:OH	1:C:227:GLY:HA2	2.08	0.53
3:L:154:VAL:O	3:L:157:ALA:HB3	2.08	0.53
3:L:189:ASP:HA	3:L:192:LYS:HD3	1.89	0.53
2:K:40:ALA:HB3	2:K:43:GLN:CB	2.37	0.53
3:M:184:THR:HG23	3:M:184:THR:O	2.08	0.53
2:X:122:LYS:NZ	2:X:123:GLY:O	2.34	0.53
1:A:224:HIS:HE1	1:B:226:GLY:H	1.56	0.53
3:L:13:VAL:CG1	3:L:82:VAL:HG21	2.35	0.53
2:K:30:THR:HA	2:K:53:PRO:HG2	1.90	0.53
2:K:124:PRO:CA	2:K:150:TYR:HB3	2.39	0.53
2:K:176:GLN:HE22	2:K:182:SER:HB2	1.72	0.53
3:Y:58:LEU:HD23	3:Y:62:VAL:CG1	2.39	0.53
2:H:40:ALA:HB3	2:H:43:GLN:CB	2.37	0.53
2:H:131:PRO:HG2	2:H:218:PRO:HB3	1.89	0.53
2:K:40:ALA:O	2:K:43:GLN:N	2.41	0.53
2:X:39:GLN:HA	2:X:44:GLY:O	2.09	0.53
1:C:190:ILE:HD11	1:C:207:ARG:HE	1.74	0.53
3:M:119:VAL:HG11	3:M:200:VAL:CG1	2.39	0.53
3:L:123:PRO:HB3	3:L:213:PHE:CE2	2.43	0.53
2:K:180:LEU:HD12	2:K:180:LEU:H	1.74	0.53
3:M:110:ILE:HG13	3:M:170:GLN:NE2	2.23	0.53
2:X:169:HIS:CD2	3:Y:141:ASN:ND2	2.75	0.53
1:A:126:VAL:C	1:A:127:ILE:HD12	2.34	0.53
1:A:149:SER:O	1:A:150:ASN:HB3	2.08	0.53
3:L:40:TYR:CD2	3:L:40:TYR:N	2.77	0.53
2:K:12:VAL:CG2	2:K:16:ALA:HB3	2.38	0.53
3:M:146:ARG:HH22	3:M:167:VAL:HB	1.74	0.53
3:Y:37:MET:HG3	3:Y:75:PHE:CD1	2.44	0.53
1:A:193:LEU:HD12	1:A:206:LEU:CD2	2.40	0.52
1:B:145:TYR:HB2	1:C:203:ARG:NE	2.22	0.52
2:K:131:PRO:HG3	2:K:194:LEU:CD2	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Y:114:VAL:HG12	3:Y:115:ALA:N	2.23	0.52
3:Y:169:GLU:O	3:Y:170:GLN:C	2.50	0.52
1:B:186:GLN:HE21	1:B:212:HIS:CE1	2.10	0.52
1:C:157:ASN:CB	1:C:159:LYS:HG2	2.39	0.52
3:L:58:LEU:HD23	3:L:62:VAL:CB	2.35	0.52
3:M:146:ARG:NH2	3:M:167:VAL:CB	2.73	0.52
2:X:143:LEU:HD23	2:X:144:GLY:N	2.25	0.52
2:X:176:GLN:NE2	2:X:182:SER:HB2	2.24	0.52
2:H:39:GLN:HA	2:H:44:GLY:O	2.09	0.52
3:L:144:TYR:CD2	3:L:145:PRO:N	2.77	0.52
3:L:189:ASP:CB	3:L:192:LYS:HE2	2.39	0.52
2:K:73:ASP:O	2:K:74:LYS:C	2.51	0.52
2:K:143:LEU:C	2:K:143:LEU:HD22	2.34	0.52
2:K:149:ASP:HB3	2:K:180:LEU:HD22	1.90	0.52
3:M:167:VAL:CG1	3:M:168:THR:N	2.72	0.52
2:H:12:VAL:HG21	2:H:16:ALA:HB3	1.91	0.52
2:H:13:LYS:H	2:H:13:LYS:HD2	1.74	0.52
2:H:120:SER:O	2:H:121:THR:C	2.52	0.52
3:L:77:LEU:HD22	3:L:78:THR:N	2.24	0.52
3:L:146:ARG:HB2	3:L:177:TYR:CE2	2.45	0.52
2:K:120:SER:O	2:K:121:THR:C	2.52	0.52
3:M:187:LYS:HD3	3:M:191:GLU:CD	2.34	0.52
3:Y:13:VAL:HA	3:Y:17:GLU:OE1	2.10	0.52
3:L:141:ASN:ND2	3:L:142:ASN:H	2.06	0.52
2:X:5:VAL:HA	2:X:110:GLN:HE21	1.74	0.52
1:C:123:ALA:HA	1:C:258:LEU:O	2.10	0.52
2:H:91:THR:O	2:H:92:ALA:HB2	2.10	0.52
2:H:175:LEU:HD13	2:H:181:TYR:CE1	2.44	0.52
2:H:175:LEU:HD22	2:H:181:TYR:CE1	2.45	0.52
3:L:58:LEU:HD11	3:L:66:PHE:O	2.08	0.52
3:M:30:SER:CB	3:M:72:GLY:H	2.19	0.52
3:M:194:LYS:HG3	3:M:214:ASN:HD22	1.75	0.52
2:H:105:MET:HG3	3:L:40:TYR:OH	2.09	0.52
2:H:149:ASP:HB3	2:H:180:LEU:HD13	1.92	0.52
3:L:167:VAL:CG1	3:L:168:THR:N	2.73	0.52
3:Y:189:ASP:HA	3:Y:192:LYS:HD3	1.92	0.52
1:A:145:TYR:HB2	1:B:203:ARG:HH21	1.75	0.52
1:C:190:ILE:O	1:C:242:THR:CG2	2.57	0.52
2:H:169:HIS:CD2	3:L:141:ASN:ND2	2.78	0.52
2:K:169:HIS:CD2	3:M:141:ASN:ND2	2.78	0.52
3:M:110:ILE:H	3:M:170:GLN:NE2	1.99	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:142:ASN:HA	3:M:177:TYR:O	2.10	0.52
3:Y:124:PRO:HB2	3:Y:129:LEU:HD11	1.90	0.52
1:B:181:ARG:N	1:B:213:SER:O	2.42	0.52
1:C:125:HIS:CE1	1:C:255:SER:HB2	2.45	0.52
2:H:206:LYS:O	2:H:208:SER:N	2.42	0.52
2:X:5:VAL:HA	2:X:110:GLN:NE2	2.25	0.52
3:Y:21:ILE:HG12	3:Y:106:THR:HG21	1.90	0.52
1:B:172:TYR:CE2	1:C:227:GLY:HA2	2.45	0.52
2:H:6:GLN:NE2	2:H:94:TYR:O	2.43	0.52
2:H:176:GLN:HG2	2:H:180:LEU:O	2.10	0.52
2:X:41:PRO:C	2:X:43:GLN:H	2.17	0.52
3:Y:39:TRP:CZ3	3:Y:92:CYS:HB3	2.45	0.52
2:H:208:SER:O	2:H:209:ASN:HB3	2.10	0.51
3:L:17:GLU:O	3:L:82:VAL:HG23	2.10	0.51
3:Y:146:ARG:HH22	3:Y:167:VAL:CB	2.23	0.51
2:K:37:VAL:CG2	2:K:105:MET:HE1	2.41	0.51
2:K:143:LEU:HD23	2:K:144:GLY:N	2.25	0.51
2:H:172:PRO:HD2	3:L:166:SER:OG	2.10	0.51
2:K:40:ALA:O	2:K:41:PRO:C	2.53	0.51
2:K:147:VAL:HG22	2:K:203:VAL:HG21	1.93	0.51
2:K:206:LYS:O	2:K:208:SER:N	2.43	0.51
2:X:136:THR:O	2:X:136:THR:HG22	2.11	0.51
2:X:208:SER:C	2:X:210:THR:H	2.17	0.51
3:Y:51:LEU:HD23	3:Y:62:VAL:CG1	2.40	0.51
3:Y:94:HIS:C	3:Y:94:HIS:CD2	2.87	0.51
1:C:124:ALA:HB2	1:C:153:VAL:HG11	1.93	0.51
1:C:130:ALA:HB2	1:C:249:HIS:CD2	2.45	0.51
1:C:168:LEU:HA	1:C:229:PHE:O	2.09	0.51
2:H:95:TYR:CE1	3:L:47:PRO:HB3	2.44	0.51
3:L:124:PRO:HG2	3:L:190:TYR:CE2	2.45	0.51
3:M:43:LYS:HD3	3:M:88:ALA:HB2	1.93	0.51
3:M:124:PRO:HG2	3:M:190:TYR:CE2	2.45	0.51
3:Y:143:PHE:O	3:Y:177:TYR:N	2.43	0.51
3:L:21:ILE:CG2	3:L:22:SER:N	2.74	0.51
1:C:131:SER:HB3	1:C:139:GLN:HG3	1.92	0.51
2:K:65:LYS:O	2:K:65:LYS:HD3	2.10	0.51
2:K:143:LEU:C	2:K:143:LEU:HD23	2.36	0.51
2:X:177:SER:O	2:X:178:SER:CB	2.57	0.51
3:Y:132:GLY:C	3:Y:187:LYS:HB2	2.36	0.51
1:B:176:THR:HG21	1:B:253:PHE:CD1	2.46	0.51
2:H:30:THR:HB	2:H:54:SER:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:176:GLN:HE22	2:H:182:SER:HB2	1.74	0.51
2:K:176:GLN:NE2	2:K:182:SER:HB2	2.26	0.51
1:A:169:TYR:CE2	1:A:260:LYS:HB2	2.45	0.51
3:Y:122:PHE:O	3:Y:136:VAL:HG23	2.11	0.51
3:Y:146:ARG:CZ	3:Y:167:VAL:HG21	2.40	0.51
3:L:171:ASP:CB	3:L:174:ASP:OD1	2.58	0.51
2:K:76:ALA:O	2:K:77:SER:C	2.54	0.51
2:X:117:SER:OG	2:X:151:PHE:CE2	2.60	0.51
3:Y:52:ILE:HD12	3:Y:77:LEU:HD23	1.92	0.51
3:Y:59:GLU:CG	3:Y:60:SER:N	2.74	0.51
1:C:157:ASN:C	1:C:159:LYS:HG2	2.35	0.51
3:L:59:GLU:HA	3:L:59:GLU:OE2	2.11	0.51
3:L:146:ARG:NH2	3:L:167:VAL:HB	2.25	0.51
2:K:47:TRP:HZ2	2:K:50:GLU:HB3	1.76	0.51
3:M:146:ARG:CZ	3:M:167:VAL:HG11	2.41	0.51
3:Y:137:VAL:HG22	3:Y:182:THR:HG23	1.93	0.51
3:Y:167:VAL:CG1	3:Y:168:THR:N	2.74	0.51
3:Y:179:LEU:C	3:Y:179:LEU:CD2	2.84	0.51
1:B:160:GLN:HB2	1:B:237:VAL:O	2.10	0.50
1:B:176:THR:HA	1:B:222:SER:HA	1.92	0.50
1:B:186:GLN:NE2	1:B:212:HIS:HE1	1.99	0.50
1:C:216:LYS:HA	1:C:217:PRO:C	2.36	0.50
2:X:17:SER:OG	2:X:84:SER:HA	2.11	0.50
2:X:147:VAL:CG2	2:X:203:VAL:HG21	2.41	0.50
2:X:169:HIS:NE2	3:Y:141:ASN:ND2	2.52	0.50
3:Y:58:LEU:HD11	3:Y:66:PHE:O	2.10	0.50
3:Y:161:GLY:O	3:Y:162:ASN:OD1	2.29	0.50
2:H:139:GLY:O	2:H:191:SER:HB2	2.11	0.50
3:M:4:LEU:CD2	3:M:25:ALA:HA	2.41	0.50
2:X:47:TRP:CE3	3:Y:100:PRO:HD2	2.47	0.50
3:Y:39:TRP:CE2	3:Y:77:LEU:HB2	2.46	0.50
3:Y:142:ASN:HA	3:Y:177:TYR:O	2.11	0.50
3:Y:158:LEU:HD22	3:Y:158:LEU:C	2.35	0.50
1:A:260:LYS:C	1:A:261:LEU:HD23	2.36	0.50
1:B:157:ASN:O	1:B:159:LYS:HE2	2.10	0.50
1:B:184:SER:O	1:B:186:GLN:N	2.44	0.50
1:C:127:ILE:N	1:C:127:ILE:CD1	2.75	0.50
1:C:175:VAL:O	1:C:223:ILE:N	2.44	0.50
2:H:147:VAL:HG22	2:H:203:VAL:HG21	1.94	0.50
2:X:131:PRO:HG3	2:X:194:LEU:CD2	2.41	0.50
3:Y:146:ARG:NH2	3:Y:167:VAL:CB	2.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:224:HIS:HE1	1:C:226:GLY:H	1.59	0.50
2:H:13:LYS:HD2	2:H:13:LYS:N	2.26	0.50
2:H:155:VAL:HG13	2:H:183:LEU:HD21	1.94	0.50
3:L:159:GLN:OE1	3:L:159:GLN:HA	2.10	0.50
3:L:193:HIS:O	3:L:215:ARG:CD	2.60	0.50
3:M:3:VAL:H	3:M:26:SER:HG	1.58	0.50
3:M:71:SER:N	3:M:75:PHE:CE2	2.80	0.50
2:X:105:MET:HG3	3:Y:40:TYR:OH	2.10	0.50
3:Y:189:ASP:CB	3:Y:192:LYS:HE2	2.41	0.50
1:C:195:LEU:HD12	1:C:196:LYS:N	2.26	0.50
2:K:5:VAL:C	2:K:110:GLN:HE22	2.20	0.50
3:M:2:ILE:HD13	3:M:27:GLN:CG	2.42	0.50
3:M:186:SER:C	3:M:188:ALA:N	2.68	0.50
3:M:194:LYS:CG	3:M:214:ASN:HD22	2.24	0.50
3:Y:4:LEU:HD23	3:Y:25:ALA:HA	1.93	0.50
1:B:249:HIS:O	1:B:250:GLY:C	2.54	0.50
3:M:40:TYR:N	3:M:40:TYR:CD2	2.80	0.50
3:M:153:LYS:HG2	3:M:158:LEU:HA	1.94	0.50
1:A:182:GLU:O	1:A:183:ALA:C	2.54	0.50
1:C:185:SER:O	1:C:186:GLN:C	2.55	0.50
2:H:208:SER:C	2:H:210:THR:H	2.20	0.50
2:K:153:GLU:OE1	2:K:173:ALA:HB3	2.11	0.50
3:M:4:LEU:CD1	3:M:37:MET:HE1	2.42	0.50
3:M:136:VAL:HG22	3:M:152:TRP:CH2	2.45	0.50
2:X:91:THR:O	2:X:92:ALA:HB2	2.12	0.50
3:Y:158:LEU:O	3:Y:158:LEU:HD13	2.11	0.50
2:H:4:LEU:CD2	2:H:34:MET:HE1	2.42	0.50
2:K:13:LYS:H	2:K:13:LYS:HZ3	1.60	0.50
2:X:127:PHE:CE2	3:Y:128:GLN:HG3	2.47	0.50
3:Y:146:ARG:NH2	3:Y:167:VAL:HG21	2.27	0.50
2:H:149:ASP:HB3	2:H:180:LEU:HD22	1.93	0.50
3:L:146:ARG:HH22	3:L:167:VAL:HG21	1.77	0.50
3:L:152:TRP:CE2	3:L:183:LEU:HB2	2.47	0.50
2:K:30:THR:HB	2:K:54:SER:HB2	1.92	0.50
2:K:152:PRO:O	2:K:205:HIS:HE1	1.95	0.50
3:M:77:LEU:HD22	3:M:77:LEU:C	2.37	0.50
3:M:112:ARG:HD3	3:M:113:THR:O	2.12	0.50
2:X:116:VAL:O	2:X:116:VAL:HG23	2.12	0.50
1:B:138:LEU:HD22	1:B:247:VAL:HG11	1.93	0.49
1:B:143:LYS:O	1:B:144:GLY:C	2.55	0.49
3:L:158:LEU:HD22	3:L:159:GLN:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:174:ASP:OD1	3:M:176:THR:OG1	2.27	0.49
2:X:206:LYS:C	2:X:208:SER:N	2.70	0.49
3:Y:114:VAL:HG21	3:Y:203:GLN:OE1	2.11	0.49
2:H:39:GLN:HB2	2:H:45:LEU:HD12	1.95	0.49
2:K:206:LYS:C	2:K:208:SER:N	2.70	0.49
2:X:93:VAL:CG2	2:X:113:LEU:HD23	2.41	0.49
2:X:186:VAL:HG12	2:X:187:VAL:N	2.27	0.49
1:A:179:SER:N	1:A:218:CYS:HB2	2.27	0.49
1:B:141:ALA:CB	1:B:143:LYS:HE3	2.41	0.49
1:B:185:SER:O	1:B:186:GLN:C	2.54	0.49
2:K:43:GLN:OE1	2:K:43:GLN:HA	2.12	0.49
2:K:178:SER:OG	2:K:179:GLY:N	2.45	0.49
3:M:34:TYR:HD1	3:M:34:TYR:N	2.07	0.49
1:B:179:SER:O	1:B:218:CYS:HA	2.13	0.49
3:L:194:LYS:HG3	3:L:214:ASN:HD22	1.78	0.49
2:K:119:ALA:HB3	2:K:151:PHE:CE2	2.48	0.49
2:K:149:ASP:HB3	2:K:180:LEU:HD13	1.94	0.49
3:M:59:GLU:HA	3:M:59:GLU:OE2	2.13	0.49
1:B:157:ASN:CB	1:B:159:LYS:HG2	2.41	0.49
3:M:186:SER:O	3:M:188:ALA:N	2.45	0.49
1:B:127:ILE:N	1:B:127:ILE:HD12	2.27	0.49
1:B:247:VAL:HG23	1:B:248:SER:N	2.28	0.49
1:C:138:LEU:HD22	1:C:247:VAL:HG11	1.95	0.49
2:H:117:SER:OG	2:H:151:PHE:CE2	2.65	0.49
3:L:9:ALA:O	3:L:106:THR:HA	2.12	0.49
2:K:52:ASN:OD1	2:K:54:SER:N	2.46	0.49
3:Y:136:VAL:CG1	3:Y:183:LEU:HB3	2.40	0.49
2:H:6:GLN:HE22	2:H:95:TYR:C	2.20	0.49
3:M:30:SER:HB3	3:M:72:GLY:N	2.21	0.49
2:H:129:LEU:HB3	3:L:122:PHE:CD1	2.48	0.49
2:K:35:TYR:CE1	2:K:99:SER:HB3	2.47	0.49
3:M:39:TRP:CE2	3:M:77:LEU:HB2	2.47	0.49
3:Y:194:LYS:HG3	3:Y:214:ASN:HD22	1.78	0.49
1:A:206:LEU:CD1	1:A:229:PHE:CZ	2.93	0.49
1:B:155:LEU:C	1:B:155:LEU:HD23	2.38	0.49
1:B:181:ARG:CG	1:B:182:GLU:N	2.71	0.49
1:B:244:PRO:HA	1:B:247:VAL:HG12	1.94	0.49
