



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 06:59 AM UTC

PDB ID : 4S20 / pdb_00004s20
Title : Structural basis for transcription reactivation by RapA
Authors : Liu, B.; Zuo, Y.; Steitz, T.A.
Deposited on : 2015-01-16
Resolution : 4.70 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

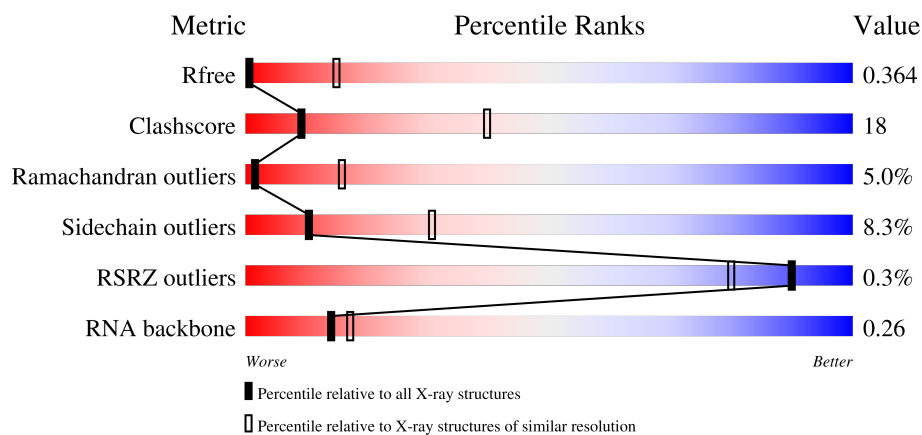
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.70 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.



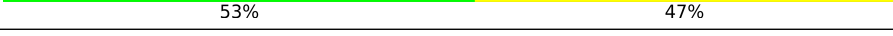
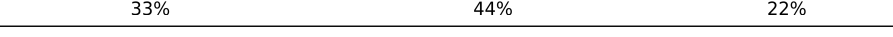
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1020 (5.48-3.92)
Clashscore	190562	1005 (5.40-3.96)
Ramachandran outliers	187476	1095 (5.50-3.90)
Sidechain outliers	187428	1077 (5.50-3.90)
RSRZ outliers	180081	1015 (5.48-3.92)
RNA backbone	3983	1042 (6.22-3.10)

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	329	62% 7% 31%
1	B	329	62% 7% 31%
1	F	329	61% 7% 31%
1	G	329	61% 7% 31%

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Mol	Chain	Length	Quality of chain
2	C	1342	
2	H	1342	
3	D	1416	
3	I	1416	
4	E	90	
4	J	90	
5	K	974	
5	L	974	
6	M	15	
6	O	15	
7	N	9	
7	P	9	

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 61154 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 DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	227	Total	C	N	O	S	0	0	0
			1759	1096	311	346	6			
1	B	227	Total	C	N	O	S	0	0	0
			1759	1096	311	346	6			
1	F	227	Total	C	N	O	S	0	0	0
			1759	1096	311	346	6			
1	G	227	Total	C	N	O	S	0	0	0
			1759	1096	311	346	6			

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1179	Total	C	N	O	S	0	0	0
			9285	5828	1620	1798	39			
2	H	1173	Total	C	N	O	S	0	0	0
			9235	5799	1609	1788	39			

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1149	Total	C	N	O	S	0	0	0
			8990	5649	1614	1681	46			
3	I	1160	Total	C	N	O	S	0	0	0
			9068	5701	1626	1695	46			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	1408	LEU	-	expression tag	UNP K0BCS5
D	1409	GLU	-	expression tag	UNP K0BCS5
D	1410	VAL	-	expression tag	UNP K0BCS5
D	1411	HIS	-	expression tag	UNP K0BCS5

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Chain	Residue	Modelled	Actual	Comment	Reference
D	1412	HIS	-	expression tag	UNP K0BCS5
D	1413	HIS	-	expression tag	UNP K0BCS5
D	1414	HIS	-	expression tag	UNP K0BCS5
D	1415	HIS	-	expression tag	UNP K0BCS5
D	1416	HIS	-	expression tag	UNP K0BCS5
I	1408	LEU	-	expression tag	UNP K0BCS5
I	1409	GLU	-	expression tag	UNP K0BCS5
I	1410	VAL	-	expression tag	UNP K0BCS5
I	1411	HIS	-	expression tag	UNP K0BCS5
I	1412	HIS	-	expression tag	UNP K0BCS5
I	1413	HIS	-	expression tag	UNP K0BCS5
I	1414	HIS	-	expression tag	UNP K0BCS5
I	1415	HIS	-	expression tag	UNP K0BCS5
I	1416	HIS	-	expression tag	UNP K0BCS5

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	75	Total	C	N	O	S	0	0	0
			600	365	114	120	1			
4	J	75	Total	C	N	O	S	0	0	0
			600	365	114	120	1			

- Molecule 5 is a protein called RNA polymerase-associated protein RapA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	K	961	Total	C	N	O	S	0	0	0
			7665	4797	1370	1468	30			
5	L	961	Total	C	N	O	S	0	0	0
			7665	4797	1370	1468	30			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	-5	HIS	-	expression tag	UNP P60240
K	-4	HIS	-	expression tag	UNP P60240
K	-3	HIS	-	expression tag	UNP P60240
K	-2	HIS	-	expression tag	UNP P60240
K	-1	HIS	-	expression tag	UNP P60240
K	0	HIS	-	expression tag	UNP P60240
K	350	CYS	ARG	engineered mutation	UNP P60240
L	-5	HIS	-	expression tag	UNP P60240

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Chain	Residue	Modelled	Actual	Comment	Reference
L	-4	HIS	-	expression tag	UNP P60240
L	-3	HIS	-	expression tag	UNP P60240
L	-2	HIS	-	expression tag	UNP P60240
L	-1	HIS	-	expression tag	UNP P60240
L	0	HIS	-	expression tag	UNP P60240
L	350	CYS	ARG	engineered mutation	UNP P60240

- Molecule 6 is a DNA chain called 5'-D(P*AP*CP*GP*AP*CP*TP*GP*AP*GP*CP*CP*GP*AP*TP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	M	15	Total	C	N	O	P	0	0	0
			311	146	61	89	15			
6	O	15	Total	C	N	O	P	0	0	0
			311	146	61	89	15			

- Molecule 7 is a RNA chain called 5'-R(P*AP*UP*CP*GP*GP*CP*UP*CP*A)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	N	9	Total	C	N	O	P	0	0	0
			191	85	33	64	9			
7	P	9	Total	C	N	O	P	0	0	0
			191	85	33	64	9			

- Molecule 8 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	D	2	Total	Zn	0	0
			2	2		
8	I	2	Total	Zn	0	0
			2	2		

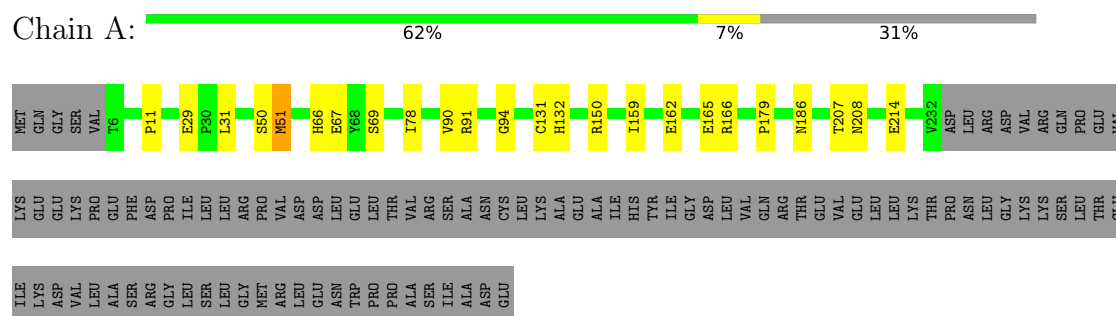
- Molecule 9 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	D	1	Total	Mg	0	0
			1	1		
9	I	1	Total	Mg	0	0
			1	1		

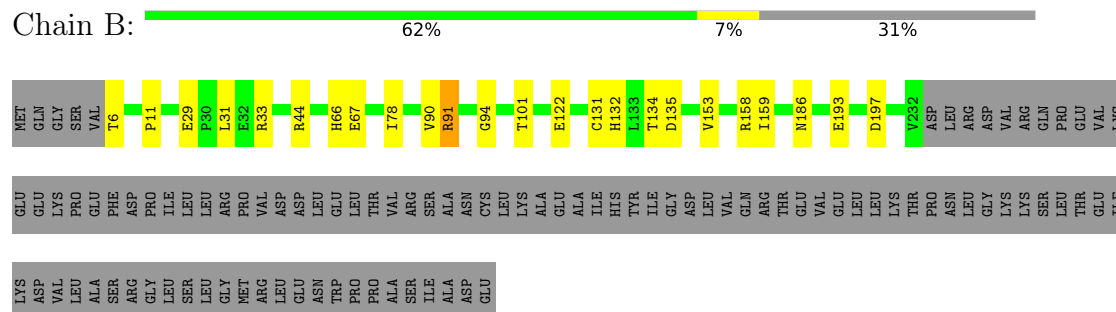
3 Residue-property plots [i](#)

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.

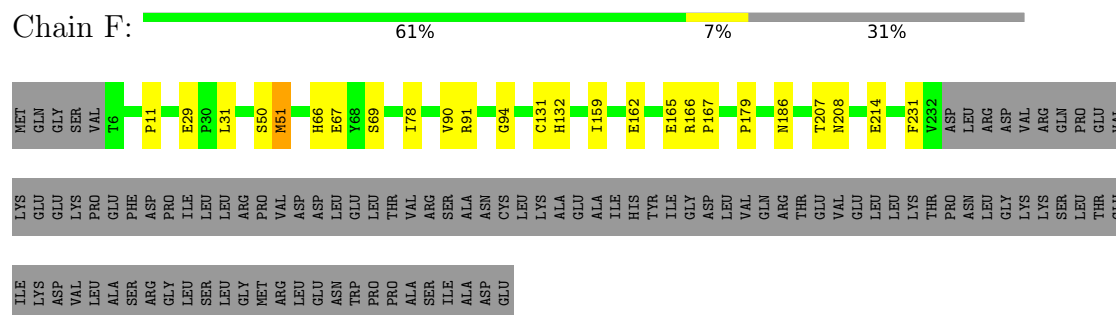
- Molecule 1: DNA-directed RNA polymerase subunit alpha