2:H:5:VAL:HA	2:H:110:GLN:HE21	1.77	0.49
2:H:41:PRO:C	2:H:43:GLN:H	2.20	0.49
2:H:47:TRP:CD2	3:L:100:PRO:HD2	2.48	0.49
2:H:125:SER:O	2:H:148:LYS:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:8:PRO:O	3:M:106:THR:OG1	2.24	0.49
2:X:200:ILE:HG23	2:X:215:LYS:CA	2.43	0.49
1:C:181:ARG:NH2	1:C:182:GLU:HB2	2.28	0.49
2:H:5:VAL:C	2:H:110:GLN:HE22	2.20	0.49
3:M:119:VAL:HA	3:M:139:LEU:O	2.12	0.49
2:X:170:THR:HA	2:X:185:SER:HA	1.95	0.49
1:A:216:LYS:HA	1:A:217:PRO:C	2.38	0.48
1:C:127:ILE:HG22	1:C:128:SER:O	2.13	0.48
1:C:190:ILE:HB	1:C:209:ALA:HB2	1.94	0.48
2:H:65:LYS:O	2:H:65:LYS:HD3	2.13	0.48
3:L:93:GLN:HG2	3:L:94:HIS:N	2.26	0.48
3:L:186:SER:O	3:L:187:LYS:C	2.56	0.48
2:K:122:LYS:HG3	2:K:123:GLY:O	2.13	0.48
2:X:157:VAL:HG11	2:X:185:SER:CB	2.43	0.48
2:X:175:LEU:HD11	2:X:179:GLY:O	2.13	0.48
3:Y:53:LYS:HG3	3:Y:54:TYR:HD1	1.78	0.48
1:A:175:VAL:O	1:A:223:ILE:N	2.47	0.48
1:C:146:TYR:CD2	1:C:146:TYR:C	2.90	0.48
2:H:121:THR:HA	2:H:151:PHE:O	2.14	0.48
2:H:136:THR:HG22	2:H:136:THR:O	2.13	0.48
2:X:119:ALA:HB3	2:X:151:PHE:CE2	2.48	0.48
1:A:244:PRO:O	1:A:246:GLN:N	2.46	0.48
1:C:177:PHE:O	1:C:220:GLN:HA	2.12	0.48
1:C:192:SER:HB3	1:C:207:ARG:HG3	1.96	0.48
2:H:5:VAL:HA	2:H:110:GLN:NE2	2.28	0.48
2:H:171:PHE:CZ	3:L:180:SER:HB3	2.49	0.48
2:K:20:LEU:N	2:K:81:MET:O	2.46	0.48
3:Y:144:TYR:HA	3:Y:145:PRO:C	2.39	0.48
1:B:132:SER:O	1:B:133:LYS:O	2.31	0.48
3:L:142:ASN:HA	3:L:177:TYR:O	2.13	0.48
2:X:12:VAL:HG22	2:X:16:ALA:HB3	1.95	0.48
2:X:52:ASN:OD1	2:X:54:SER:N	2.47	0.48
1:A:143:LYS:O	1:A:146:TYR:HB3	2.13	0.48
1:B:160:GLN:HG3	1:B:236:SER:OG	2.14	0.48
1:C:155:LEU:HD21	1:C:158:GLY:HA2	1.94	0.48
2:H:95:TYR:CE1	2:H:111:GLY:HA3	2.48	0.48
2:H:175:LEU:HD13	2:H:181:TYR:CD1	2.48	0.48
2:K:121:THR:HA	2:K:151:PHE:O	2.14	0.48
2:K:144:GLY:HA2	2:K:159:TRP:HH2	1.76	0.48
2:K:171:PHE:CZ	3:M:180:SER:HB3	2.48	0.48
3:M:132:GLY:C	3:M:187:LYS:HB2	2.39	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:158:LEU:HD22	3:M:158:LEU:C	2.38	0.48
3:Y:192:LYS:HG2	3:Y:193:HIS:CD2	2.48	0.48
1:B:131:SER:HB3	1:B:139:GLN:HG3	1.95	0.48
3:Y:51:LEU:HA	3:Y:62:VAL:CG2	2.43	0.48
3:Y:187:LYS:HD3	3:Y:191:GLU:CD	2.38	0.48
1:A:157:ASN:O	1:A:159:LYS:HE2	2.13	0.48
1:C:214:SER:O	1:C:215:ALA:C	2.56	0.48
2:H:125:SER:HB3	2:H:127:PHE:CE2	2.49	0.48
3:L:51:LEU:HD22	3:L:66:PHE:CG	2.48	0.48
2:K:176:GLN:O	2:K:177:SER:O	2.32	0.48
3:M:202:HIS:ND1	3:M:202:HIS:C	2.72	0.48
2:X:60:PHE:CG	2:X:65:LYS:HE2	2.48	0.48
2:X:63:LYS:HG3	2:X:63:LYS:O	2.12	0.48
3:Y:197:ALA:CB	3:Y:212:SER:HB3	2.39	0.48
2:H:105:MET:HE2	3:L:102:PHE:HZ	1.78	0.48
2:K:39:GLN:HA	2:K:44:GLY:O	2.12	0.48
2:K:61:ASN:O	2:K:62:GLU:C	2.57	0.48
3:M:27:GLN:C	3:M:73:THR:HG22	2.39	0.48
2:X:67:LYS:HE2	2:X:90:ASP:OD1	2.14	0.48
1:A:177:PHE:O	1:A:220:GLN:HA	2.14	0.48
1:B:171:ILE:O	1:B:226:GLY:HA2	2.14	0.48
1:C:184:SER:O	1:C:186:GLN:N	2.46	0.48
3:M:213:PHE:CD2	3:M:213:PHE:C	2.92	0.48
2:X:73:ASP:OD2	2:X:76:ALA:CB	2.62	0.48
1:A:203:ARG:NE	1:C:145:TYR:HB2	2.22	0.48
1:B:143:LYS:O	1:B:144:GLY:O	2.31	0.48
1:B:149:SER:O	1:B:150:ASN:HB3	2.14	0.48
3:L:179:LEU:HD23	3:L:179:LEU:C	2.39	0.48
2:K:67:LYS:HE2	2:K:90:ASP:OD1	2.14	0.48
2:K:186:VAL:HG11	3:M:139:LEU:HD22	1.96	0.48
3:M:117:PRO:HB3	3:M:143:PHE:CB	2.37	0.48
3:M:117:PRO:CB	3:M:143:PHE:HB3	2.36	0.48
2:X:18:VAL:HG12	2:X:86:LEU:HD11	1.96	0.48
3:Y:155:ASP:OD2	3:Y:193:HIS:ND1	2.47	0.48
1:C:139:GLN:NE2	1:C:159:LYS:HD3	2.25	0.47
1:C:142:GLU:HG2	1:C:146:TYR:CZ	2.48	0.47
2:H:30:THR:HA	2:H:53:PRO:HG2	1.95	0.47
3:M:146:ARG:NH2	3:M:167:VAL:HG21	2.28	0.47
2:X:40:ALA:O	2:X:41:PRO:C	2.57	0.47
3:Y:179:LEU:HD23	3:Y:180:SER:CA	2.44	0.47
1:B:138:LEU:CD2	1:B:247:VAL:HG11	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:159:TRP:O	2:H:160:ASN:C	2.57	0.47
2:K:120:SER:O	2:K:121:THR:O	2.32	0.47
3:M:121:ILE:HG23	3:M:121:ILE:O	2.14	0.47
2:X:139:GLY:O	2:X:191:SER:HB2	2.14	0.47
3:Y:20:THR:CB	3:Y:78:THR:HB	2.45	0.47
1:A:169:TYR:CZ	1:A:260:LYS:HD2	2.49	0.47
1:C:133:LYS:HA	1:C:133:LYS:NZ	2.29	0.47
1:C:143:LYS:O	1:C:146:TYR:HB3	2.14	0.47
1:C:246:GLN:HE21	1:C:246:GLN:HB3	1.45	0.47
2:K:12:VAL:HG12	2:K:116:VAL:HG12	1.95	0.47
3:M:122:PHE:O	3:M:136:VAL:HG23	2.14	0.47
3:M:189:ASP:HA	3:M:192:LYS:HD3	1.95	0.47
2:X:5:VAL:C	2:X:110:GLN:HE22	2.20	0.47
3:Y:158:LEU:HD22	3:Y:159:GLN:O	2.15	0.47
1:B:133:LYS:HA	1:B:133:LYS:NZ	2.27	0.47
1:B:175:VAL:O	1:B:223:ILE:HB	2.15	0.47
1:C:135:THR:HB	1:C:137:VAL:H	1.79	0.47
2:H:52:ASN:OD1	2:H:54:SER:N	2.47	0.47
2:H:103:ASN:ND2	3:L:36:TYR:HD1	2.12	0.47
2:X:169:HIS:HE1	3:Y:142:ASN:HD21	1.61	0.47
3:Y:186:SER:O	3:Y:188:ALA:N	2.47	0.47
1:B:215:ALA:HB3	1:B:219:GLY:CA	2.45	0.47
2:H:105:MET:HE2	2:H:108:TRP:CZ2	2.50	0.47
2:H:177:SER:C	2:H:178:SER:O	2.54	0.47
3:L:49:LYS:NZ	3:L:50:LEU:O	2.41	0.47
2:K:24:ALA:HB1	2:K:27:TYR:CE1	2.50	0.47
2:K:70:LEU:C	2:K:71:THR:HG22	2.40	0.47
2:X:13:LYS:HD2	2:X:13:LYS:N	2.29	0.47
2:X:113:LEU:HD13	2:X:115:THR:HG22	1.95	0.47
2:X:172:PRO:HG2	3:Y:166:SER:OG	2.15	0.47
3:Y:146:ARG:HH22	3:Y:167:VAL:HB	1.78	0.47
2:H:33:TYR:CG	2:H:102:ARG:HD2	2.50	0.47
2:H:157:VAL:HG11	2:H:185:SER:CB	2.44	0.47
3:L:52:ILE:HD12	3:L:77:LEU:CD2	2.44	0.47
2:X:13:LYS:H	2:X:13:LYS:HZ3	1.61	0.47
3:Y:119:VAL:HA	3:Y:139:LEU:O	2.15	0.47
1:C:169:TYR:CD2	1:C:260:LYS:HB2	2.50	0.47
2:H:152:PRO:O	2:H:205:HIS:HE1	1.97	0.47
3:L:7:SER:HA	3:L:8:PRO:C	2.38	0.47
2:K:170:THR:HA	2:K:185:SER:HA	1.96	0.47
3:M:54:TYR:HB2	3:M:57:ASN:ND2	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:112:ARG:HD3	3:M:112:ARG:C	2.38	0.47
2:X:131:PRO:HG2	2:X:218:PRO:HB3	1.95	0.47
3:Y:192:LYS:CG	3:Y:193:HIS:CD2	2.98	0.47
1:A:157:ASN:HB3	1:A:159:LYS:HG3	1.95	0.47
1:B:143:LYS:HZ3	2:K:103:ASN:HD21	1.58	0.47
2:H:125:SER:O	2:H:147:VAL:HA	2.14	0.47
2:H:206:LYS:C	2:H:208:SER:N	2.72	0.47
2:X:13:LYS:H	2:X:13:LYS:HD2	1.78	0.47
2:X:73:ASP:OD2	2:X:76:ALA:HB3	2.14	0.47
2:X:98:ARG:NH1	2:X:106:ASP:OD2	2.48	0.47
1:A:176:THR:HG23	1:A:253:PHE:HB3	1.96	0.47
1:C:178:CYS:O	2:X:55:ASN:OD1	2.33	0.47
1:C:182:GLU:C	1:C:185:SER:HB2	2.40	0.47
2:H:146:LEU:HD12	2:H:147:VAL:N	2.29	0.47
2:H:175:LEU:HD11	2:H:179:GLY:O	2.15	0.47
3:L:108:LEU:HD12	3:L:108:LEU:HA	1.70	0.47
2:K:73:ASP:OD2	2:K:76:ALA:HB3	2.15	0.47
3:M:70:GLY:O	3:M:71:SER:HB3	2.15	0.47
2:X:4:LEU:O	2:X:109:GLY:HA2	2.15	0.47
1:A:125:HIS:CE1	1:A:255:SER:HB2	2.50	0.47
1:B:145:TYR:H	1:C:203:ARG:HH21	1.63	0.47
1:C:175:VAL:O	1:C:223:ILE:HB	2.14	0.47
1:C:176:THR:HG21	1:C:253:PHE:CD1	2.49	0.47
3:M:140:LEU:HD12	3:M:140:LEU:N	2.30	0.47
3:Y:186:SER:C	3:Y:188:ALA:N	2.72	0.47
1:A:194:CYS:CB	1:A:238:PHE:CZ	2.99	0.46
1:A:201:PHE:C	1:A:202:GLU:O	2.57	0.46
1:B:244:PRO:HA	1:B:247:VAL:CG1	2.45	0.46
2:H:127:PHE:CE1	3:L:128:GLN:HA	2.50	0.46
2:H:134:LYS:H	2:H:134:LYS:HG3	1.45	0.46
2:H:186:VAL:HG11	3:L:139:LEU:CD2	2.44	0.46
2:H:200:ILE:HG23	2:H:215:LYS:CA	2.45	0.46
2:K:29:PHE:CD2	2:K:77:SER:HA	2.49	0.46
2:K:144:GLY:HA2	2:K:159:TRP:CZ2	2.50	0.46
3:M:6:GLN:OE1	3:M:91:TYR:HA	2.15	0.46
3:M:143:PHE:HE1	3:M:179:LEU:H	1.63	0.46
3:Y:39:TRP:C	3:Y:40:TYR:CD2	2.93	0.46
1:A:190:ILE:CD1	1:A:207:ARG:HE	2.27	0.46
1:C:150:ASN:O	1:C:153:VAL:O	2.33	0.46
3:L:20:THR:CB	3:L:78:THR:HB	2.44	0.46
2:X:12:VAL:HG23	2:X:13:LYS:CE	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:52:ASN:OD1	2:X:52:ASN:C	2.58	0.46
3:Y:51:LEU:HD22	3:Y:66:PHE:CG	2.50	0.46
1:B:135:THR:HB	1:B:137:VAL:H	1.80	0.46
1:C:136:SER:O	1:C:240:ASN:OD1	2.34	0.46
2:H:4:LEU:HD13	2:H:96:CYS:SG	2.55	0.46
2:X:4:LEU:CD2	2:X:34:MET:HE1	2.45	0.46
2:X:30:THR:HB	2:X:54:SER:CB	2.44	0.46
2:X:143:LEU:C	2:X:143:LEU:HD22	2.40	0.46
1:A:185:SER:O	1:A:186:GLN:C	2.58	0.46
1:B:126:VAL:C	1:B:127:ILE:HD12	2.41	0.46
2:H:40:ALA:HA	2:H:92:ALA:CB	2.45	0.46
3:L:124:PRO:HG2	3:L:190:TYR:CZ	2.49	0.46
3:L:153:LYS:HG2	3:L:158:LEU:HA	1.97	0.46
2:K:156:THR:HG23	2:K:204:ASN:HB3	1.98	0.46
2:X:124:PRO:HB3	2:X:150:TYR:HB3	1.96	0.46
3:Y:36:TYR:O	3:Y:94:HIS:HA	2.15	0.46
3:Y:77:LEU:HD22	3:Y:77:LEU:C	2.41	0.46
3:Y:110:ILE:HG13	3:Y:170:GLN:HE22	1.79	0.46
1:B:176:THR:HG23	1:B:253:PHE:HB3	1.98	0.46
3:M:179:LEU:C	3:M:179:LEU:CD2	2.87	0.46
2:X:152:PRO:O	2:X:205:HIS:HE1	1.97	0.46
2:X:193:SER:C	2:X:195:GLY:N	2.74	0.46
3:Y:153:LYS:HG2	3:Y:158:LEU:HA	1.96	0.46
2:H:158:SER:O	2:H:202:ASN:N	2.44	0.46
2:K:13:LYS:HD2	2:K:13:LYS:N	2.31	0.46
3:M:30:SER:HB2	3:M:35:SER:CB	2.46	0.46
2:X:73:ASP:OD1	2:X:73:ASP:C	2.58	0.46
3:Y:136:VAL:HG22	3:Y:152:TRP:CH2	2.48	0.46
3:L:83:GLU:O	3:L:84:PRO:C	2.58	0.46
2:K:177:SER:O	2:K:178:SER:CB	2.61	0.46
3:M:51:LEU:HD22	3:M:66:PHE:CD1	2.50	0.46
2:X:124:PRO:HA	2:X:150:TYR:HB3	1.98	0.46
1:A:146:TYR:CD2	1:A:147:THR:N	2.84	0.46
1:B:186:GLN:NE2	1:B:187:ALA:O	2.48	0.46
1:C:192:SER:HB3	1:C:207:ARG:CG	2.45	0.46
1:C:215:ALA:HB3	1:C:219:GLY:CA	2.46	0.46
2:H:43:GLN:OE1	2:H:43:GLN:HA	2.15	0.46
3:L:197:ALA:CB	3:L:212:SER:HB3	2.40	0.46
3:M:110:ILE:N	3:M:170:GLN:HE22	2.01	0.46
3:Y:27:GLN:O	3:Y:73:THR:HG22	2.15	0.46
3:Y:194:LYS:CG	3:Y:214:ASN:HD22	2.28	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:GLY:O	1:A:230:GLU:HA	2.16	0.46
1:C:190:ILE:HD12	1:C:191:ALA:C	2.41	0.46
1:C:244:PRO:HA	1:C:247:VAL:CG1	2.45	0.46
3:L:201:THR:CG2	3:L:208:PRO:HG3	2.36	0.46
3:M:94:HIS:C	3:M:94:HIS:CD2	2.93	0.46
2:X:175:LEU:HD13	2:X:181:TYR:CD1	2.50	0.46
1:B:135:THR:CB	1:B:137:VAL:CG1	2.93	0.46
1:B:145:TYR:HB2	1:C:203:ARG:HH21	1.80	0.46
1:B:157:ASN:C	1:B:159:LYS:HG2	2.40	0.46
1:C:179:SER:O	1:C:218:CYS:HA	2.15	0.46
2:K:47:TRP:CD2	3:M:100:PRO:HD2	2.50	0.46
2:X:208:SER:O	2:X:209:ASN:HB3	2.16	0.46
3:Y:43:LYS:HB2	3:Y:46:GLN:HG3	1.97	0.46
3:Y:110:ILE:HG22	3:Y:111:LYS:O	2.16	0.46
1:A:145:TYR:HB2	1:B:203:ARG:NE	2.25	0.45
1:A:186:GLN:NE2	1:A:187:ALA:O	2.49	0.45
1:A:194:CYS:HB2	1:A:238:PHE:CZ	2.51	0.45
1:B:189:PHE:CD1	1:B:189:PHE:O	2.69	0.45
2:H:131:PRO:HA	2:H:135:SER:OG	2.16	0.45
2:H:148:LYS:HD2	2:H:149:ASP:CG	2.41	0.45
2:H:170:THR:HA	2:H:185:SER:HA	1.98	0.45
2:X:20:LEU:N	2:X:20:LEU:CD1	2.79	0.45
1:C:182:GLU:HA	1:C:185:SER:CB	2.46	0.45
2:H:78:THR:HG22	2:H:80:TYR:CE2	2.52	0.45
3:L:11:LEU:HD13	3:L:11:LEU:C	2.41	0.45
3:M:129:LEU:C	3:M:131:SER:N	2.72	0.45
2:K:39:GLN:NE2	2:K:45:LEU:HD13	2.32	0.45
2:K:63:LYS:O	2:K:63:LYS:HG3	2.15	0.45
3:M:193:HIS:O	3:M:215:ARG:NE	2.49	0.45
2:X:125:SER:N	2:X:148:LYS:O	2.49	0.45
2:X:147:VAL:CG2	2:X:203:VAL:CG2	2.95	0.45
2:X:149:ASP:HB3	2:X:180:LEU:HD13	1.99	0.45
3:Y:122:PHE:HA	3:Y:123:PRO:HD3	1.84	0.45
1:A:133:LYS:HA	1:A:133:LYS:NZ	2.31	0.45
1:A:142:GLU:HG2	1:A:146:TYR:CZ	2.51	0.45
1:A:160:GLN:HG3	1:A:236:SER:OG	2.17	0.45
2:H:93:VAL:HA	2:H:112:THR:O	2.16	0.45
2:K:125:SER:N	2:K:148:LYS:O	2.49	0.45
3:M:110:ILE:HG13	3:M:170:GLN:HE22	1.81	0.45
2:X:183:LEU:C	2:X:183:LEU:CD1	2.89	0.45
3:Y:59:GLU:OE2	3:Y:59:GLU:CA	2.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Y:125:SER:O	3:Y:126:ASP:C	2.58	0.45
1:B:150:ASN:O	1:B:153:VAL:O	2.35	0.45
3:M:51:LEU:HA	3:M:62:VAL:CG2	2.40	0.45
2:X:12:VAL:HG13	2:X:116:VAL:HG12	1.98	0.45
2:X:103:ASN:ND2	3:Y:36:TYR:HD1	2.15	0.45
3:Y:69:SER:OG	3:Y:70:GLY:N	2.48	0.45
3:Y:124:PRO:HG2	3:Y:190:TYR:CE2	2.52	0.45
3:Y:159:GLN:HG3	3:Y:183:LEU:HD13	1.95	0.45
3:Y:189:ASP:O	3:Y:192:LYS:CG	2.63	0.45
1:B:139:GLN:HE22	1:B:159:LYS:CD	2.26	0.45
3:L:159:GLN:HG3	3:L:183:LEU:HD13	1.99	0.45
2:K:123:GLY:HA2	2:K:205:HIS:CD2	2.39	0.45
3:M:14:SER:O	3:M:17:GLU:HB2	2.16	0.45
2:X:55:ASN:HB3	2:X:57:ASP:H	1.82	0.45
3:Y:25:ALA:C	3:Y:27:GLN:H	2.24	0.45
1:C:176:THR:HB	1:C:222:SER:HG	1.78	0.45
2:H:124:PRO:HB3	2:H:150:TYR:HB3	1.99	0.45
3:L:90:TYR:N	3:L:90:TYR:CD1	2.85	0.45
2:X:50:GLU:OE2	2:X:59:ASN:HB2	2.17	0.45
3:Y:7:SER:HA	3:Y:8:PRO:C	2.42	0.45
1:A:226:GLY:H	1:C:224:HIS:HE1	1.64	0.45
1:B:201:PHE:C	1:B:202:GLU:O	2.59	0.45
2:H:63:LYS:O	2:H:63:LYS:HG3	2.17	0.45
3:L:39:TRP:CZ3	3:L:92:CYS:HB3	2.52	0.45
3:M:14:SER:O	3:M:17:GLU:CB	2.65	0.45
3:M:94:HIS:CD2	3:M:101:THR:H	2.34	0.45
1:B:172:TYR:HA	1:B:225:LEU:O	2.17	0.45
1:C:149:SER:O	1:C:150:ASN:HB3	2.17	0.45
1:C:157:ASN:O	1:C:159:LYS:HG2	2.17	0.45
2:H:108:TRP:CH2	3:L:48:PRO:HG2	2.52	0.45
2:K:124:PRO:HD3	2:K:205:HIS:HB2	1.99	0.45
3:M:7:SER:HA	3:M:8:PRO:C	2.42	0.45
3:Y:25:ALA:HB1	3:Y:27:GLN:O	2.17	0.45
3:L:25:ALA:C	3:L:27:GLN:N	2.75	0.45
3:L:112:ARG:NH1	3:L:113:THR:O	2.37	0.45
2:K:136:THR:O	2:K:136:THR:HG22	2.16	0.45
3:M:52:ILE:CD1	3:M:77:LEU:HD23	2.46	0.45
3:M:118:SER:O	3:M:120:PHE:CE2	2.70	0.45
3:M:144:TYR:CD2	3:M:145:PRO:CA	3.00	0.45
2:X:180:LEU:HD12	2:X:180:LEU:H	1.82	0.45
1:B:127:ILE:HG22	1:B:128:SER:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:187:ALA:CB	1:B:188:PRO:HD2	2.30	0.44
3:L:77:LEU:HD22	3:L:77:LEU:C	2.42	0.44
3:L:119:VAL:HG11	3:L:200:VAL:CG1	2.44	0.44
3:L:146:ARG:HH22	3:L:167:VAL:CB	2.30	0.44
2:K:193:SER:C	2:K:195:GLY:N	2.74	0.44
2:X:70:LEU:C	2:X:71:THR:HG22	2.41	0.44
2:X:150:TYR:CD2	2:X:150:TYR:N	2.84	0.44
3:Y:13:VAL:CG1	3:Y:82:VAL:HG21	2.36	0.44
1:A:182:GLU:HA	1:A:185:SER:CB	2.48	0.44
1:A:215:ALA:HB3	1:A:219:GLY:CA	2.47	0.44
1:B:136:SER:O	1:B:240:ASN:OD1	2.35	0.44
1:C:127:ILE:N	1:C:127:ILE:HD12	2.32	0.44
1:C:146:TYR:HD2	1:C:147:THR:N	2.16	0.44
2:H:186:VAL:CG1	2:H:187:VAL:N	2.80	0.44
3:L:6:GLN:CD	3:L:105:GLY:H	2.25	0.44
3:L:141:ASN:ND2	3:L:178:SER:OG	2.50	0.44
3:L:155:ASP:C	3:L:157:ALA:H	2.24	0.44
3:M:8:PRO:HG3	3:M:11:LEU:HD23	1.98	0.44
3:M:39:TRP:CZ3	3:M:92:CYS:HB3	2.53	0.44
2:X:12:VAL:HG12	2:X:116:VAL:HG12	1.98	0.44
3:Y:25:ALA:C	3:Y:27:GLN:N	2.73	0.44
1:B:181:ARG:NH2	1:B:182:GLU:HB2	2.32	0.44
1:B:192:SER:HB3	1:B:207:ARG:HG3	2.00	0.44
3:L:205:LEU:CD1	3:L:205:LEU:N	2.79	0.44
2:K:12:VAL:HG22	2:K:13:LYS:N	2.31	0.44
3:M:43:LYS:HB2	3:M:46:GLN:HG3	1.99	0.44
3:Y:184:THR:O	3:Y:184:THR:CG2	2.66	0.44
2:H:17:SER:OG	2:H:84:SER:HA	2.17	0.44
2:H:81:MET:HE1	2:H:94:TYR:CD2	2.53	0.44
3:L:39:TRP:C	3:L:40:TYR:CD2	2.95	0.44
2:K:51:ILE:O	2:K:51:ILE:HG23	2.17	0.44
3:M:193:HIS:O	3:M:215:ARG:CD	2.65	0.44
1:B:182:GLU:O	1:B:183:ALA:O	2.36	0.44
1:B:194:CYS:HB2	1:B:238:PHE:CZ	2.52	0.44
1:B:244:PRO:O	1:B:245:SER:C	2.60	0.44
2:H:43:GLN:CD	2:H:44:GLY:H	2.24	0.44
3:L:36:TYR:CD2	3:L:36:TYR:N	2.85	0.44
3:L:154:VAL:HG23	3:L:159:GLN:HG2	1.99	0.44
3:M:9:ALA:O	3:M:106:THR:HA	2.18	0.44
3:Y:174:ASP:O	3:Y:176:THR:HG23	2.18	0.44
1:C:155:LEU:CD2	1:C:158:GLY:HA2	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:12:VAL:HG23	2:H:13:LYS:CE	2.45	0.44
2:H:113:LEU:HD13	2:H:115:THR:HG22	2.00	0.44
2:H:151:PHE:C	2:H:151:PHE:HD1	2.24	0.44
3:M:30:SER:HB2	3:M:35:SER:OG	2.18	0.44
3:Y:2:ILE:HD13	3:Y:27:GLN:CG	2.47	0.44
1:A:137:VAL:HG13	1:A:137:VAL:O	2.17	0.44
1:B:216:LYS:HA	1:B:217:PRO:C	2.42	0.44
2:H:4:LEU:O	2:H:109:GLY:HA2	2.18	0.44
2:H:4:LEU:HD21	2:H:34:MET:HE1	1.99	0.44
3:L:43:LYS:HD3	3:L:88:ALA:HB2	1.98	0.44
3:L:167:VAL:HG12	3:L:168:THR:H	1.82	0.44
2:K:41:PRO:C	2:K:43:GLN:H	2.25	0.44
2:K:193:SER:O	2:K:194:LEU:C	2.61	0.44
2:K:208:SER:C	2:K:210:THR:N	2.74	0.44
3:Y:119:VAL:CG1	3:Y:200:VAL:HG11	2.45	0.44
3:Y:167:VAL:HG12	3:Y:168:THR:H	1.79	0.44
3:Y:194:LYS:HE3	3:Y:194:LYS:HA	1.99	0.44
1:B:190:ILE:CD1	1:B:207:ARG:NE	2.80	0.44
1:C:192:SER:CB	1:C:207:ARG:HG2	2.48	0.44
2:H:76:ALA:O	2:H:77:SER:C	2.60	0.44
3:L:140:LEU:HD12	3:L:140:LEU:N	2.33	0.44
3:L:146:ARG:NH2	3:L:167:VAL:HG21	2.33	0.44
2:K:73:ASP:O	2:K:73:ASP:CG	2.59	0.44
3:M:124:PRO:HG2	3:M:190:TYR:CZ	2.53	0.44
2:H:156:THR:HG23	2:H:204:ASN:HB3	2.00	0.44
2:H:171:PHE:HB3	2:H:172:PRO:HD2	2.00	0.44
3:L:187:LYS:HD3	3:L:191:GLU:CD	2.43	0.44
2:K:150:TYR:CD2	2:K:150:TYR:N	2.86	0.44
3:M:49:LYS:HD3	3:M:49:LYS:C	2.43	0.44
3:M:59:GLU:HG3	3:M:60:SER:N	2.32	0.44
2:X:65:LYS:O	2:X:65:LYS:NZ	2.43	0.44
2:X:73:ASP:CG	2:X:76:ALA:H	2.26	0.44
2:X:186:VAL:HG11	3:Y:139:LEU:CD2	2.48	0.44
3:Y:42:GLN:NE2	3:Y:46:GLN:O	2.46	0.44
1:B:180:ASN:ND2	1:B:216:LYS:HD3	2.32	0.43
2:H:12:VAL:CG2	2:H:16:ALA:CB	2.94	0.43
2:H:13:LYS:H	2:H:13:LYS:HZ3	1.65	0.43
2:H:124:PRO:HA	2:H:150:TYR:HB3	2.00	0.43
2:H:131:PRO:HD3	2:H:143:LEU:CB	2.41	0.43
3:L:24:ARG:CZ	3:L:74:ASP:OD1	2.66	0.43
2:K:12:VAL:HG21	2:K:16:ALA:HB3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:99:SER:OG	2:K:102:ARG:HA	2.18	0.43
2:K:124:PRO:HA	2:K:150:TYR:HB3	2.00	0.43
3:M:155:ASP:C	3:M:157:ALA:H	2.25	0.43
3:M:170:GLN:HG2	3:M:177:TYR:CZ	2.53	0.43
2:X:187:VAL:HG22	2:X:188:THR:N	2.33	0.43
2:X:208:SER:C	2:X:210:THR:N	2.76	0.43
3:Y:49:LYS:NZ	3:Y:50:LEU:O	2.42	0.43
1:A:182:GLU:C	1:A:185:SER:HB2	2.41	0.43
1:A:201:PHE:O	1:A:202:GLU:O	2.36	0.43
1:A:228:VAL:HG21	1:C:259:LEU:HB3	1.99	0.43
1:C:193:LEU:HD12	1:C:206:LEU:CD2	2.47	0.43
2:H:50:GLU:OE2	2:H:59:ASN:HB2	2.18	0.43
2:H:79:ALA:C	2:H:80:TYR:CD2	2.96	0.43
3:L:54:TYR:HB2	3:L:57:ASN:HD21	1.83	0.43
3:M:12:SER:HA	3:M:109:GLU:O	2.18	0.43
2:X:51:ILE:HD12	2:X:58:THR:HG22	2.00	0.43
3:Y:54:TYR:O	3:Y:56:SER:N	2.49	0.43
3:Y:114:VAL:HG22	3:Y:145:PRO:HD3	2.00	0.43
3:L:59:GLU:HG3	3:L:60:SER:N	2.33	0.43
3:L:112:ARG:HD3	3:L:112:ARG:C	2.44	0.43
3:M:169:GLU:O	3:M:170:GLN:C	2.61	0.43
3:Y:8:PRO:HG3	3:Y:11:LEU:HD23	2.00	0.43
1:A:150:ASN:O	1:A:153:VAL:O	2.36	0.43
1:A:196:LYS:HA	1:A:196:LYS:HD2	1.87	0.43
1:B:190:ILE:HD11	1:B:192:SER:OG	2.17	0.43
2:H:129:LEU:HD11	2:H:184:SER:HG	1.83	0.43
3:L:146:ARG:NH2	3:L:167:VAL:CB	2.81	0.43
3:M:39:TRP:CD2	3:M:77:LEU:HB2	2.53	0.43
3:M:52:ILE:HD12	3:M:77:LEU:HD23	2.00	0.43
3:M:152:TRP:O	3:M:159:GLN:HB2	2.19	0.43
1:A:127:ILE:HG22	1:A:128:SER:O	2.19	0.43
1:A:143:LYS:HE2	3:L:36:TYR:CE1	2.53	0.43
3:L:67:SER:O	3:L:77:LEU:HD22	2.18	0.43
3:L:140:LEU:HD21	3:L:200:VAL:HG21	2.01	0.43
3:L:146:ARG:HH22	3:L:167:VAL:HB	1.82	0.43
2:K:35:TYR:CD2	2:K:47:TRP:NE1	2.86	0.43
2:K:73:ASP:OD2	2:K:76:ALA:CB	2.67	0.43
2:K:164:LEU:HD12	2:K:164:LEU:HA	1.79	0.43
3:M:154:VAL:HG23	3:M:159:GLN:HG2	2.01	0.43
3:Y:195:VAL:O	3:Y:195:VAL:CG2	2.63	0.43
1:C:157:ASN:O	1:C:159:LYS:HE2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:60:PHE:CG	2:H:65:LYS:HE2	2.54	0.43
2:K:12:VAL:HG23	2:K:13:LYS:CE	2.47	0.43
3:M:90:TYR:CD1	3:M:90:TYR:N	2.86	0.43
2:X:151:PHE:CD1	2:X:152:PRO:N	2.87	0.43
3:Y:40:TYR:N	3:Y:40:TYR:HD2	2.13	0.43
1:B:168:LEU:HA	1:B:229:PHE:O	2.18	0.43
1:C:157:ASN:HB3	1:C:159:LYS:HG3	1.98	0.43
1:C:177:PHE:HB2	1:C:246:GLN:O	2.19	0.43
3:M:136:VAL:CG1	3:M:183:LEU:HB3	2.45	0.43
3:M:144:TYR:CD2	3:M:145:PRO:HA	2.54	0.43
2:X:125:SER:O	2:X:148:LYS:N	2.51	0.43
2:X:159:TRP:O	2:X:160:ASN:C	2.61	0.43
3:Y:109:GLU:HG2	3:Y:170:GLN:NE2	2.34	0.43
3:Y:188:ALA:O	3:Y:189:ASP:C	2.61	0.43
2:K:60:PHE:CG	2:K:65:LYS:HE2	2.54	0.43
2:K:105:MET:HE2	2:K:108:TRP:CH2	2.53	0.43
2:X:32:TYR:CD1	2:X:98:ARG:HD3	2.53	0.43
2:X:40:ALA:HA	2:X:92:ALA:CB	2.49	0.43
1:B:155:LEU:HD21	1:B:158:GLY:HA2	1.99	0.43
2:H:33:TYR:CD1	2:H:102:ARG:HD2	2.54	0.43
2:H:73:ASP:C	2:H:73:ASP:OD1	2.60	0.43
3:L:144:TYR:CG	3:L:145:PRO:HA	2.54	0.43
3:L:194:LYS:CG	3:L:214:ASN:HD22	2.31	0.43
2:K:13:LYS:H	2:K:13:LYS:HD2	1.79	0.43
3:Y:152:TRP:CE2	3:Y:183:LEU:HB2	2.54	0.43
1:A:178:CYS:O	2:H:55:ASN:OD1	2.37	0.43
3:L:36:TYR:O	3:L:94:HIS:HA	2.19	0.43
3:L:50:LEU:HG	3:L:59:GLU:CB	2.49	0.43
2:K:191:SER:C	2:K:193:SER:N	2.77	0.43
3:M:17:GLU:CD	3:M:111:LYS:HE3	2.44	0.43
2:X:148:LYS:HD2	2:X:149:ASP:CG	2.44	0.43
2:H:18:VAL:HG12	2:H:86:LEU:HD11	2.01	0.42
2:H:119:ALA:HB3	2:H:151:PHE:CD2	2.54	0.42
2:H:147:VAL:CG2	2:H:203:VAL:HG21	2.48	0.42
2:H:150:TYR:CD2	2:H:150:TYR:N	2.87	0.42
3:L:6:GLN:OE1	3:L:91:TYR:HA	2.19	0.42
3:L:99:PRO:O	3:L:101:THR:HG23	2.19	0.42
2:X:20:LEU:N	2:X:81:MET:O	2.52	0.42
3:Y:52:ILE:CD1	3:Y:77:LEU:HD23	2.48	0.42
2:H:108:TRP:N	2:H:108:TRP:CD1	2.87	0.42
3:L:188:ALA:O	3:L:189:ASP:C	2.60	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:93:GLN:HG2	3:M:94:HIS:N	2.33	0.42
2:X:52:ASN:CG	2:X:55:ASN:HB2	2.43	0.42
3:Y:129:LEU:C	3:Y:131:SER:N	2.77	0.42
1:B:125:HIS:H	1:B:147:THR:HB	1.84	0.42
1:C:250:GLY:O	1:C:251:THR:C	2.61	0.42
3:L:144:TYR:HA	3:L:145:PRO:C	2.43	0.42
2:K:47:TRP:CH2	2:K:49:GLY:HA2	2.54	0.42
2:X:108:TRP:N	2:X:108:TRP:CD1	2.87	0.42
2:X:127:PHE:CE1	3:Y:128:GLN:HA	2.54	0.42