- Molecule 1: DNA-directed RNA polymerase subunit alpha

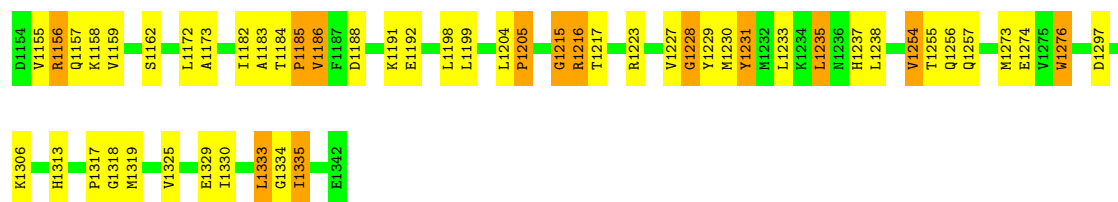


- Molecule 1: DNA-directed RNA polymerase subunit alpha



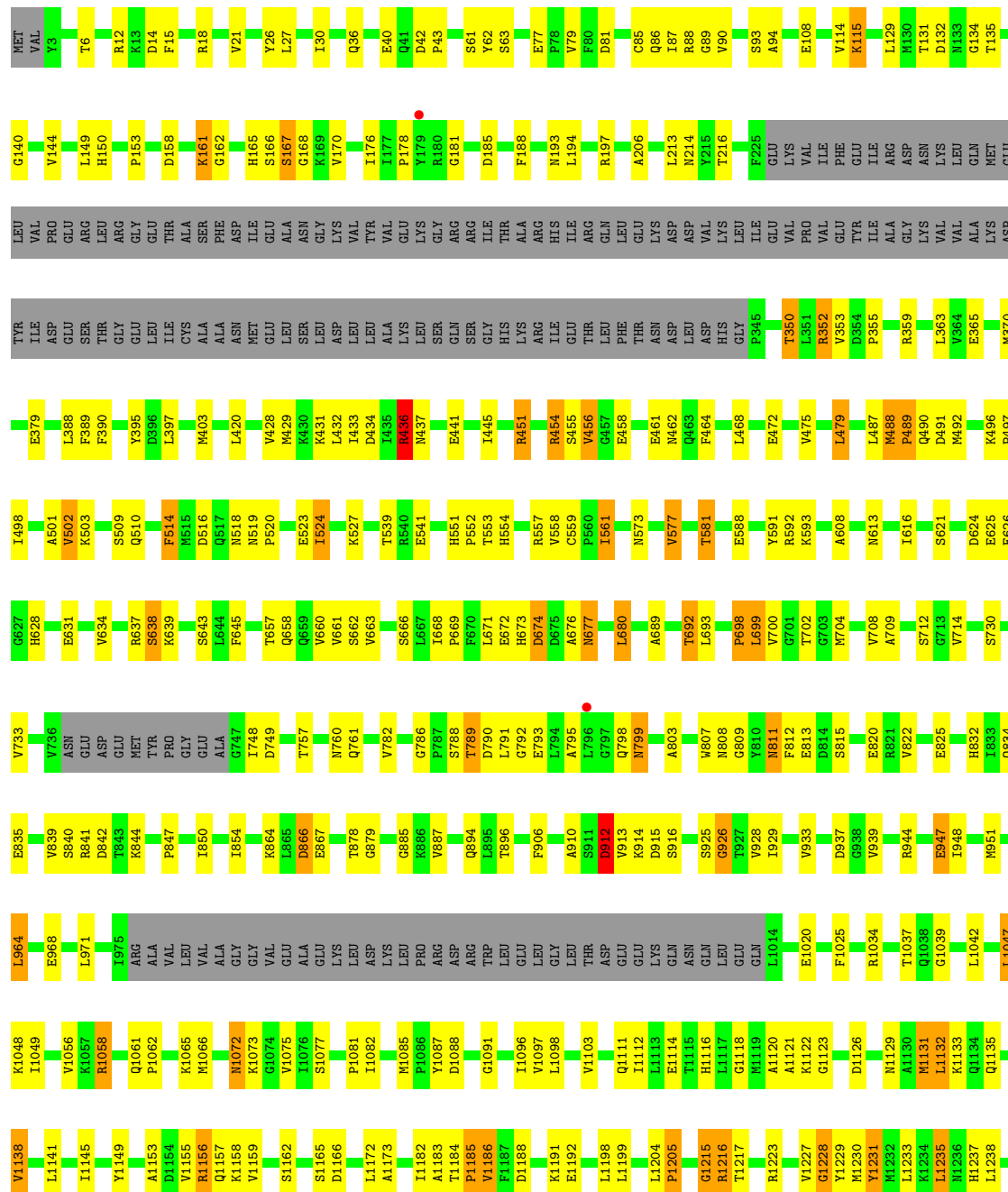
- Molecule 1: DNA-directed RNA polymerase subunit alpha

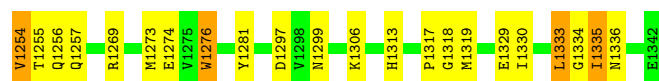




• Molecule 2: DNA-directed RNA polymerase subunit beta

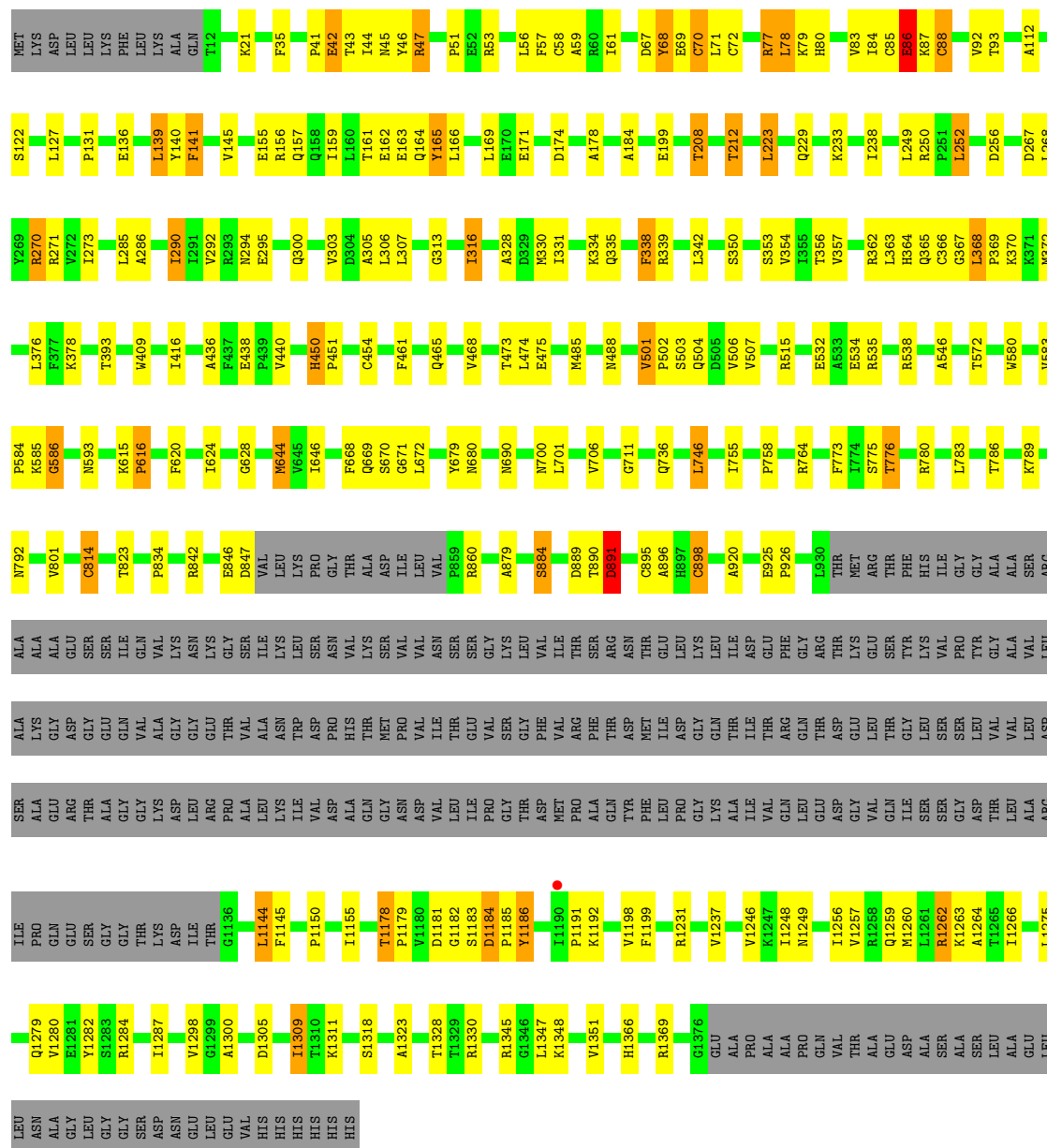
Chain H: 61% 23% 13%





• Molecule 3: DNA-directed RNA polymerase subunit beta'

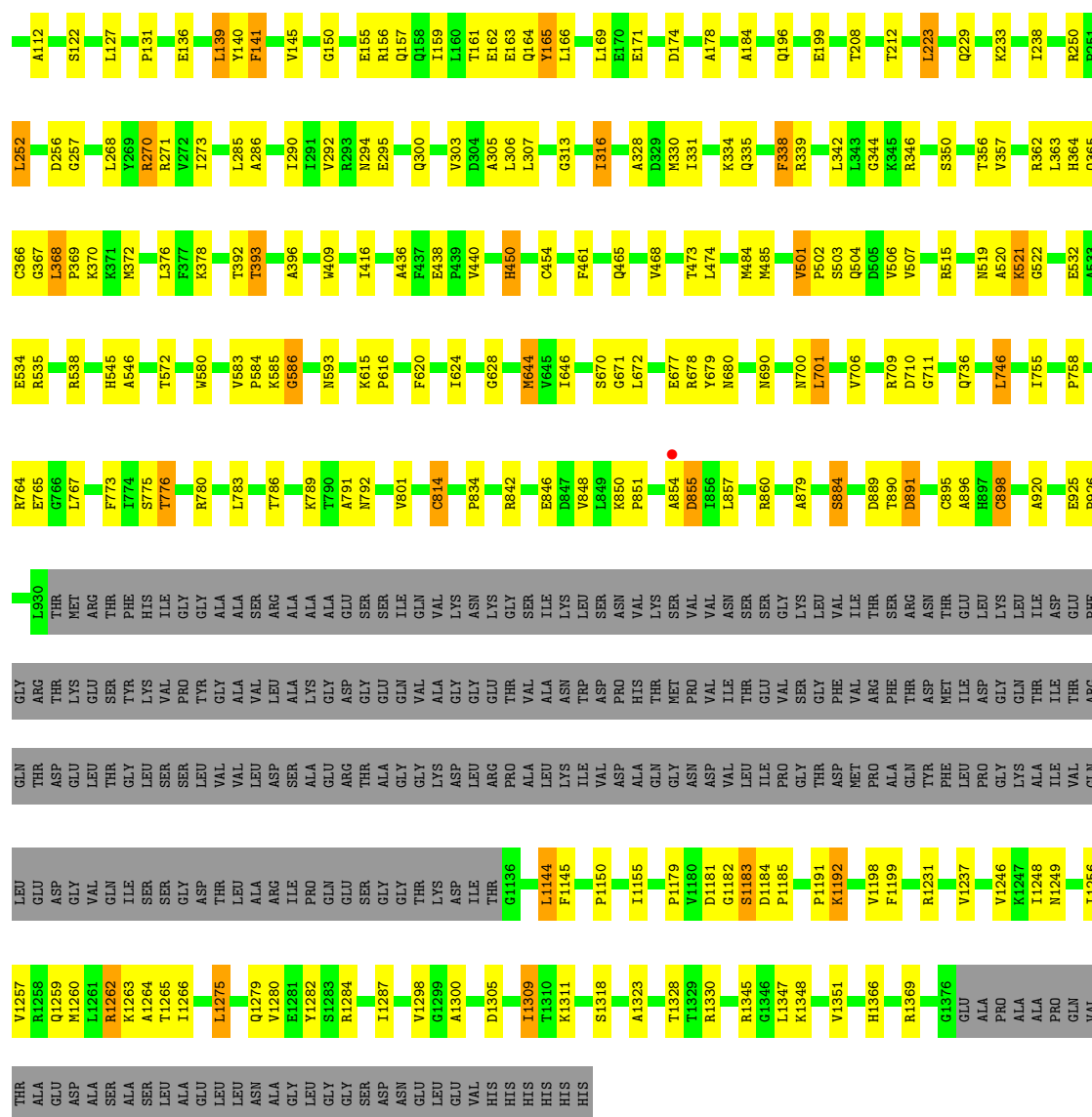
Chain D: 64% 15% 19%



• Molecule 3: DNA-directed RNA polymerase subunit beta'