2:X:151:PHE:C	2:X:151:PHE:HD1	2.27	0.42
3:Y:137:VAL:CG2	3:Y:182:THR:HG23	2.49	0.42
1:A:190:ILE:O	1:A:242:THR:CG2	2.67	0.42
1:A:249:HIS:O	1:A:250:GLY:C	2.61	0.42
1:B:192:SER:HB3	1:B:207:ARG:CG	2.49	0.42
1:B:206:LEU:CD1	1:B:229:PHE:CZ	2.96	0.42
1:B:206:LEU:O	1:B:207:ARG:HG3	2.20	0.42
1:C:206:LEU:HD11	1:C:229:PHE:CZ	2.51	0.42
2:H:201:CYS:O	2:H:213:ASP:HA	2.19	0.42
2:X:60:PHE:CZ	2:X:70:LEU:HG	2.54	0.42
2:X:125:SER:O	2:X:147:VAL:HA	2.19	0.42
1:B:157:ASN:HB3	1:B:159:LYS:CE	2.50	0.42
1:C:125:HIS:H	1:C:147:THR:HB	1.84	0.42
1:C:206:LEU:HD23	1:C:225:LEU:HB2	2.01	0.42
2:H:178:SER:OG	2:H:179:GLY:N	2.52	0.42
3:L:186:SER:C	3:L:188:ALA:N	2.75	0.42
3:L:205:LEU:C	3:L:207:SER:N	2.74	0.42
2:K:201:CYS:O	2:K:213:ASP:HA	2.19	0.42
2:X:47:TRP:CH2	2:X:49:GLY:HA2	2.55	0.42
3:Y:25:ALA:CB	3:Y:27:GLN:O	2.68	0.42
1:A:132:SER:O	1:A:133:LYS:O	2.38	0.42
3:L:149:LYS:HG3	3:L:150:VAL:N	2.34	0.42
3:L:155:ASP:OD2	3:L:193:HIS:ND1	2.52	0.42
2:K:5:VAL:HA	2:K:110:GLN:HE21	1.85	0.42
2:K:125:SER:HB3	2:K:127:PHE:CE2	2.55	0.42
2:K:157:VAL:HG11	2:K:185:SER:CB	2.49	0.42
2:X:47:TRP:CG	3:Y:100:PRO:HG2	2.55	0.42
2:X:132:SER:O	2:X:133:SER:C	2.58	0.42
3:Y:202:HIS:ND1	3:Y:202:HIS:C	2.77	0.42
1:A:243:ASP:O	1:A:246:GLN:HG2	2.19	0.42
1:B:128:SER:HB3	1:B:254:THR:HB	2.01	0.42
2:H:193:SER:C	2:H:195:GLY:N	2.75	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:194:LYS:HA	3:L:194:LYS:HE3	2.00	0.42
2:K:151:PHE:CD1	2:K:152:PRO:N	2.87	0.42
3:M:149:LYS:HG3	3:M:150:VAL:N	2.34	0.42
2:X:20:LEU:O	2:X:80:TYR:HA	2.20	0.42
2:X:43:GLN:OE1	2:X:43:GLN:HA	2.19	0.42
2:X:81:MET:HE1	2:X:94:TYR:HD2	1.85	0.42
1:A:132:SER:C	1:A:133:LYS:O	2.63	0.42
1:A:194:CYS:HB2	1:A:238:PHE:CE2	2.55	0.42
1:A:261:LEU:N	1:A:261:LEU:CD2	2.61	0.42
1:B:175:VAL:O	1:B:223:ILE:N	2.53	0.42
1:B:195:LEU:HB2	1:B:237:VAL:HG12	2.01	0.42
2:H:24:ALA:HB1	2:H:27:TYR:CE1	2.55	0.42
2:H:60:PHE:CZ	2:H:70:LEU:HG	2.55	0.42
2:H:149:ASP:HA	2:H:180:LEU:HB2	2.02	0.42
2:H:193:SER:O	2:H:194:LEU:C	2.63	0.42
3:M:79:ILE:HG21	3:M:86:ASP:OD2	2.20	0.42
2:X:12:VAL:HG21	2:X:16:ALA:HB3	2.02	0.42
2:X:73:ASP:CG	2:X:73:ASP:O	2.60	0.42
2:X:129:LEU:HB3	3:Y:122:PHE:CD1	2.54	0.42
2:X:160:ASN:O	2:X:161:SER:C	2.63	0.42
3:Y:202:HIS:O	3:Y:203:GLN:C	2.62	0.42
1:A:179:SER:O	1:A:218:CYS:HA	2.19	0.42
1:B:176:THR:HB	1:B:222:SER:HG	1.84	0.42
2:H:95:TYR:HE1	2:H:110:GLN:O	2.03	0.42
2:H:212:VAL:HG12	2:H:213:ASP:N	2.35	0.42
2:K:14:PRO:HD3	2:K:117:SER:C	2.44	0.42
2:X:4:LEU:HD23	2:X:24:ALA:HA	2.01	0.42
2:X:24:ALA:O	2:X:25:SER:HB3	2.20	0.42
3:Y:117:PRO:CD	3:Y:205:LEU:HD13	2.34	0.42
1:A:125:HIS:H	1:A:147:THR:HB	1.84	0.42
2:H:47:TRP:HE3	2:H:61:ASN:HB2	1.85	0.42
2:H:52:ASN:CG	2:H:55:ASN:HB2	2.45	0.42
2:H:73:ASP:OD2	2:H:76:ALA:CB	2.68	0.42
2:H:84:SER:O	2:H:85:SER:C	2.63	0.42
3:M:159:GLN:HG3	3:M:183:LEU:HD13	1.99	0.42
2:X:51:ILE:O	2:X:51:ILE:HG23	2.19	0.42
1:A:203:ARG:HH21	1:C:145:TYR:HB2	1.84	0.41
1:B:196:LYS:HD3	1:B:202:GLU:HG2	2.01	0.41
1:C:258:LEU:HD12	1:C:258:LEU:C	2.45	0.41
2:H:14:PRO:HD3	2:H:117:SER:C	2.45	0.41
2:H:61:ASN:O	2:H:62:GLU:C	2.62	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:191:SER:C	2:H:193:SER:N	2.77	0.41
3:L:25:ALA:C	3:L:27:GLN:H	2.26	0.41
3:L:186:SER:O	3:L:188:ALA:N	2.53	0.41
3:M:6:GLN:CD	3:M:105:GLY:H	2.28	0.41
2:X:14:PRO:HD3	2:X:117:SER:C	2.45	0.41
2:X:172:PRO:HD2	3:Y:166:SER:OG	2.20	0.41
3:Y:146:ARG:NH2	3:Y:167:VAL:CG2	2.81	0.41
1:C:126:VAL:HG22	1:C:256:PHE:O	2.20	0.41
1:C:193:LEU:C	1:C:193:LEU:CD2	2.94	0.41
1:C:205:LEU:C	1:C:206:LEU:HD13	2.45	0.41
2:K:5:VAL:HA	2:K:110:GLN:NE2	2.36	0.41
2:K:63:LYS:HG3	2:K:64:PHE:CD1	2.55	0.41
2:K:78:THR:CG2	2:K:80:TYR:CE2	3.02	0.41
2:X:24:ALA:HB1	2:X:27:TYR:CE1	2.55	0.41
2:X:47:TRP:CZ2	2:X:49:GLY:C	2.98	0.41
2:X:156:THR:HG23	2:X:204:ASN:HB3	2.02	0.41
3:Y:192:LYS:HE3	3:Y:193:HIS:HD2	1.82	0.41
1:B:182:GLU:HA	1:B:185:SER:CB	2.50	0.41
1:B:189:PHE:CD1	1:B:189:PHE:C	2.98	0.41
2:H:13:LYS:CD	2:H:13:LYS:N	2.77	0.41
3:L:71:SER:HA	3:L:75:PHE:CE2	2.55	0.41
2:K:86:LEU:HD23	2:K:90:ASP:OD2	2.21	0.41
3:M:93:GLN:HB2	3:M:102:PHE:CD2	2.54	0.41
2:X:2:VAL:HG23	2:X:27:TYR:CD1	2.55	0.41
2:X:91:THR:HA	2:X:114:VAL:O	2.20	0.41
2:X:183:LEU:HD12	2:X:183:LEU:O	2.19	0.41
1:A:128:SER:HB3	1:A:254:THR:O	2.20	0.41
1:B:146:TYR:CD2	1:B:146:TYR:C	2.98	0.41
3:L:11:LEU:C	3:L:11:LEU:CD1	2.94	0.41
2:X:73:ASP:O	2:X:74:LYS:C	2.63	0.41
3:Y:17:GLU:O	3:Y:82:VAL:HG23	2.20	0.41
1:C:195:LEU:HD12	1:C:196:LYS:H	1.83	0.41
2:H:127:PHE:CE2	3:L:128:GLN:HG3	2.55	0.41
3:L:193:HIS:O	3:L:215:ARG:NE	2.53	0.41
2:K:43:GLN:CD	2:K:44:GLY:H	2.28	0.41
3:M:27:GLN:O	3:M:73:THR:HG22	2.21	0.41
1:A:258:LEU:C	1:A:258:LEU:HD12	2.45	0.41
1:B:250:GLY:O	1:B:251:THR:C	2.60	0.41
3:L:59:GLU:OE2	3:L:59:GLU:CA	2.68	0.41
2:K:125:SER:O	2:K:148:LYS:N	2.50	0.41
2:K:129:LEU:HD12	2:K:144:GLY:C	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:186:VAL:HG12	2:K:187:VAL:N	2.36	0.41
3:M:143:PHE:HE1	3:M:179:LEU:N	2.18	0.41
2:X:41:PRO:C	2:X:43:GLN:N	2.78	0.41
2:X:124:PRO:CB	2:X:150:TYR:HB3	2.51	0.41
2:X:191:SER:C	2:X:193:SER:N	2.77	0.41
2:X:193:SER:O	2:X:194:LEU:C	2.63	0.41
3:Y:124:PRO:HG2	3:Y:190:TYR:CZ	2.56	0.41
3:Y:144:TYR:HA	3:Y:145:PRO:O	2.21	0.41
1:A:161:LEU:HD12	1:A:256:PHE:CZ	2.55	0.41
1:A:180:ASN:O	1:A:212:HIS:HB3	2.20	0.41
1:A:190:ILE:CD1	1:A:207:ARG:NE	2.84	0.41
1:A:246:GLN:HE21	1:A:246:GLN:HB3	1.51	0.41
1:B:196:LYS:HA	1:B:196:LYS:HD2	1.89	0.41
2:H:104:ASP:HB2	3:L:50:LEU:HD22	2.02	0.41
3:L:21:ILE:HD12	3:L:77:LEU:HD12	2.02	0.41
2:K:102:ARG:HH11	2:K:102:ARG:HD3	1.64	0.41
3:M:71:SER:HA	3:M:75:PHE:CE2	2.56	0.41
2:X:2:VAL:HA	2:X:26:GLY:HA3	2.02	0.41
2:X:120:SER:C	2:X:121:THR:O	2.63	0.41
2:X:121:THR:HA	2:X:151:PHE:O	2.20	0.41
3:Y:112:ARG:HD3	3:Y:113:THR:O	2.20	0.41
3:Y:202:HIS:CE1	3:Y:204:GLY:H	2.39	0.41
1:A:196:LYS:HD3	1:A:202:GLU:HG2	2.03	0.41
1:B:132:SER:C	1:B:133:LYS:O	2.63	0.41
1:B:182:GLU:C	1:B:185:SER:HB2	2.46	0.41
1:C:167:GLY:O	1:C:230:GLU:HA	2.21	0.41
1:C:169:TYR:CE2	1:C:260:LYS:HD2	2.55	0.41
3:L:2:ILE:HG13	3:L:94:HIS:CE1	2.54	0.41
3:L:167:VAL:CG1	3:L:168:THR:H	2.34	0.41
2:K:186:VAL:HG11	3:M:139:LEU:CD2	2.51	0.41
2:X:105:MET:HE2	2:X:108:TRP:CH2	2.55	0.41
2:X:162:GLY:O	2:X:163:ALA:C	2.63	0.41
2:X:177:SER:C	2:X:178:SER:O	2.59	0.41
1:A:131:SER:CB	1:A:139:GLN:HG3	2.50	0.41
1:A:244:PRO:HA	1:A:247:VAL:HG12	2.02	0.41
1:B:124:ALA:O	1:B:257:GLY:HA3	2.21	0.41
1:B:190:ILE:O	1:B:242:THR:CG2	2.67	0.41
1:C:161:LEU:HD12	1:C:256:PHE:CZ	2.56	0.41
2:H:67:LYS:HE2	2:H:90:ASP:OD1	2.20	0.41
2:H:151:PHE:CD1	2:H:152:PRO:N	2.88	0.41
3:L:13:VAL:CG2	3:L:17:GLU:HB3	2.22	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:110:ILE:HG13	3:L:170:GLN:NE2	2.35	0.41
2:K:132:SER:OG	2:K:134:LYS:HD2	2.21	0.41
2:K:134:LYS:H	2:K:134:LYS:HG3	1.50	0.41
2:K:189:VAL:HG11	2:K:199:TYR:CZ	2.56	0.41
3:M:114:VAL:HG21	3:M:203:GLN:OE1	2.21	0.41
3:M:179:LEU:HD23	3:M:180:SER:CA	2.49	0.41
2:X:70:LEU:N	2:X:70:LEU:HD23	2.35	0.41
2:X:191:SER:O	2:X:193:SER:N	2.54	0.41
3:Y:40:TYR:OH	3:Y:93:GLN:NE2	2.52	0.41
3:Y:193:HIS:O	3:Y:215:ARG:NE	2.53	0.41
1:A:141:ALA:CB	1:A:143:LYS:HE3	2.51	0.41
1:A:153:VAL:O	1:A:153:VAL:HG12	2.20	0.41
1:A:211:THR:O	1:A:212:HIS:C	2.63	0.41
1:C:135:THR:CB	1:C:137:VAL:CG1	2.95	0.41
1:C:211:THR:O	1:C:212:HIS:C	2.64	0.41
3:L:43:LYS:HB2	3:L:46:GLN:HG3	2.03	0.41
3:L:54:TYR:O	3:L:56:SER:N	2.52	0.41
3:L:146:ARG:HG2	3:L:146:ARG:O	2.19	0.41
3:L:206:SER:C	3:L:207:SER:OG	2.64	0.41
3:M:67:SER:O	3:M:77:LEU:CD2	2.68	0.41
2:X:65:LYS:O	2:X:65:LYS:HD3	2.21	0.41
3:Y:39:TRP:CD2	3:Y:77:LEU:HB2	2.56	0.41
3:Y:170:GLN:HG2	3:Y:177:TYR:CZ	2.56	0.41
1:A:206:LEU:HD23	1:A:225:LEU:HB2	2.02	0.40
1:C:134:THR:O	1:C:135:THR:HG23	2.22	0.40
2:K:43:GLN:NE2	2:K:44:GLY:N	2.64	0.40
2:K:50:GLU:OE2	2:K:59:ASN:HB2	2.21	0.40
3:M:10:THR:HG22	3:M:11:LEU:N	2.35	0.40
3:M:58:LEU:HD11	3:M:66:PHE:O	2.19	0.40
3:Y:9:ALA:O	3:Y:106:THR:HA	2.21	0.40
3:Y:155:ASP:C	3:Y:157:ALA:H	2.29	0.40
1:B:185:SER:HB3	1:B:186:GLN:H	1.69	0.40
2:H:12:VAL:HG22	2:H:13:LYS:N	2.36	0.40
2:K:2:VAL:HA	2:K:26:GLY:HA3	2.03	0.40
2:K:6:GLN:HE22	2:K:96:CYS:N	2.18	0.40
3:M:54:TYR:O	3:M:56:SER:N	2.53	0.40
2:X:104:ASP:HB2	3:Y:50:LEU:HD22	2.04	0.40
2:X:171:PHE:HB3	2:X:172:PRO:HD2	2.03	0.40
3:Y:6:GLN:O	3:Y:7:SER:CB	2.69	0.40
3:Y:155:ASP:CG	3:Y:193:HIS:HB3	2.46	0.40
3:Y:213:PHE:CD2	3:Y:213:PHE:C	2.98	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:LEU:HD21	1:A:158:GLY:HA2	2.03	0.40
1:B:139:GLN:C	1:B:140:TRP:CG	2.99	0.40
2:H:150:TYR:CE1	2:H:155:VAL:CG1	3.03	0.40
2:H:150:TYR:CE1	2:H:155:VAL:HB	2.55	0.40
2:H:180:LEU:HD12	2:H:180:LEU:H	1.85	0.40
2:H:183:LEU:HD12	2:H:183:LEU:O	2.20	0.40
3:L:36:TYR:HB3	3:L:95:SER:HG	1.85	0.40
3:L:71:SER:CA	3:L:75:PHE:CE2	3.04	0.40
2:K:52:ASN:OD1	2:K:52:ASN:C	2.64	0.40
2:K:126:VAL:HA	2:K:146:LEU:O	2.21	0.40
2:K:171:PHE:HB3	2:K:172:PRO:HD2	2.02	0.40
3:M:146:ARG:CZ	3:M:167:VAL:HG21	2.52	0.40
2:X:144:GLY:HA2	2:X:159:TRP:CZ2	2.56	0.40
2:X:150:TYR:CE1	2:X:155:VAL:CG1	3.05	0.40
2:X:171:PHE:CE2	3:Y:180:SER:HB3	2.56	0.40
3:Y:71:SER:N	3:Y:75:PHE:CE2	2.88	0.40
1:A:145:TYR:CB	1:B:203:ARG:HH21	2.35	0.40
2:H:20:LEU:O	2:H:80:TYR:HA	2.21	0.40
2:H:107:SER:C	2:H:108:TRP:CD1	2.99	0.40
2:H:144:GLY:HA2	2:H:159:TRP:CZ2	2.56	0.40
3:L:62:VAL:HA	3:L:63:PRO:HD3	1.80	0.40
2:K:124:PRO:HB3	2:K:150:TYR:HB3	2.03	0.40
3:M:25:ALA:C	3:M:27:GLN:N	2.80	0.40
2:X:86:LEU:HD23	2:X:90:ASP:OD2	2.20	0.40
2:X:143:LEU:HD22	2:X:187:VAL:HG13	2.04	0.40
3:Y:144:TYR:CD2	3:Y:145:PRO:N	2.89	0.40
1:C:189:PHE:CD1	1:C:189:PHE:C	3.00	0.40
1:C:193:LEU:C	1:C:193:LEU:HD22	2.47	0.40
2:H:62:GLU:C	2:H:64:PHE:N	2.79	0.40
3:M:159:GLN:NE2	3:M:183:LEU:HD11	2.28	0.40
2:X:134:LYS:H	2:X:134:LYS:HG3	1.51	0.40
3:Y:183:LEU:HG	3:Y:184:THR:N	2.37	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:24:ARG:NH1	3:M:24:ARG:NH2[2_655]	2.03	0.17
3:L:24:ARG:NH2	3:Y:24:ARG:NH2[4_555]	2.06	0.14
3:L:24:ARG:NH2	3:Y:24:ARG:NH1[4_555]	2.11	0.09
3:L:24:ARG:NH1	3:Y:24:ARG:NH2[4_555]	2.13	0.07