Chain I: 63% 16% 18%





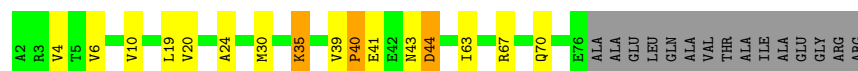
- Molecule 4: DNA-directed RNA polymerase subunit omega

Chain E: 63% 17% 17%

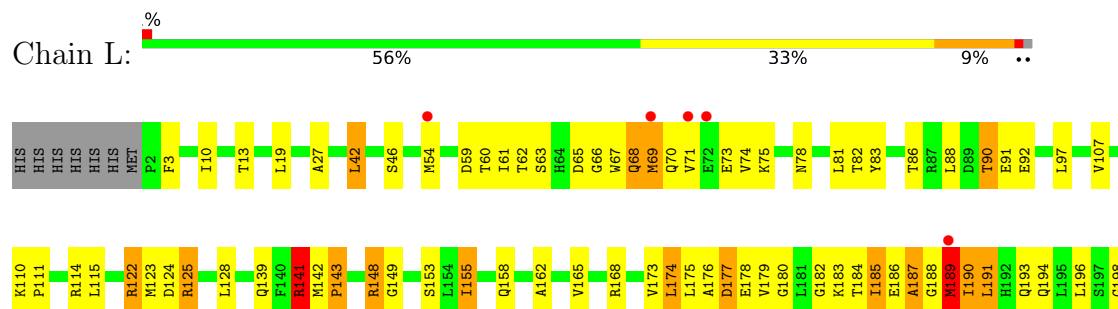


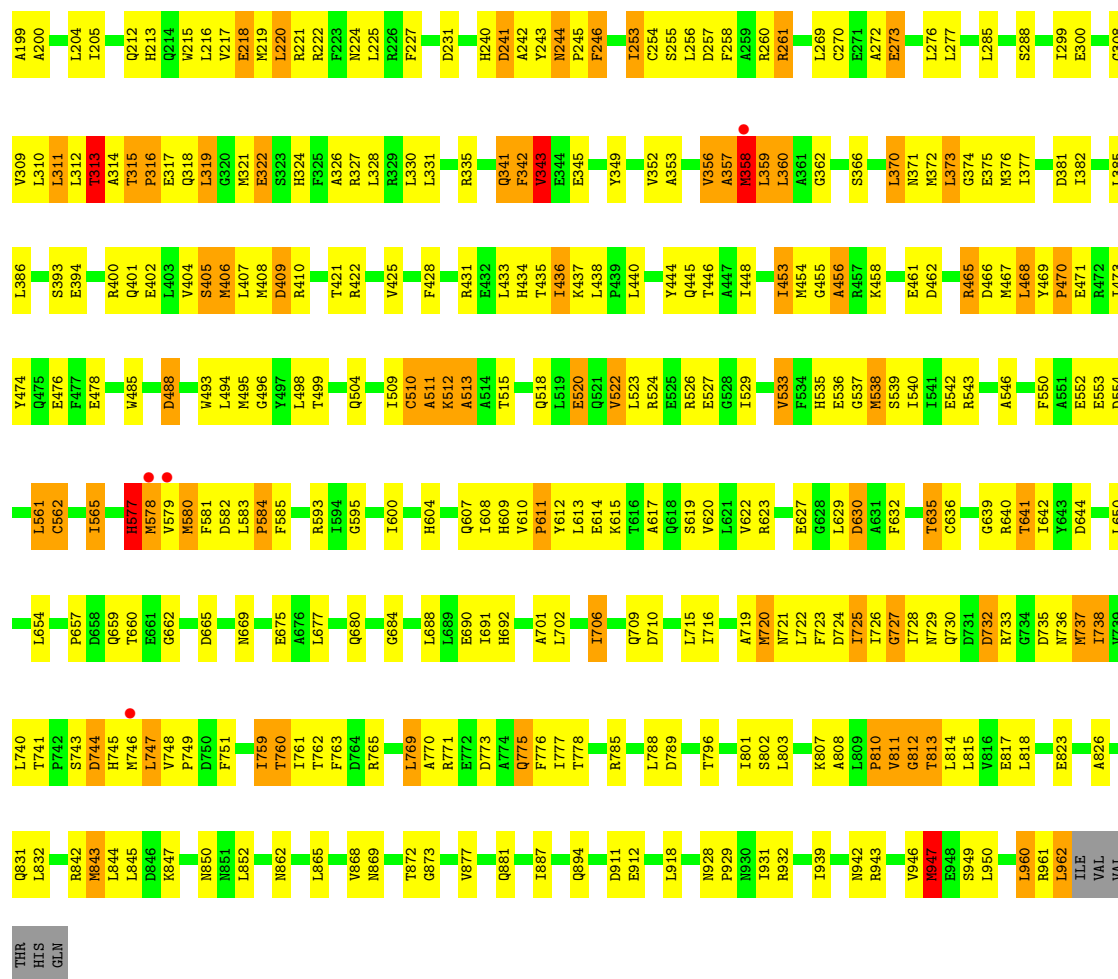
- Molecule 4: DNA-directed RNA polymerase subunit omega

Chain J: 66% 14% 17%



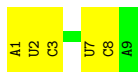
- Molecule 5: RNA polymerase-associated protein RapA





- Molecule 7: 5'-R(P*AP*UP*CP*GP*GP*CP*UP*CP*A)-3'

Chain P:  44% 56%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	336.09Å 158.93Å 255.01Å 90.00° 101.28° 90.00°	Depositor
Resolution (Å)	20.00 – 4.70 20.00 – 4.70	Depositor EDS
% Data completeness (in resolution range)	93.2 (20.00-4.70) 93.2 (20.00-4.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.21 (at 4.74Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.273 , 0.369 0.288 , 0.364	Depositor DCC
R_{free} test set	3240 reflections (4.77%)	wwPDB-VP
Wilson B-factor (Å ²)	196.2	Xtriage
Anisotropy	0.118	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.20 , 251.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	61154	wwPDB-VP
Average B, all atoms (Å ²)	292.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.40% 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: MG, 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	0.51	0/1781	0.76	1/2414 (0.0%)
1	B	0.51	0/1781	0.77	1/2414 (0.0%)
1	F	0.52	0/1781	0.76	1/2414 (0.0%)
1	G	0.52	0/1781	0.77	1/2414 (0.0%)
2	C	0.54	0/9435	0.84	8/12729 (0.1%)
2	H	0.54	0/9385	0.83	9/12662 (0.1%)
3	D	0.55	0/9128	0.82	7/12313 (0.1%)
3	I	0.55	0/9208	0.82	2/12426 (0.0%)
4	E	0.59	0/602	0.74	0/810
4	J	0.57	0/602	0.73	0/810
5	K	0.58	3/7808 (0.0%)	0.94	30/10576 (0.3%)
5	L	0.57	2/7808 (0.0%)	0.97	35/10576 (0.3%)
6	M	0.28	0/349	0.56	0/535
6	O	0.28	0/349	0.59	0/535
7	N	0.41	0/212	0.68	0/326
7	P	0.40	0/212	0.72	0/326
All	All	0.55	5/62222 (0.0%)	0.85	95/84280 (0.1%)

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
5	L	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	68	GLN	CA-C	5.98	1.59	1.52
5	K	69	MET	CA-C	5.81	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	947	MET	C-N	-5.77	1.25	1.33
5	K	70	GLN	CA-C	5.35	1.59	1.52
5	K	68	GLN	CA-C	5.20	1.59	1.52

All (95) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	461	GLU	N-CA-C	11.43	123.74	111.28
5	L	947	MET	N-CA-C	-11.41	100.15	112.93
5	L	465	ARG	N-CA-C	11.15	123.43	111.28
5	L	141	ARG	N-CA-C	-10.90	99.29	112.59
5	K	70	GLN	CA-C-N	-10.65	109.26	122.90
5	K	70	GLN	C-N-CA	-10.65	109.26	122.90
5	K	375	GLU	N-CA-C	-10.49	99.85	111.28
5	L	406	MET	N-CA-C	-10.24	100.11	111.07
5	K	373	LEU	CA-C-N	9.88	130.87	120.00
5	K	373	LEU	C-N-CA	9.88	130.87	120.00
5	K	143	PRO	N-CA-C	-9.47	100.36	113.53
5	K	141	ARG	N-CA-C	-9.34	101.10	111.28
5	L	122	ARG	N-CA-C	9.09	123.41	110.23
5	L	578	MET	N-CA-C	9.03	122.32	108.42
5	L	409	ASP	N-CA-C	-8.00	102.56	111.28
5	L	744	ASP	N-CA-C	-7.95	102.62	111.28
5	K	71	VAL	N-CA-C	7.89	119.51	107.99
5	K	373	LEU	N-CA-C	-7.82	101.15	111.24
3	D	814	CYS	N-CA-C	-7.75	96.60	109.07
3	I	814	CYS	N-CA-C	-7.55	96.92	109.07
5	K	538	MET	N-CA-C	7.51	119.47	111.28
5	K	496	GLY	N-CA-C	-7.45	103.79	112.73
5	L	538	MET	N-CA-C	7.21	120.69	110.23
5	L	468	LEU	N-CA-C	-7.17	103.47	111.28
5	K	222	ARG	N-CA-C	-7.14	104.19	113.12
5	K	68	GLN	N-CA-C	6.98	120.88	109.85
5	L	537	GLY	N-CA-C	6.94	121.66	112.77
5	L	220	LEU	N-CA-C	6.81	118.71	111.28
5	L	577	HIS	CA-C-N	-6.66	108.39	121.91
5	L	577	HIS	C-N-CA	-6.66	108.39	121.91
5	L	187	ALA	CA-C-N	-6.62	112.51	119.99
5	L	187	ALA	C-N-CA	-6.62	112.51	119.99
2	H	864	LYS	N-CA-C	-6.52	103.79	111.03
5	K	577	HIS	N-CA-C	-6.50	96.77	108.48
5	L	405	SER	CA-C-N	-6.48	112.02	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	405	SER	C-N-CA	-6.48	112.02	120.44
2	C	864	LYS	N-CA-C	-6.43	103.90	111.03
5	K	320	GLY	N-CA-C	-6.41	102.12	110.45
5	L	580	MET	N-CA-C	-6.33	101.12	110.48
5	K	466	ASP	N-CA-C	6.28	121.03	112.68
5	K	841	VAL	O-C-N	6.27	130.41	122.57
5	L	743	SER	N-CA-C	6.21	118.93	110.55
5	K	373	LEU	O-C-N	6.21	129.31	122.11
2	C	181	GLY	N-CA-C	6.19	119.48	110.63
5	L	373	LEU	N-CA-C	6.14	122.92	113.28
2	H	167	SER	N-CA-C	6.13	117.76	111.14
5	L	218	GLU	N-CA-C	6.10	117.96	107.28
5	L	747	LEU	N-CA-C	6.07	118.08	108.79
5	L	462	ASP	N-CA-C	6.06	117.88	111.28
5	L	189	MET	CA-C-N	6.01	129.34	120.74
5	L	189	MET	C-N-CA	6.01	129.34	120.74
5	K	842	ARG	N-CA-C	-6.01	102.03	110.50
5	K	190	ILE	CA-C-N	5.88	128.63	120.29
5	K	190	ILE	C-N-CA	5.88	128.63	120.29
2	H	42	ASP	CA-C-N	5.86	127.17	119.84
2	H	42	ASP	C-N-CA	5.86	127.17	119.84
5	L	370	LEU	N-CA-C	-5.79	104.97	111.28
5	K	743	SER	CA-C-N	5.78	132.10	121.70
5	K	743	SER	C-N-CA	5.78	132.10	121.70
3	D	1178	THR	CA-C-N	-5.73	114.06	119.85
3	D	1178	THR	C-N-CA	-5.73	114.06	119.85
2	H	181	GLY	N-CA-C	5.69	118.77	110.63
5	L	356	VAL	N-CA-C	-5.68	104.83	110.62
1	A	94	GLY	N-CA-C	5.67	115.37	110.21
2	C	42	ASP	CA-C-N	5.65	126.90	119.84
2	C	42	ASP	C-N-CA	5.65	126.90	119.84
2	C	1228	GLY	N-CA-C	5.55	118.07	110.69
2	H	1228	GLY	N-CA-C	5.55	118.07	110.69
2	H	896	THR	CA-C-N	5.54	126.77	119.84
2	H	896	THR	C-N-CA	5.54	126.77	119.84
2	C	896	THR	CA-C-N	5.54	126.77	119.84
2	C	896	THR	C-N-CA	5.54	126.77	119.84
1	B	94	GLY	N-CA-C	5.51	115.23	110.21
1	G	94	GLY	N-CA-C	5.50	115.21	110.21
1	F	94	GLY	N-CA-C	5.47	115.19	110.21
5	L	319	LEU	N-CA-C	5.47	117.39	109.07
3	D	1184	ASP	CA-C-N	-5.38	114.42	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1184	ASP	C-N-CA	-5.38	114.42	119.85
2	C	524	ILE	N-CA-C	5.34	116.42	111.45
5	K	67	TRP	CA-C-N	5.20	131.54	122.81
5	K	67	TRP	C-N-CA	5.20	131.54	122.81
5	L	611	PRO	CA-N-CD	-5.17	104.76	112.00
5	K	372	MET	N-CA-C	5.17	121.80	110.80
5	K	219	MET	N-CA-C	-5.16	106.96	113.20
5	L	246	PHE	N-CA-C	5.16	117.49	108.52
5	L	322	GLU	N-CA-C	5.14	118.50	108.18
5	L	143	PRO	CA-C-N	-5.08	114.91	122.74
5	L	143	PRO	C-N-CA	-5.08	114.91	122.74
5	K	225	LEU	N-CA-C	-5.08	100.13	108.41
5	K	125	ARG	N-CA-C	-5.07	105.75	111.28
3	D	823	THR	CA-C-N	5.05	126.16	119.84
3	D	823	THR	C-N-CA	5.05	126.16	119.84
3	I	1192	LYS	N-CA-C	5.05	118.53	111.30
2	H	524	ILE	N-CA-C	5.03	116.13	111.45
5	K	580	MET	N-CA-C	-5.03	99.10	107.99

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	L	148	ARG	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	1759	0	1785	10	0
1	B	1759	0	1785	11	0
1	F	1759	0	1785	11	0
1	G	1759	0	1785	11	0
2	C	9285	0	9291	166	0
2	H	9235	0	9242	176	0
3	D	8990	0	9174	160	0
3	I	9068	0	9265	159	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	600	0	607	10	0
4	J	600	0	607	6	0
5	K	7665	0	7524	748	0
5	L	7665	0	7524	824	0
6	M	311	0	168	19	0
6	O	311	0	168	5	0
7	N	191	0	98	12	0
7	P	191	0	98	7	0
8	D	2	0	0	1	0
8	I	2	0	0	0	0
9	D	1	0	0	0	0
9	I	1	0	0	0	0
All	All	61154	0	60906	2212	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 18.

All (2212) 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)
5:K:69:MET:CG	5:K:97:LEU:HD22	1.28	1.61
5:L:184:THR:HG22	5:L:312:LEU:CD2	1.17	1.61
5:L:219:MET:HG2	5:L:227:PHE:CE1	1.37	1.60
5:L:468:LEU:HA	5:L:617:ALA:CB	1.24	1.59
5:L:720:MET:CE	5:L:723:PHE:HE2	1.17	1.57
5:L:434:HIS:CD2	5:L:436:ILE:HD11	1.39	1.51
5:L:720:MET:HE3	5:L:723:PHE:CE2	1.42	1.50
3:D:77:ARG:CD	5:L:747:LEU:HB2	1.41	1.49
5:L:737:MET:HB3	5:L:738:ILE:CG2	1.06	1.49
5:K:578:MET:SD	5:K:608:ILE:HG12	1.50	1.49
5:L:737:MET:CB	5:L:738:ILE:HG22	1.44	1.48
5:L:123:MET:CG	5:L:865:LEU:HB2	1.43	1.47
5:L:494:LEU:CD1	5:L:523:LEU:HD21	1.44	1.45
5:L:494:LEU:CD2	5:L:523:LEU:HD22	1.48	1.41
5:L:219:MET:SD	5:L:227:PHE:CD1	2.14	1.40
5:L:74:VAL:CG1	5:L:81:LEU:HD11	1.51	1.39
5:K:408:MET:HE1	5:K:691:ILE:CG2	1.53	1.36
5:K:376:MET:O	5:K:377:ILE:HG12	1.24	1.36
5:L:737:MET:CB	5:L:738:ILE:CG2	1.94	1.36
5:K:407:LEU:HD11	5:K:408:MET:CE	1.53	1.35
5:K:468:LEU:HD21	5:K:469:TYR:CD2	1.60	1.35

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:K:407:LEU:CD1	5:K:408:MET:HE3	1.56	1.35
5:L:139:GLN:O	5:L:142:MET:HB2	1.17	1.34
5:L:139:GLN:O	5:L:142:MET:CB	1.75	1.34
5:L:185:ILE:HG13	5:L:222:ARG:CZ	1.55	1.34
5:L:727:GLY:HA3	5:L:746:MET:N	1.41	1.33
5:K:69:MET:HG3	5:K:97:LEU:CD2	1.58	1.33
5:K:69:MET:CG	5:K:97:LEU:CD2	2.06	1.32
5:L:244:ASN:HB3	5:L:245:PRO:CD	1.56	1.31
5:L:216:LEU:HA	5:L:219:MET:SD	1.71	1.31
5:L:61:ILE:HG23	5:L:70:GLN:NE2	1.45	1.30
3:D:77:ARG:NE	5:L:747:LEU:HB2	1.47	1.29
3:D:814:CYS:SG	3:D:898:CYS:SG	1.29	1.28
5:L:434:HIS:HD2	5:L:436:ILE:CD1	1.47	1.28
5:K:468:LEU:CD2	5:K:469:TYR:CD2	2.16	1.28
5:L:219:MET:CG	5:L:227:PHE:CE1	2.16	1.28
6:M:15:DG:N1	7:N:1:A:C2	2.02	1.28
5:K:52:ARG:HG3	5:K:54:MET:SD	1.74	1.27
5:L:468:LEU:CA	5:L:617:ALA:CB	2.12	1.27
3:I:814:CYS:SG	3:I:898:CYS:SG	1.28	1.27
3:D:77:ARG:HE	5:L:747:LEU:CB	1.46	1.27
5:L:184:THR:CG2	5:L:312:LEU:CD2	2.13	1.27
5:L:727:GLY:CA	5:L:746:MET:H	1.48	1.27
5:K:123:MET:HG3	5:K:865:LEU:CD1	1.63	1.26
5:K:843:MET:HE2	5:K:850:ASN:ND2	1.49	1.26
5:L:737:MET:CA	5:L:738:ILE:HB	1.67	1.25
5:L:372:MET:C	5:L:374:GLY:HA3	1.59	1.25
5:L:353:ALA:HA	5:L:356:VAL:CG2	1.66	1.24
6:M:15:DG:C2	7:N:1:A:H2	1.55	1.24
3:D:77:ARG:NE	5:L:747:LEU:CB	2.01	1.23
5:L:538:MET:HG2	5:L:542:GLU:CD	1.62	1.23
5:L:148:ARG:NH1	5:L:709:GLN:HB3	1.50	1.23
5:L:185:ILE:CG1	5:L:222:ARG:CZ	2.16	1.23
5:L:726:ILE:O	5:L:746:MET:CG	1.86	1.23
5:K:720:MET:HB3	5:K:730:GLN:OE1	1.39	1.22
5:L:720:MET:CE	5:L:723:PHE:CE2	2.07	1.22
5:K:61:ILE:CB	5:K:69:MET:HE2	1.70	1.22
5:L:220:LEU:O	5:L:224:ASN:HA	1.38	1.21
5:L:728:ILE:CD1	5:L:747:LEU:HD21	1.69	1.21
2:H:912:ASP:CB	2:H:913:VAL:HG13	1.70	1.21
5:L:68:GLN:O	5:L:69:MET:HG2	1.04	1.20
5:L:493:TRP:CZ2	5:L:609:HIS:NE2	2.08	1.20