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	141/146 (97%)	121 (86%)	14 (10%)	6 (4%)	2	12
1	B	141/146 (97%)	119 (84%)	15 (11%)	7 (5%)	1	11
1	C	141/146 (97%)	121 (86%)	14 (10%)	6 (4%)	2	12
2	H	217/219 (99%)	179 (82%)	27 (12%)	11 (5%)	1	10
2	K	217/219 (99%)	176 (81%)	32 (15%)	9 (4%)	2	13
2	X	217/219 (99%)	182 (84%)	27 (12%)	8 (4%)	2	15
3	L	213/218 (98%)	181 (85%)	28 (13%)	4 (2%)	6	27
3	M	213/218 (98%)	182 (85%)	25 (12%)	6 (3%)	4	20
3	Y	213/218 (98%)	179 (84%)	28 (13%)	6 (3%)	4	20
All	All	1713/1749 (98%)	1440 (84%)	210 (12%)	63 (4%)	2	15

All (63) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	183	ALA
1	A	202	GLU
1	B	133	LYS
1	B	183	ALA
1	B	202	GLU
1	C	133	LYS
1	C	183	ALA
2	H	121	THR
2	H	177	SER
2	H	194	LEU
2	K	121	THR
2	K	177	SER
2	K	194	LEU
2	X	121	THR
2	X	177	SER
2	X	194	LEU

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Mol	Chain	Res	Type
3	Y	160	SER
1	A	133	LYS
1	A	185	SER
1	B	185	SER
1	C	185	SER
1	C	202	GLU
1	C	245	SER
2	H	149	ASP
3	L	160	SER
2	K	149	ASP
3	M	160	SER
2	X	149	ASP
1	A	215	ALA
1	A	245	SER
1	B	144	GLY
1	B	215	ALA
1	B	245	SER
1	C	215	ALA
2	H	92	ALA
2	K	74	LYS
2	K	92	ALA
2	X	92	ALA
2	X	207	PRO
2	H	63	LYS
2	H	119	ALA
2	H	207	PRO
3	L	95	SER
3	L	142	ASN
2	K	16	ALA
2	K	207	PRO
3	M	55	ALA
3	M	203	GLN
2	X	63	LYS
2	X	119	ALA
3	Y	95	SER
2	K	161	SER
3	M	95	SER
3	Y	55	ALA
3	Y	142	ASN
2	H	74	LYS
2	H	161	SER
3	M	114	VAL

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Mol	Chain	Res	Type
3	M	142	ASN
2	H	41	PRO
3	L	124	PRO
3	Y	114	VAL
3	Y	124	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	120/122 (98%)	79 (66%)	41 (34%)	0	0
1	B	120/122 (98%)	79 (66%)	41 (34%)	0	0
1	C	120/122 (98%)	81 (68%)	39 (32%)	0	0
2	H	187/187 (100%)	132 (71%)	55 (29%)	0	1
2	K	187/187 (100%)	130 (70%)	57 (30%)	0	0
2	X	187/187 (100%)	134 (72%)	53 (28%)	0	1
3	L	190/192 (99%)	136 (72%)	54 (28%)	0	1
3	M	190/192 (99%)	137 (72%)	53 (28%)	0	1
3	Y	190/192 (99%)	133 (70%)	57 (30%)	0	1
All	All	1491/1503 (99%)	1041 (70%)	450 (30%)	0	0