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:K:408:MET:SD	5:K:691:ILE:HG22	1.80	1.20
5:L:244:ASN:CB	5:L:245:PRO:HD2	1.70	1.20
3:I:78:LEU:HB2	5:K:746:MET:N	1.54	1.19
5:L:148:ARG:HH12	5:L:709:GLN:CB	1.56	1.19
5:L:54:MET:SD	5:L:81:LEU:CD1	2.32	1.18
5:L:62:THR:HA	5:L:68:GLN:OE1	1.39	1.18
5:L:852:LEU:HD12	5:L:852:LEU:O	1.43	1.18
5:K:72:GLU:O	5:K:73:GLU:CG	1.90	1.17
5:K:72:GLU:O	5:K:73:GLU:HG2	1.02	1.17
5:L:720:MET:HB3	5:L:730:GLN:OE1	1.37	1.17
5:L:494:LEU:CD2	5:L:523:LEU:CD2	2.21	1.17
5:K:580:MET:HB2	5:K:610:VAL:CG1	1.75	1.17
2:C:912:ASP:CB	2:C:913:VAL:HG13	1.72	1.16
5:K:70:GLN:HE21	5:K:86:THR:HB	1.07	1.16
5:K:372:MET:H	5:K:375:GLU:CG	1.56	1.16
5:L:219:MET:HA	5:L:225:LEU:CD1	1.73	1.16
5:K:376:MET:O	5:K:377:ILE:CG1	1.94	1.16
5:K:843:MET:SD	5:K:850:ASN:HB3	1.85	1.16
5:L:70:GLN:HB3	5:L:71:VAL:CB	1.75	1.16
5:L:494:LEU:CD1	5:L:523:LEU:CD2	2.24	1.15
3:I:78:LEU:HD12	5:K:746:MET:SD	1.85	1.15
5:L:69:MET:HB2	5:L:86:THR:O	1.45	1.15
5:L:123:MET:HG2	5:L:865:LEU:CB	1.74	1.15
5:L:353:ALA:HA	5:L:356:VAL:HG23	1.23	1.15
5:L:843:MET:HG2	5:L:850:ASN:HD22	1.11	1.15
6:M:15:DG:N1	7:N:1:A:H2	1.35	1.15
5:K:61:ILE:HB	5:K:69:MET:HE2	1.23	1.14
5:L:220:LEU:HA	5:L:225:LEU:N	1.59	1.14
5:L:376:MET:HG3	5:L:410:ARG:HD2	1.29	1.14
2:C:912:ASP:HB2	2:C:913:VAL:CG1	1.77	1.14
5:L:68:GLN:O	5:L:69:MET:CG	1.93	1.14
6:M:15:DG:N2	7:N:1:A:C2	2.15	1.14
3:D:78:LEU:HB3	5:L:746:MET:HB2	1.29	1.14
5:L:219:MET:CA	5:L:225:LEU:HD12	1.77	1.14
5:L:434:HIS:CD2	5:L:436:ILE:CD1	2.25	1.14
5:L:70:GLN:CB	5:L:71:VAL:HB	1.76	1.13
5:L:843:MET:HG2	5:L:850:ASN:ND2	1.62	1.13
2:H:912:ASP:HB2	2:H:913:VAL:CG1	1.78	1.12
5:L:407:LEU:HG	5:L:688:LEU:HD13	1.20	1.12
5:K:123:MET:CG	5:K:865:LEU:HD13	1.79	1.12
5:K:408:MET:HA	5:K:688:LEU:CD1	1.80	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:184:THR:HG22	5:L:312:LEU:HD23	1.16	1.12
5:L:581:PHE:HD2	5:L:582:ASP:OD1	1.31	1.11
5:L:175:LEU:HD22	5:L:187:ALA:HB1	1.25	1.11
5:K:467:MET:HE2	5:K:654:LEU:HB3	1.26	1.11
3:D:814:CYS:SG	3:D:898:CYS:CB	2.39	1.11
5:K:720:MET:CE	5:K:738:ILE:HD13	1.80	1.11
5:K:408:MET:CE	5:K:691:ILE:HG22	1.81	1.10
5:L:495:MET:HE3	5:L:499:THR:CG2	1.81	1.10
5:L:184:THR:HG22	5:L:312:LEU:HD21	1.12	1.10
5:L:376:MET:CG	5:L:410:ARG:HD2	1.81	1.10
5:L:123:MET:CG	5:L:865:LEU:CB	2.30	1.10
5:K:371:ASN:ND2	5:K:375:GLU:HG3	1.67	1.10
5:K:408:MET:HE1	5:K:691:ILE:HG21	1.11	1.10
5:K:726:ILE:HG23	5:K:747:LEU:HD22	1.29	1.10
5:L:74:VAL:CG1	5:L:81:LEU:CD1	2.30	1.10
5:K:578:MET:SD	5:K:608:ILE:CG1	2.40	1.09
5:K:69:MET:HG2	5:K:97:LEU:HD22	1.14	1.09
5:L:123:MET:H	5:L:865:LEU:HD22	1.03	1.09
3:I:78:LEU:CB	5:K:746:MET:HA	1.82	1.09
5:L:468:LEU:CA	5:L:617:ALA:HB3	1.80	1.09
5:L:60:THR:HA	5:L:70:GLN:HB2	1.24	1.09
5:L:494:LEU:HD11	5:L:523:LEU:CD1	1.82	1.09
6:M:3:DG:H2''	6:M:4:DA:H5'	1.29	1.09
3:D:77:ARG:HD2	5:L:747:LEU:HB2	1.11	1.09
5:L:407:LEU:CG	5:L:688:LEU:HD13	1.82	1.09
5:L:468:LEU:HA	5:L:617:ALA:HB2	1.09	1.09
3:I:814:CYS:SG	3:I:898:CYS:CB	2.39	1.08
5:K:69:MET:HE3	5:K:83:TYR:HB3	1.32	1.08
5:K:408:MET:CE	5:K:691:ILE:CG2	2.29	1.08
3:D:77:ARG:HE	5:L:747:LEU:HB3	1.07	1.08
5:K:322:GLU:CG	5:K:324:HIS:CD2	2.35	1.08
5:K:371:ASN:HD22	5:K:375:GLU:HG3	0.92	1.08
5:L:737:MET:HA	5:L:738:ILE:CB	1.74	1.08
3:D:77:ARG:CD	5:L:747:LEU:CB	2.32	1.08
5:K:408:MET:HA	5:K:688:LEU:HD12	1.09	1.08
5:L:726:ILE:O	5:L:746:MET:HG2	1.47	1.08
5:K:408:MET:CA	5:K:688:LEU:HD12	1.84	1.08
5:L:468:LEU:HG	5:L:617:ALA:HB1	1.36	1.08
5:K:720:MET:CB	5:K:730:GLN:OE1	2.02	1.07
5:L:148:ARG:HH12	5:L:709:GLN:HB3	0.94	1.07
5:L:219:MET:HA	5:L:225:LEU:HD12	1.08	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:728:ILE:HD11	5:L:747:LEU:HD21	1.12	1.07
5:K:322:GLU:CG	5:K:324:HIS:HD2	1.66	1.07
5:K:406:MET:HG2	5:K:410:ARG:HE	1.19	1.07
3:I:78:LEU:HB3	5:K:746:MET:HA	1.14	1.07
5:K:843:MET:CE	5:K:850:ASN:CG	2.27	1.07
5:K:358:MET:HG3	5:K:365:LEU:HD22	1.29	1.07
5:L:720:MET:HE3	5:L:720:MET:HA	1.08	1.07
5:K:578:MET:HB3	5:K:607:GLN:O	1.52	1.06
5:L:358:MET:HE2	5:L:358:MET:HA	1.32	1.06
5:K:466:ASP:H	5:K:467:MET:HB3	1.13	1.06
5:K:746:MET:HB3	5:K:747:LEU:HB2	1.37	1.06
5:L:139:GLN:HG3	5:L:142:MET:HE3	1.37	1.06
5:K:372:MET:H	5:K:375:GLU:HG2	1.20	1.06
5:K:843:MET:HE2	5:K:850:ASN:CG	1.80	1.06
5:L:737:MET:HB3	5:L:738:ILE:HG21	1.30	1.06
5:K:61:ILE:HD11	5:K:83:TYR:CZ	1.91	1.06
5:K:123:MET:CG	5:K:865:LEU:CD1	2.34	1.06
5:K:322:GLU:HG2	5:K:324:HIS:HD2	1.19	1.05
3:D:77:ARG:HD2	5:L:747:LEU:CB	1.86	1.05
5:K:61:ILE:HB	5:K:69:MET:HB2	1.37	1.05
5:K:406:MET:HG3	5:K:410:ARG:CZ	1.86	1.05
5:K:580:MET:HB2	5:K:610:VAL:HG12	1.37	1.05
5:L:494:LEU:HD11	5:L:523:LEU:HD11	1.29	1.05
5:K:720:MET:HE1	5:K:738:ILE:CD1	1.85	1.05
5:K:727:GLY:CA	5:K:745:HIS:O	2.05	1.05
5:L:139:GLN:HG3	5:L:142:MET:CE	1.87	1.05
5:K:69:MET:SD	5:K:97:LEU:HB3	1.96	1.04
5:L:494:LEU:HD21	5:L:523:LEU:HD22	1.06	1.04
5:K:52:ARG:HG3	5:K:54:MET:CE	1.86	1.04
5:K:214:GLN:HG2	5:K:218:GLU:OE2	1.53	1.04
5:L:720:MET:HE1	5:L:723:PHE:HE2	1.20	1.04
5:K:467:MET:CE	5:K:654:LEU:HB3	1.87	1.04
5:L:219:MET:CE	5:L:253:ILE:HG21	1.87	1.04
5:L:581:PHE:CD2	5:L:582:ASP:OD1	2.11	1.04
5:K:322:GLU:HG3	5:K:324:HIS:CD2	1.94	1.03
5:K:407:LEU:HG	5:K:408:MET:HG2	1.40	1.03
5:K:720:MET:SD	5:K:730:GLN:NE2	2.31	1.03
5:L:728:ILE:HD11	5:L:747:LEU:CD2	1.87	1.03
5:L:435:THR:HG21	5:L:437:LYS:HZ1	1.19	1.03
5:L:577:HIS:NE2	5:L:607:GLN:OE1	1.92	1.03
5:L:74:VAL:HG13	5:L:81:LEU:CD1	1.89	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:433:LEU:HD12	5:L:632:PHE:CG	1.93	1.03
5:L:580:MET:N	5:L:609:HIS:O	1.92	1.03
5:K:52:ARG:CG	5:K:54:MET:SD	2.47	1.02
5:L:737:MET:CA	5:L:738:ILE:CB	2.33	1.02
5:K:188:GLY:C	5:K:223:PHE:CE1	2.37	1.02
5:K:188:GLY:HA3	5:K:223:PHE:CZ	1.94	1.02
5:K:743:SER:O	5:K:746:MET:O	1.77	1.02
5:L:69:MET:HG3	5:L:88:LEU:HB2	1.39	1.02
3:I:78:LEU:HB2	5:K:746:MET:H	0.89	1.02
5:K:123:MET:H	5:K:865:LEU:CD1	1.72	1.02
5:K:406:MET:HG3	5:K:410:ARG:NH2	1.74	1.02
5:K:70:GLN:NE2	5:K:86:THR:CB	2.22	1.02
5:L:353:ALA:CA	5:L:356:VAL:HG23	1.88	1.02
5:L:184:THR:CG2	5:L:312:LEU:HD23	1.85	1.02
5:L:356:VAL:HG12	5:L:358:MET:HE3	1.40	1.02
5:K:843:MET:HA	5:K:850:ASN:HD22	1.19	1.01
5:L:62:THR:CA	5:L:68:GLN:OE1	2.08	1.01