All (450) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	119	ASN
1	A	121	GLN
1	A	122	ILE
1	A	127	ILE
1	A	129	GLU
1	A	131	SER
1	A	132	SER
1	A	133	LYS
1	A	134	THR

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Mol	Chain	Res	Type
1	A	135	THR
1	A	137	VAL
1	A	152	LEU
1	A	153	VAL
1	A	154	THR
1	A	155	LEU
1	A	159	LYS
1	A	160	GLN
1	A	165	ARG
1	A	168	LEU
1	A	174	GLN
1	A	176	THR
1	A	181	ARG
1	A	184	SER
1	A	185	SER
1	A	190	ILE
1	A	192	SER
1	A	193	LEU
1	A	195	LEU
1	A	196	LYS
1	A	203	ARG
1	A	206	LEU
1	A	211	THR
1	A	223	ILE
1	A	225	LEU
1	A	236	SER
1	A	241	VAL
1	A	242	THR
1	A	247	VAL
1	A	251	THR
1	A	255	SER
1	A	261	LEU
1	B	119	ASN
1	B	122	ILE
1	B	127	ILE
1	B	129	GLU
1	B	131	SER
1	B	132	SER
1	B	133	LYS
1	B	134	THR
1	B	135	THR
1	B	137	VAL

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Mol	Chain	Res	Type
1	B	143	LYS
1	B	152	LEU
1	B	153	VAL
1	B	154	THR
1	B	155	LEU
1	B	159	LYS
1	B	160	GLN
1	B	165	ARG
1	B	168	LEU
1	B	174	GLN
1	B	176	THR
1	B	181	ARG
1	B	184	SER
1	B	185	SER
1	B	190	ILE
1	B	192	SER
1	B	193	LEU
1	B	195	LEU
1	B	203	ARG
1	B	206	LEU
1	B	211	THR
1	B	213	SER
1	B	223	ILE
1	B	225	LEU
1	B	236	SER
1	B	241	VAL
1	B	242	THR
1	B	247	VAL
1	B	251	THR
1	B	255	SER
1	B	261	LEU
1	C	119	ASN
1	C	121	GLN
1	C	122	ILE
1	C	127	ILE
1	C	131	SER
1	C	132	SER
1	C	133	LYS
1	C	134	THR
1	C	135	THR
1	C	137	VAL
1	C	152	LEU

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Mol	Chain	Res	Type
1	C	153	VAL
1	C	154	THR
1	C	155	LEU
1	C	159	LYS
1	C	160	GLN
1	C	165	ARG
1	C	168	LEU
1	C	174	GLN
1	C	176	THR
1	C	181	ARG
1	C	184	SER
1	C	185	SER
1	C	190	ILE
1	C	192	SER
1	C	193	LEU
1	C	195	LEU
1	C	203	ARG
1	C	206	LEU
1	C	211	THR
1	C	223	ILE
1	C	225	LEU
1	C	236	SER
1	C	241	VAL
1	C	242	THR
1	C	247	VAL
1	C	251	THR
1	C	255	SER
1	C	261	LEU
2	H	1	GLN
2	H	2	VAL
2	H	6	GLN
2	H	10	GLU
2	H	11	VAL
2	H	13	LYS
2	H	21	SER
2	H	22	CYS
2	H	38	LYS
2	H	43	GLN
2	H	45	LEU
2	H	52	ASN
2	H	54	SER
2	H	65	LYS

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Mol	Chain	Res	Type
2	H	67	LYS
2	H	71	THR
2	H	72	VAL
2	H	74	LYS
2	H	75	SER
2	H	84	SER
2	H	88	SER
2	H	97	THR
2	H	98	ARG
2	H	105	MET
2	H	113	LEU
2	H	114	VAL
2	H	115	THR
2	H	117	SER
2	H	118	SER
2	H	122	LYS
2	H	133	SER
2	H	134	LYS
2	H	140	THR
2	H	143	LEU
2	H	146	LEU
2	H	148	LYS
2	H	149	ASP
2	H	150	TYR
2	H	155	VAL
2	H	158	SER
2	H	161	SER
2	H	170	THR
2	H	175	LEU
2	H	178	SER
2	H	180	LEU
2	H	183	LEU
2	H	184	SER
2	H	191	SER
2	H	192	SER
2	H	196	THR
2	H	200	ILE
2	H	203	VAL
2	H	209	ASN
2	H	214	LYS
2	H	219	LYS
3	L	2	ILE

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Mol	Chain	Res	Type
3	L	7	SER
3	L	11	LEU
3	L	18	ARG
3	L	20	THR
3	L	24	ARG
3	L	30	SER
3	L	33	THR
3	L	34	TYR
3	L	40	TYR
3	L	46	GLN
3	L	49	LYS
3	L	50	LEU
3	L	51	LEU
3	L	53	LYS
3	L	56	SER
3	L	57	ASN
3	L	58	LEU
3	L	60	SER
3	L	65	ARG
3	L	69	SER
3	L	77	LEU
3	L	78	THR
3	L	89	THR
3	L	93	GLN
3	L	98	ILE
3	L	106	THR
3	L	109	GLU
3	L	119	VAL
3	L	125	SER
3	L	130	LYS
3	L	131	SER
3	L	133	THR
3	L	136	VAL
3	L	139	LEU
3	L	149	LYS
3	L	150	VAL
3	L	151	GLN
3	L	153	LYS
3	L	158	LEU
3	L	169	GLU
3	L	173	LYS
3	L	179	LEU

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Mol	Chain	Res	Type
3	L	183	LEU
3	L	187	LYS
3	L	189	ASP
3	L	191	GLU
3	L	192	LYS
3	L	194	LYS
3	L	195	VAL
3	L	198	CYS
3	L	200	VAL
3	L	201	THR
3	L	207	SER
2	K	1	GLN
2	K	2	VAL
2	K	6	GLN
2	K	10	GLU
2	K	11	VAL
2	K	13	LYS
2	K	21	SER
2	K	38	LYS
2	K	43	GLN
2	K	45	LEU
2	K	52	ASN
2	K	54	SER
2	K	65	LYS
2	K	67	LYS
2	K	69	THR
2	K	71	THR
2	K	72	VAL
2	K	74	LYS
2	K	75	SER
2	K	84	SER
2	K	88	SER
2	K	97	THR
2	K	98	ARG
2	K	105	MET
2	K	113	LEU
2	K	114	VAL
2	K	115	THR
2	K	117	SER
2	K	118	SER
2	K	122	LYS
2	K	133	SER

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Mol	Chain	Res	Type
2	K	134	LYS
2	K	140	THR
2	K	143	LEU
2	K	146	LEU
2	K	148	LYS
2	K	149	ASP
2	K	155	VAL
2	K	158	SER
2	K	161	SER
2	K	165	THR
2	K	170	THR
2	K	174	VAL
2	K	175	LEU
2	K	178	SER
2	K	180	LEU
2	K	183	LEU
2	K	184	SER
2	K	191	SER
2	K	192	SER
2	K	196	THR
2	K	200	ILE
2	K	202	ASN
2	K	203	VAL
2	K	209	ASN
2	K	214	LYS
2	K	219	LYS
3	M	2	ILE
3	M	7	SER
3	M	11	LEU
3	M	13	VAL
3	M	18	ARG
3	M	20	THR
3	M	24	ARG
3	M	26	SER
3	M	30	SER
3	M	33	THR
3	M	34	TYR
3	M	40	TYR
3	M	46	GLN
3	M	49	LYS
3	M	53	LYS
3	M	56	SER

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Mol	Chain	Res	Type
3	M	57	ASN
3	M	58	LEU
3	M	60	SER
3	M	65	ARG
3	M	67	SER
3	M	69	SER
3	M	77	LEU
3	M	78	THR
3	M	89	THR
3	M	93	GLN
3	M	98	ILE
3	M	106	THR
3	M	119	VAL
3	M	125	SER
3	M	130	LYS
3	M	131	SER
3	M	133	THR
3	M	136	VAL
3	M	138	CYS
3	M	141	ASN
3	M	149	LYS
3	M	150	VAL
3	M	151	GLN
3	M	158	LEU
3	M	169	GLU
3	M	173	LYS
3	M	179	LEU
3	M	183	LEU
3	M	187	LYS
3	M	189	ASP
3	M	192	LYS
3	M	194	LYS
3	M	195	VAL
3	M	198	CYS
3	M	200	VAL
3	M	201	THR
3	M	207	SER
2	X	1	GLN
2	X	2	VAL
2	X	6	GLN
2	X	10	GLU
2	X	11	VAL

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Mol	Chain	Res	Type
2	X	13	LYS
2	X	21	SER
2	X	38	LYS
2	X	43	GLN
2	X	45	LEU
2	X	52	ASN
2	X	54	SER
2	X	65	LYS
2	X	67	LYS
2	X	71	THR
2	X	72	VAL
2	X	74	LYS
2	X	75	SER
2	X	84	SER
2	X	88	SER
2	X	98	ARG
2	X	105	MET
2	X	113	LEU
2	X	114	VAL
2	X	115	THR
2	X	117	SER
2	X	118	SER
2	X	122	LYS
2	X	133	SER
2	X	134	LYS
2	X	140	THR
2	X	143	LEU
2	X	146	LEU
2	X	148	LYS
2	X	149	ASP
2	X	150	TYR
2	X	155	VAL
2	X	158	SER
2	X	161	SER
2	X	165	THR
2	X	170	THR
2	X	178	SER
2	X	180	LEU
2	X	183	LEU
2	X	184	SER
2	X	191	SER
2	X	192	SER

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Mol	Chain	Res	Type
2	X	196	THR
2	X	200	ILE
2	X	203	VAL
2	X	209	ASN
2	X	214	LYS
2	X	219	LYS
3	Y	2	ILE
3	Y	7	SER
3	Y	11	LEU
3	Y	13	VAL
3	Y	18	ARG
3	Y	20	THR
3	Y	24	ARG
3	Y	26	SER
3	Y	30	SER
3	Y	33	THR
3	Y	34	TYR
3	Y	40	TYR
3	Y	46	GLN
3	Y	49	LYS
3	Y	50	LEU
3	Y	51	LEU
3	Y	53	LYS
3	Y	57	ASN
3	Y	58	LEU
3	Y	60	SER
3	Y	65	ARG
3	Y	67	SER
3	Y	69	SER
3	Y	77	LEU
3	Y	78	THR
3	Y	89	THR
3	Y	93	GLN
3	Y	98	ILE
3	Y	99	PRO
3	Y	106	THR
3	Y	109	GLU
3	Y	119	VAL
3	Y	125	SER
3	Y	130	LYS
3	Y	131	SER
3	Y	133	THR

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Mol	Chain	Res	Type
3	Y	136	VAL
3	Y	139	LEU
3	Y	141	ASN
3	Y	146	ARG
3	Y	149	LYS
3	Y	150	VAL
3	Y	151	GLN
3	Y	153	LYS
3	Y	158	LEU
3	Y	169	GLU
3	Y	173	LYS
3	Y	179	LEU
3	Y	183	LEU
3	Y	187	LYS
3	Y	189	ASP
3	Y	192	LYS
3	Y	194	LYS
3	Y	195	VAL
3	Y	200	VAL
3	Y	201	THR
3	Y	207	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (75) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	139	GLN
1	A	151	ASN
1	A	160	GLN
1	A	174	GLN
1	A	180	ASN
1	A	212	HIS
1	A	224	HIS
1	A	246	GLN
1	B	121	GLN
1	B	139	GLN
1	B	151	ASN
1	B	174	GLN
1	B	180	ASN
1	B	212	HIS
1	B	224	HIS
1	B	246	GLN
1	C	121	GLN

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Mol	Chain	Res	Type
1	C	139	GLN
1	C	151	ASN
1	C	160	GLN
1	C	174	GLN
1	C	180	ASN
1	C	212	HIS
1	C	224	HIS
1	C	246	GLN
2	H	6	GLN
2	H	43	GLN
2	H	55	ASN
2	H	103	ASN
2	H	110	GLN
2	H	205	HIS
3	L	41	GLN
3	L	57	ASN
3	L	93	GLN
3	L	94	HIS
3	L	141	ASN
3	L	151	GLN
3	L	159	GLN
3	L	164	GLN
3	L	170	GLN
3	L	214	ASN
2	K	1	GLN
2	K	6	GLN
2	K	39	GLN
2	K	43	GLN
2	K	55	ASN
2	K	103	ASN
2	K	110	GLN
2	K	205	HIS
3	M	41	GLN
3	M	57	ASN
3	M	93	GLN
3	M	94	HIS
3	M	128	GLN
3	M	141	ASN
3	M	159	GLN
3	M	164	GLN
3	M	170	GLN
3	M	214	ASN

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Mol	Chain	Res	Type
2	X	6	GLN
2	X	43	GLN
2	X	55	ASN
2	X	103	ASN
2	X	110	GLN
2	X	205	HIS
3	Y	41	GLN
3	Y	57	ASN
3	Y	93	GLN
3	Y	94	HIS
3	Y	141	ASN
3	Y	151	GLN
3	Y	159	GLN
3	Y	164	GLN
3	Y	170	GLN
3	Y	214	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 3 ligands modelled in this entry, 3 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

There are no such residues in this entry.

5.8 Polymer linkage issues

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	142/146 (97%)	-0.28	2 (1%) 73 53	2, 12, 51, 78	0
1	B	142/146 (97%)	-0.35	2 (1%) 73 53	3, 12, 50, 76	0
1	C	142/146 (97%)	-0.29	3 (2%) 63 42	2, 12, 49, 78	0
2	H	219/219 (100%)	0.04	1 (0%) 87 73	4, 30, 56, 70	3 (1%)
2	K	219/219 (100%)	-0.02	3 (1%) 73 53	3, 28, 53, 68	3 (1%)
2	X	219/219 (100%)	-0.06	3 (1%) 73 53	2, 26, 52, 68	3 (1%)
3	L	215/218 (98%)	-0.20	1 (0%) 87 73	3, 16, 61, 69	0
3	M	215/218 (98%)	-0.24	1 (0%) 87 73	3, 14, 58, 68	0
3	Y	215/218 (98%)	-0.24	2 (0%) 81 63	2, 15, 58, 68	0
All	All	1728/1749 (98%)	-0.16	18 (1%) 79 61	2, 19, 57, 78	9 (0%)

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	185	SER	4.5
1	A	185	SER	4.1
1	B	185	SER	3.5
2	K	209	ASN	3.3
3	Y	133	THR	2.9
3	Y	125	SER	2.8
2	X	209	ASN	2.6
2	H	43	GLN	2.5
2	K	137	SER	2.4
1	B	184	SER	2.4
2	K	43	GLN	2.4
1	C	134	THR	2.3
3	L	162	ASN	2.3
1	C	186	GLN	2.3
1	A	183	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
2	X	43	GLN	2.1
2	X	121	THR	2.1
3	M	133	THR	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($\text{\AA}^2$)	Q<0.9
4	ZN	K	499	1/1	0.91	0.05	38,38,38,38	0
4	ZN	X	500	1/1	0.96	0.07	38,38,38,38	0
4	ZN	H	498	1/1	0.98	0.06	39,39,39,39	0

6.5 Other polymers [i](#)

There are no such residues in this entry.