5:L:123:MET:H	5:L:865:LEU:CD2	1.72	1.01
5:L:726:ILE:O	5:L:746:MET:HG3	1.54	1.01
5:K:377:ILE:O	5:K:379:GLU:HB3	1.59	1.01
3:D:78:LEU:HD12	5:L:746:MET:HE3	1.43	1.01
5:K:123:MET:H	5:K:865:LEU:HD13	1.25	1.01
5:K:727:GLY:HA2	5:K:745:HIS:O	1.60	1.01
5:L:720:MET:CE	5:L:720:MET:HA	1.90	1.01
5:L:123:MET:HB3	5:L:865:LEU:HD13	1.39	1.01
5:L:219:MET:HE1	5:L:253:ILE:HG21	1.41	1.01
5:L:720:MET:HG3	5:L:730:GLN:NE2	1.75	1.01
2:H:912:ASP:CB	2:H:913:VAL:CG1	2.37	1.01
5:K:69:MET:HG2	5:K:97:LEU:CD2	1.81	1.01
5:K:355:ALA:HA	5:K:358:MET:HG2	1.40	1.01
5:L:468:LEU:CA	5:L:617:ALA:HB2	1.81	1.01
5:L:123:MET:N	5:L:865:LEU:HD22	1.75	1.00
5:K:468:LEU:HD23	5:K:469:TYR:CG	1.95	1.00
5:L:74:VAL:HG13	5:L:81:LEU:HD11	1.06	1.00
5:L:468:LEU:HA	5:L:617:ALA:HB3	1.02	1.00
5:K:70:GLN:NE2	5:K:86:THR:HB	1.76	1.00
5:L:219:MET:CG	5:L:227:PHE:CD1	2.40	1.00
5:L:352:VAL:O	5:L:356:VAL:HG23	1.61	0.99
5:L:727:GLY:HA2	5:L:745:HIS:O	1.62	0.99
3:I:78:LEU:CB	5:K:746:MET:H	1.74	0.99
5:L:61:ILE:CG2	5:L:70:GLN:NE2	2.23	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:396:ALA:HB2	5:K:733:ARG:HD2	1.39	0.99
5:L:494:LEU:HD22	5:L:523:LEU:CD2	1.91	0.99
3:I:396:ALA:CB	5:K:733:ARG:HH11	1.73	0.99
5:K:61:ILE:CG1	5:K:69:MET:HE2	1.90	0.99
5:K:406:MET:HG2	5:K:410:ARG:NE	1.78	0.99
5:K:69:MET:CE	5:K:83:TYR:CB	2.41	0.99
5:L:356:VAL:O	5:L:358:MET:N	1.96	0.99
5:L:747:LEU:HD22	5:L:751:PHE:HE2	1.26	0.99
5:L:220:LEU:HA	5:L:225:LEU:H	1.23	0.98
5:K:720:MET:HA	5:K:723:PHE:CE2	1.98	0.98
5:L:185:ILE:HG13	5:L:222:ARG:NE	1.77	0.98
5:L:494:LEU:HD22	5:L:523:LEU:HD22	1.45	0.98
5:K:150:GLN:HG2	5:K:189:MET:SD	2.03	0.98
5:L:498:LEU:HD21	5:L:529:ILE:HG12	1.45	0.98
6:M:15:DG:C2	7:N:1:A:C2	2.42	0.98
5:L:493:TRP:CZ2	5:L:609:HIS:CE1	2.51	0.98
5:L:716:ILE:HD12	5:L:761:ILE:HD13	1.46	0.97
3:I:78:LEU:CB	5:K:746:MET:CA	2.41	0.97
5:L:494:LEU:HD13	5:L:523:LEU:HD21	0.97	0.97
5:K:720:MET:HE1	5:K:738:ILE:HD13	0.98	0.97
5:K:498:LEU:HD21	5:K:529:ILE:HG12	1.46	0.97
5:K:580:MET:CB	5:K:610:VAL:HG12	1.94	0.97
5:L:162:ALA:HB2	5:L:189:MET:HB3	1.43	0.97
5:L:175:LEU:HD22	5:L:187:ALA:CB	1.93	0.97
5:K:69:MET:HG3	5:K:97:LEU:HD22	0.97	0.97
5:L:219:MET:HE1	5:L:253:ILE:CG2	1.93	0.96
5:K:843:MET:CE	5:K:850:ASN:ND2	2.29	0.96
5:L:720:MET:HA	5:L:723:PHE:CE2	2.00	0.96
3:I:78:LEU:CB	5:K:746:MET:N	2.27	0.96
5:L:123:MET:HG2	5:L:865:LEU:HB2	0.98	0.96
5:L:219:MET:CE	5:L:253:ILE:CG2	2.44	0.96
5:L:435:THR:HG21	5:L:437:LYS:NZ	1.80	0.96
2:C:912:ASP:CB	2:C:913:VAL:CG1	2.38	0.96
5:K:843:MET:SD	5:K:850:ASN:CB	2.54	0.96
5:L:376:MET:CB	5:L:410:ARG:HD2	1.95	0.96
5:L:184:THR:HG22	5:L:312:LEU:HD22	1.48	0.96
5:K:720:MET:HB3	5:K:730:GLN:CD	1.90	0.95
5:L:728:ILE:HG13	5:L:747:LEU:HD11	1.46	0.95
5:K:70:GLN:HB3	5:K:86:THR:CB	1.94	0.95
5:L:580:MET:HE1	5:L:593:ARG:HD3	1.47	0.95
5:L:509:ILE:O	5:L:581:PHE:HB3	1.66	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:721:ASN:O	5:L:725:ILE:HD13	1.64	0.95
5:K:408:MET:HE1	5:K:691:ILE:HG22	1.43	0.95
5:K:726:ILE:HG23	5:K:747:LEU:CD2	1.95	0.95
5:K:727:GLY:HA3	5:K:746:MET:HB2	1.47	0.95
5:L:123:MET:CB	5:L:865:LEU:HB2	1.96	0.95
5:K:69:MET:HE1	5:K:83:TYR:CG	2.00	0.95
5:K:185:ILE:HG13	5:K:222:ARG:HD3	1.47	0.95
3:I:77:ARG:HB3	5:K:746:MET:O	1.66	0.94
3:I:396:ALA:CB	5:K:733:ARG:NH1	2.28	0.94
5:L:359:LEU:HD23	5:L:359:LEU:H	1.32	0.94
3:I:396:ALA:HB1	5:K:733:ARG:NH1	1.82	0.94
5:K:70:GLN:HE21	5:K:86:THR:CB	1.77	0.94
5:K:72:GLU:C	5:K:73:GLU:HG2	1.89	0.94
5:K:143:PRO:HD2	5:K:148:ARG:NH2	1.82	0.94
5:L:54:MET:SD	5:L:81:LEU:HD13	2.07	0.94
5:L:433:LEU:HD12	5:L:632:PHE:CB	1.97	0.94
5:K:69:MET:SD	5:K:97:LEU:CB	2.55	0.94
5:L:911:ASP:OD2	5:L:947:MET:HE1	1.66	0.94
5:K:162:ALA:HA	5:K:190:ILE:CD1	1.97	0.94
5:K:371:ASN:HD22	5:K:375:GLU:CG	1.78	0.94
3:I:77:ARG:HB3	5:K:746:MET:C	1.93	0.94
5:K:123:MET:HG3	5:K:865:LEU:HD13	0.96	0.94
3:I:78:LEU:HB3	5:K:746:MET:CA	1.96	0.94
5:K:466:ASP:N	5:K:467:MET:HB3	1.82	0.94
5:K:580:MET:CB	5:K:610:VAL:CG1	2.45	0.94
5:L:842:ARG:O	5:L:843:MET:HG2	1.68	0.93
5:K:468:LEU:HD21	5:K:469:TYR:CE2	2.01	0.93
5:K:580:MET:HB2	5:K:610:VAL:HG13	1.49	0.93
5:K:818:LEU:O	5:K:843:MET:HB2	1.68	0.93
5:L:219:MET:CA	5:L:225:LEU:HB2	1.99	0.93
5:K:70:GLN:CB	5:K:86:THR:HB	1.99	0.93
2:C:912:ASP:HB2	2:C:913:VAL:HG13	0.93	0.93
5:L:61:ILE:HG23	5:L:70:GLN:HE22	1.24	0.93
5:L:433:LEU:HD23	5:L:434:HIS:N	1.82	0.93
2:H:912:ASP:HB2	2:H:913:VAL:HG13	0.93	0.93
5:L:843:MET:HE1	5:L:894:GLN:O	1.68	0.92
5:L:220:LEU:O	5:L:224:ASN:CA	2.16	0.92
5:L:465:ARG:O	5:L:469:TYR:HD2	1.50	0.92
5:L:185:ILE:HG13	5:L:222:ARG:NH1	1.84	0.92
5:L:74:VAL:HG11	5:L:81:LEU:HD11	1.52	0.92
5:K:69:MET:CE	5:K:83:TYR:HB3	1.98	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:K:188:GLY:HA3	5:K:223:PHE:CE2	2.04	0.92
5:K:578:MET:CB	5:K:607:GLN:O	2.17	0.92
5:K:70:GLN:HB3	5:K:86:THR:HB	1.52	0.92
5:K:321:MET:O	5:K:322:GLU:C	2.03	0.92
5:L:353:ALA:HA	5:L:356:VAL:HG21	1.49	0.92
5:L:188:GLY:O	5:L:190:ILE:N	2.02	0.92
6:M:2:DC:H2'	6:M:3:DG:N7	1.85	0.92
5:K:222:ARG:HH11	5:K:222:ARG:HG3	1.35	0.91
5:L:376:MET:HG3	5:L:410:ARG:CD	2.00	0.91
5:K:578:MET:N	5:K:607:GLN:O	2.03	0.91
5:L:737:MET:HB2	5:L:760:THR:HA	1.51	0.91
5:K:373:LEU:O	5:K:376:MET:O	1.88	0.91
5:L:494:LEU:HD13	5:L:523:LEU:CD2	1.94	0.91
5:K:468:LEU:CD2	5:K:469:TYR:CG	2.50	0.91
5:K:61:ILE:HD11	5:K:83:TYR:CE1	2.06	0.91
5:L:911:ASP:CG	5:L:947:MET:HE1	1.96	0.90
5:L:727:GLY:CA	5:L:746:MET:N	2.17	0.90
3:D:78:LEU:CB	5:L:746:MET:HB2	2.02	0.90
5:L:139:GLN:C	5:L:142:MET:HB2	1.96	0.90
5:L:720:MET:CB	5:L:730:GLN:OE1	2.20	0.90
5:L:158:GLN:HG2	5:L:186:GLU:CG	2.01	0.90
5:L:466:ASP:O	5:L:468:LEU:N	2.03	0.90
5:K:863:ARG:HB3	5:K:961:ARG:HH21	1.34	0.90
5:L:495:MET:HE3	5:L:499:THR:HG21	1.53	0.90
5:K:185:ILE:HG13	5:K:222:ARG:CD	2.02	0.90
5:K:72:GLU:HB2	5:K:84:ILE:O	1.70	0.89
5:L:60:THR:HA	5:L:70:GLN:CB	2.02	0.89
3:D:668:PHE:CE2	3:D:669:GLN:NE2	2.41	0.89
5:L:911:ASP:OD1	5:L:947:MET:CE	2.21	0.89
6:M:2:DC:H2'	6:M:3:DG:C8	2.08	0.89
6:M:15:DG:N2	7:N:1:A:N3	2.14	0.89
5:K:406:MET:CG	5:K:410:ARG:NH2	2.36	0.89
5:K:69:MET:HE1	5:K:83:TYR:CB	2.01	0.89
5:K:466:ASP:HB3	5:K:467:MET:HB2	1.53	0.89
5:L:538:MET:HG2	5:L:542:GLU:OE1	1.72	0.89
5:L:737:MET:HE3	5:L:761:ILE:HG22	1.54	0.89
5:L:842:ARG:O	5:L:843:MET:CG	2.21	0.88
3:I:78:LEU:HB2	5:K:746:MET:CA	2.03	0.88
5:K:318:GLN:O	5:K:319:LEU:HD23	1.72	0.88
5:K:406:MET:CG	5:K:410:ARG:CZ	2.50	0.88
5:K:406:MET:CG	5:K:410:ARG:NE	2.36	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:216:LEU:CA	5:L:219:MET:SD	2.60	0.88
5:L:219:MET:SD	5:L:227:PHE:CE1	2.66	0.88
5:K:378:GLY:HA2	5:K:379:GLU:CB	2.02	0.88
5:L:184:THR:CG2	5:L:312:LEU:HD21	1.91	0.88
5:K:123:MET:SD	5:K:124:ASP:N	2.46	0.88
5:K:467:MET:SD	5:K:654:LEU:O	2.32	0.88
5:K:408:MET:SD	5:K:691:ILE:C	2.57	0.88
5:L:219:MET:HE1	5:L:253:ILE:HD12	1.54	0.88
5:K:54:MET:HA	5:K:83:TYR:OH	1.74	0.88
5:K:372:MET:N	5:K:375:GLU:CG	2.36	0.88
5:K:374:GLY:O	5:K:378:GLY:C	2.16	0.88
5:K:720:MET:SD	5:K:730:GLN:CD	2.56	0.87
5:L:494:LEU:HD11	5:L:523:LEU:HD21	1.56	0.87
5:L:494:LEU:O	5:L:498:LEU:CB	2.22	0.87
5:L:726:ILE:O	5:L:746:MET:O	1.91	0.87
5:K:907:ARG:HH21	5:K:947:MET:HE3	1.37	0.87
5:L:942:ASN:O	5:L:946:VAL:HG23	1.72	0.87
6:M:15:DG:N2	7:N:1:A:H2	1.62	0.87
3:D:78:LEU:HB2	5:L:746:MET:HA	1.55	0.87
5:K:372:MET:HA	5:K:375:GLU:HB2	1.57	0.87
5:K:53:VAL:N	5:K:54:MET:HE2	1.89	0.87
5:K:737:MET:SD	5:K:771:ARG:NH1	2.48	0.87
5:L:54:MET:HA	5:L:83:TYR:OH	1.74	0.87
5:L:219:MET:O	5:L:225:LEU:HG	1.75	0.87
5:L:373:LEU:N	5:L:374:GLY:HA3	1.78	0.86
5:L:468:LEU:CB	5:L:617:ALA:CB	2.54	0.86
5:K:70:GLN:NE2	5:K:86:THR:CG2	2.39	0.86
5:K:19:LEU:HD13	5:K:102:LEU:HD23	1.56	0.86
5:K:818:LEU:O	5:K:843:MET:CB	2.22	0.86
5:L:219:MET:N	5:L:225:LEU:HD12	1.90	0.86
5:L:737:MET:CB	5:L:738:ILE:CB	2.53	0.86
5:K:727:GLY:HA3	5:K:745:HIS:O	1.73	0.86
5:L:139:GLN:CG	5:L:142:MET:HE3	2.06	0.86
5:K:223:PHE:O	5:K:225:LEU:HD12	1.75	0.86
5:K:535:HIS:HE1	5:K:538:MET:HG2	1.41	0.86
5:L:158:GLN:HG2	5:L:186:GLU:HG2	1.56	0.86
5:L:219:MET:HA	5:L:225:LEU:HB2	1.57	0.86
5:K:223:PHE:O	5:K:225:LEU:CD1	2.24	0.86
5:K:244:ASN:HB3	5:K:245:PRO:CD	2.05	0.86
3:I:396:ALA:HB2	5:K:733:ARG:HH11	1.41	0.85
5:K:863:ARG:HD2	5:K:961:ARG:HE	1.41	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:K:61:ILE:HG13	5:K:69:MET:HE2	1.57	0.85
5:K:122:ARG:O	5:K:125:ARG:HG2	1.76	0.85
5:K:70:GLN:NE2	5:K:86:THR:HG21	1.91	0.85
5:K:214:GLN:O	5:K:218:GLU:HG3	1.75	0.85
5:K:189:MET:N	5:K:223:PHE:CE1	2.45	0.85
5:L:535:HIS:CE1	5:L:538:MET:H	1.94	0.85
5:L:244:ASN:HB3	5:L:245:PRO:HD2	0.85	0.85
5:L:493:TRP:CH2	5:L:609:HIS:CE1	2.64	0.85
5:L:509:ILE:O	5:L:581:PHE:CB	2.25	0.85
5:L:220:LEU:C	5:L:224:ASN:HA	2.01	0.84
5:L:578:MET:HB3	5:L:607:GLN:O	1.76	0.84
5:L:720:MET:HE3	5:L:720:MET:CA	1.99	0.84
6:M:3:DG:H2''	6:M:4:DA:C5'	2.07	0.84
5:K:42:LEU:HG	5:K:242:ALA:HB1	1.59	0.84
5:L:583:LEU:HD11	5:L:622:VAL:HG22	1.60	0.84
5:K:214:GLN:CG	5:K:218:GLU:OE2	2.26	0.84
5:L:494:LEU:HD11	5:L:523:LEU:CD2	2.02	0.84
5:K:162:ALA:HA	5:K:190:ILE:HD11	1.57	0.84
5:K:369:GLU:O	5:K:373:LEU:HG	1.78	0.84
5:K:378:GLY:HA2	5:K:379:GLU:HB3	1.57	0.84
5:K:188:GLY:CA	5:K:223:PHE:CZ	2.60	0.84
5:K:322:GLU:HG2	5:K:324:HIS:CD2	2.07	0.84
5:L:42:LEU:HG	5:L:242:ALA:HB1	1.59	0.84
5:K:843:MET:CA	5:K:850:ASN:HD22	1.90	0.84
5:K:61:ILE:HG13	5:K:69:MET:CE	2.07	0.83
5:L:185:ILE:HG23	5:L:222:ARG:HD3	1.58	0.83
5:K:57:PRO:HA	5:K:71:VAL:HG11	1.61	0.83
5:K:61:ILE:CD1	5:K:83:TYR:CE1	2.60	0.83
5:K:408:MET:SD	5:K:691:ILE:CG2	2.64	0.83
3:I:501:VAL:HG12	3:I:502:PRO:HD2	1.59	0.83
5:L:139:GLN:CG	5:L:142:MET:CE	2.56	0.83
5:L:538:MET:CG	5:L:542:GLU:CD	2.50	0.83
5:L:435:THR:CG2	5:L:437:LYS:NZ	2.40	0.83
5:L:577:HIS:O	5:L:578:MET:HB2	1.77	0.83
5:K:322:GLU:O	5:K:323:SER:OG	1.95	0.83
5:K:843:MET:HA	5:K:850:ASN:ND2	1.94	0.83
5:K:69:MET:HG3	5:K:97:LEU:HD23	1.61	0.83
5:K:355:ALA:CA	5:K:358:MET:HG2	2.08	0.83
5:L:407:LEU:HG	5:L:688:LEU:CD1	2.07	0.83
5:L:737:MET:HE3	5:L:761:ILE:CG2	2.08	0.83
5:L:182:GLY:O	5:L:186:GLU:HG3	1.79	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:535:HIS:CE1	5:L:538:MET:HB2	2.13	0.83
5:K:863:ARG:HD2	5:K:961:ARG:NE	1.94	0.82
5:L:720:MET:HE1	5:L:740:LEU:HD21	1.60	0.82
5:L:494:LEU:HD21	5:L:523:LEU:CD2	1.99	0.82
5:L:538:MET:O	5:L:543:ARG:CZ	2.27	0.82
5:K:408:MET:SD	5:K:692:HIS:N	2.52	0.82
5:L:737:MET:HA	5:L:738:ILE:HB	0.87	0.82
5:K:322:GLU:HG3	5:K:324:HIS:NE2	1.93	0.82
5:K:818:LEU:HB2	5:K:843:MET:HB3	1.59	0.82
5:L:220:LEU:CA	5:L:225:LEU:H	1.92	0.82
3:D:501:VAL:HG12	3:D:502:PRO:HD2	1.60	0.82
5:K:726:ILE:CG2	5:K:747:LEU:HD22	2.10	0.82
5:K:150:GLN:NE2	5:K:189:MET:HE1	1.95	0.82
5:L:220:LEU:HD12	5:L:224:ASN:HA	1.62	0.82
5:L:408:MET:HA	5:L:688:LEU:HD12	1.59	0.82
5:L:538:MET:O	5:L:543:ARG:NH2	2.13	0.82
5:L:747:LEU:HD22	5:L:751:PHE:CE2	2.14	0.82
5:K:378:GLY:CA	5:K:379:GLU:CB	2.57	0.81
3:I:396:ALA:HB2	5:K:733:ARG:CD	2.08	0.81
5:K:69:MET:HG2	5:K:97:LEU:CG	2.10	0.81
5:L:69:MET:CG	5:L:88:LEU:HB2	2.10	0.81
5:L:468:LEU:CG	5:L:617:ALA:HB1	2.09	0.81
5:L:407:LEU:HD13	5:L:410:ARG:NH2	1.96	0.81
5:L:535:HIS:NE2	5:L:538:MET:HB2	1.95	0.81
3:D:814:CYS:CB	3:D:898:CYS:SG	2.69	0.80
5:K:70:GLN:HE22	5:K:86:THR:HG21	1.46	0.80
5:L:720:MET:HG3	5:L:730:GLN:HE22	1.42	0.80
7:P:1:A:H2'	7:P:2:U:C5	2.16	0.80
5:K:720:MET:CB	5:K:730:GLN:CD	2.53	0.80
5:L:219:MET:HA	5:L:225:LEU:CG	2.09	0.80
5:L:538:MET:HE3	5:L:542:GLU:OE1	1.82	0.80
5:L:219:MET:HA	5:L:225:LEU:CB	2.11	0.80
5:K:466:ASP:HB3	5:K:467:MET:CB	2.11	0.80
5:L:54:MET:SD	5:L:81:LEU:HD12	2.22	0.80
5:K:186:GLU:O	5:K:190:ILE:HD13	1.80	0.80
5:K:364:LYS:HG2	5:K:391:SER:HB3	1.64	0.80
5:K:506:VAL:HG13	5:K:577:HIS:HB3	1.64	0.80
5:L:219:MET:C	5:L:225:LEU:HB2	2.06	0.80
5:L:737:MET:CG	5:L:738:ILE:HG21	2.12	0.80
5:K:467:MET:HA	5:K:617:ALA:HB2	1.64	0.79
5:L:185:ILE:HD11	5:L:222:ARG:NH2	1.95	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:407:LEU:O	5:L:409:ASP:N	2.15	0.79
5:L:219:MET:SD	5:L:227:PHE:CG	2.76	0.79
5:K:377:ILE:HD12	5:K:410:ARG:HE	1.46	0.79
5:K:378:GLY:HA2	5:K:380:GLN:H	1.48	0.79
5:K:946:VAL:O	5:K:949:SER:N	2.16	0.79
5:L:59:ASP:O	5:L:70:GLN:HB2	1.83	0.79
5:K:185:ILE:H	5:K:185:ILE:HD12	1.48	0.79
5:K:407:LEU:CD1	5:K:408:MET:CE	2.36	0.79
5:L:123:MET:HB2	5:L:961:ARG:NH2	1.98	0.79
5:L:818:LEU:O	5:L:843:MET:HB2	1.83	0.78
5:L:494:LEU:O	5:L:498:LEU:HB3	1.82	0.78
5:L:843:MET:CG	5:L:850:ASN:HD22	1.93	0.78
3:D:77:ARG:CD	5:L:747:LEU:HD12	2.11	0.78
3:I:814:CYS:CB	3:I:898:CYS:SG	2.70	0.78
5:L:436:ILE:HG12	5:L:609:HIS:CE1	2.17	0.78
3:D:78:LEU:HB3	5:L:746:MET:CB	2.11	0.78
5:K:123:MET:CG	5:K:865:LEU:HD12	2.13	0.78
5:K:185:ILE:HG13	5:K:222:ARG:NE	1.99	0.78
5:L:738:ILE:HG23	5:L:759:ILE:HG22	1.65	0.78
5:L:148:ARG:NH1	5:L:709:GLN:CB	2.29	0.77
5:L:407:LEU:CD1	5:L:688:LEU:HD13	2.15	0.77
5:L:455:GLY:O	5:L:456:ALA:HB2	1.82	0.77
5:K:578:MET:HE2	5:K:580:MET:SD	2.24	0.77
5:L:434:HIS:CD2	5:L:609:HIS:ND1	2.53	0.77
5:L:468:LEU:HG	5:L:617:ALA:CB	2.12	0.77
5:L:122:ARG:HB3	5:L:124:ASP:OD1	1.84	0.77
5:L:175:LEU:CD2	5:L:187:ALA:HB1	2.09	0.77
5:L:495:MET:CE	5:L:499:THR:CG2	2.62	0.77
3:D:78:LEU:CB	5:L:746:MET:CB	2.61	0.77
5:K:185:ILE:O	5:K:223:PHE:HZ	1.67	0.77
5:K:733:ARG:O	5:K:733:ARG:HD3	1.84	0.77
5:K:244:ASN:HB3	5:K:245:PRO:HD3	1.65	0.77
5:K:53:VAL:CA	5:K:54:MET:HE2	2.15	0.77
5:K:69:MET:HG2	5:K:97:LEU:CB	2.14	0.77
5:K:726:ILE:CG2	5:K:747:LEU:CD2	2.63	0.76
5:K:747:LEU:HG	5:K:748:VAL:HG23	1.66	0.76
5:K:69:MET:HE1	5:K:83:TYR:CD1	2.19	0.76
5:L:162:ALA:CB	5:L:189:MET:HB3	2.15	0.76
3:I:519:ASN:ND2	3:I:709:ARG:HB2	2.00	0.76
5:L:60:THR:CG2	5:L:69:MET:HA	2.16	0.76
5:L:352:VAL:O	5:L:356:VAL:CG2	2.33	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:356:VAL:CG1	5:L:358:MET:HE3	2.15	0.76
5:L:494:LEU:O	5:L:498:LEU:HB2	1.84	0.76
5:L:737:MET:CE	5:L:761:ILE:CG2	2.63	0.76
5:K:369:GLU:CG	5:K:373:LEU:HD11	2.15	0.76
5:L:373:LEU:N	5:L:374:GLY:CA	2.48	0.76
3:D:77:ARG:NE	5:L:747:LEU:HB3	1.85	0.76
5:K:719:ALA:C	5:K:723:PHE:CE1	2.63	0.76
5:L:352:VAL:C	5:L:356:VAL:HG23	2.11	0.76
5:K:578:MET:CA	5:K:607:GLN:O	2.32	0.76
5:L:220:LEU:HA	5:L:224:ASN:C	2.09	0.76
3:I:393:THR:OG1	5:K:733:ARG:HG3	1.86	0.76
5:K:722:LEU:HD11	5:K:726:ILE:HD11	1.66	0.76
5:K:19:LEU:HD13	5:K:102:LEU:CD2	2.16	0.76
5:K:53:VAL:C	5:K:54:MET:HE2	2.11	0.75
5:K:151:ARG:HB3	5:K:222:ARG:HA	1.67	0.75
5:K:123:MET:CB	5:K:865:LEU:CD1	2.64	0.75
5:K:357:ALA:C	5:K:359:LEU:H	1.94	0.75
5:K:377:ILE:HD12	5:K:406:MET:HG2	1.68	0.75
5:L:219:MET:CG	5:L:227:PHE:HE1	1.77	0.75
5:L:186:GLU:O	5:L:189:MET:CG	2.34	0.75
5:L:220:LEU:HD12	5:L:224:ASN:CA	2.17	0.75
5:K:52:ARG:C	5:K:54:MET:HE2	2.12	0.75
5:L:42:LEU:CD1	5:L:242:ALA:HB2	2.16	0.75
5:L:372:MET:O	5:L:374:GLY:HA3	1.87	0.75
5:K:320:GLY:CA	5:K:321:MET:HB2	2.17	0.75
5:L:215:TRP:O	5:L:219:MET:HG3	1.87	0.75
5:K:494:LEU:O	5:K:498:LEU:HB3	1.87	0.75
5:L:498:LEU:HD21	5:L:529:ILE:CG1	2.16	0.75
5:K:407:LEU:HG	5:K:408:MET:N	2.02	0.75
5:L:185:ILE:CD1	5:L:222:ARG:CZ	2.64	0.75
5:L:374:GLY:O	5:L:376:MET:N	2.20	0.75
5:L:376:MET:HB2	5:L:410:ARG:HD2	1.67	0.75
5:K:376:MET:C	5:K:377:ILE:HG12	2.09	0.74
5:K:863:ARG:CB	5:K:961:ARG:NH2	2.49	0.74
5:L:185:ILE:CG1	5:L:222:ARG:NE	2.43	0.74
5:K:377:ILE:CG2	5:K:410:ARG:HD2	2.17	0.74
5:K:907:ARG:NH2	5:K:947:MET:HE3	2.02	0.74
5:L:60:THR:CA	5:L:70:GLN:HB2	2.12	0.74
5:L:139:GLN:O	5:L:142:MET:N	2.20	0.74
5:L:158:GLN:CG	5:L:186:GLU:HG2	2.17	0.74
5:L:358:MET:HA	5:L:358:MET:CE	2.16	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:737:MET:CA	5:L:738:ILE:CG2	2.65	0.74
5:L:139:GLN:HG2	5:L:142:MET:SD	2.26	0.74
5:K:372:MET:H	5:K:375:GLU:HG3	1.53	0.74
5:K:538:MET:O	5:K:539:SER:HB2	1.86	0.74
5:L:186:GLU:O	5:L:189:MET:HG2	1.87	0.74
5:L:407:LEU:HG	5:L:408:MET:H	1.53	0.74
5:K:498:LEU:HD21	5:K:529:ILE:CG1	2.17	0.74
5:L:468:LEU:HD22	5:L:469:TYR:CE2	2.22	0.74
5:K:377:ILE:HG13	5:K:378:GLY:H	1.51	0.74
5:L:139:GLN:O	5:L:142:MET:HB3	1.85	0.74
5:L:721:ASN:O	5:L:725:ILE:CD1	2.36	0.74
5:L:727:GLY:CA	5:L:745:HIS:C	2.61	0.74
5:K:42:LEU:CD1	5:K:242:ALA:HB2	2.17	0.73
5:K:69:MET:CG	5:K:97:LEU:CB	2.67	0.73
5:K:150:GLN:CD	5:K:189:MET:HE1	2.13	0.73
5:K:364:LYS:NZ	5:K:392:ASP:OD2	2.20	0.73
5:K:733:ARG:HD3	5:K:733:ARG:C	2.13	0.73
3:D:85:CYS:SG	3:D:86:GLU:N	2.61	0.73
5:L:54:MET:SD	5:L:74:VAL:HG11	2.29	0.73
5:L:175:LEU:CD2	5:L:187:ALA:CB	2.66	0.73
5:L:720:MET:HE3	5:L:723:PHE:CZ	2.18	0.73
5:K:371:ASN:O	5:K:372:MET:HB2	1.88	0.73
5:K:377:ILE:HG13	5:K:378:GLY:N	2.03	0.73
5:L:578:MET:O	5:L:609:HIS:HB3	1.88	0.73
5:L:60:THR:HG23	5:L:69:MET:HA	1.70	0.73
5:K:358:MET:CG	5:K:365:LEU:HD22	2.15	0.73
5:L:495:MET:SD	5:L:527:GLU:HB3	2.29	0.73
5:K:863:ARG:CB	5:K:961:ARG:HH21	2.02	0.73
5:K:69:MET:SD	5:K:97:LEU:HB2	2.29	0.72
5:L:436:ILE:N	5:L:436:ILE:HD12	2.04	0.72
5:L:468:LEU:HD23	5:L:468:LEU:O	1.89	0.72
5:L:495:MET:O	5:L:499:THR:N	2.18	0.72
5:K:123:MET:N	5:K:865:LEU:CD1	2.52	0.72
5:K:123:MET:N	5:K:865:LEU:HD13	2.02	0.72
5:K:143:PRO:HD2	5:K:148:ARG:HH22	1.52	0.72
5:L:577:HIS:CE1	5:L:607:GLN:OE1	2.42	0.72
5:L:727:GLY:HA2	5:L:745:HIS:C	2.13	0.72
3:D:70:CYS:SG	3:D:72:CYS:N	2.63	0.72
5:K:69:MET:HG2	5:K:97:LEU:HB2	1.70	0.72
5:K:468:LEU:HD23	5:K:468:LEU:C	2.14	0.72
5:L:727:GLY:HA3	5:L:746:MET:H	0.62	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:K:188:GLY:C	5:K:223:PHE:CZ	2.67	0.72
5:K:369:GLU:HG2	5:K:373:LEU:HD11	1.70	0.72
5:K:408:MET:HB3	5:K:688:LEU:HB2	1.70	0.72
5:L:215:TRP:O	5:L:219:MET:SD	2.47	0.72
5:L:220:LEU:CA	5:L:225:LEU:N	2.47	0.72
5:K:403:LEU:HA	5:K:407:LEU:HB2	1.72	0.72
5:K:407:LEU:HG	5:K:408:MET:H	1.54	0.72
5:K:61:ILE:CG1	5:K:69:MET:CE	2.64	0.72
5:L:139:GLN:O	5:L:142:MET:CA	2.37	0.72
3:D:1185:PRO:O	3:D:1186:TYR:HB2	1.89	0.72
3:I:78:LEU:HD12	5:K:746:MET:CE	2.20	0.72
5:L:123:MET:HB3	5:L:865:LEU:CD1	2.16	0.72
5:L:217:VAL:HG12	5:L:218:GLU:HG3	1.71	0.72
5:K:56:ASN:O	5:K:71:VAL:HG21	1.89	0.71
5:L:219:MET:C	5:L:225:LEU:H	1.98	0.71
5:L:435:THR:C	5:L:436:ILE:HD12	2.13	0.71
5:L:943:ARG:HG2	5:L:947:MET:SD	2.30	0.71
6:O:2:DC:H2"	6:O:3:DG:OP1	1.90	0.71
5:L:453:ILE:HD12	5:L:453:ILE:N	2.05	0.71
5:L:733:ARG:O	5:L:733:ARG:HD3	1.91	0.71
5:K:219:MET:CB	5:K:227:PHE:HE1	2.02	0.71
5:K:720:MET:HB2	5:K:730:GLN:OE1	1.90	0.71
5:L:190:ILE:N	5:L:190:ILE:HD12	2.06	0.71
5:L:370:LEU:O	5:L:370:LEU:HD23	1.91	0.71
3:D:78:LEU:HG	5:L:746:MET:HB3	1.70	0.71
5:L:538:MET:HG2	5:L:542:GLU:CB	2.21	0.71
5:K:59:ASP:O	5:K:71:VAL:HG23	1.89	0.71
5:L:61:ILE:HG23	5:L:70:GLN:CD	2.15	0.71
5:L:720:MET:HE1	5:L:723:PHE:CE2	2.01	0.71
5:L:727:GLY:CA	5:L:745:HIS:O	2.37	0.71
5:L:583:LEU:O	5:L:584:PRO:O	2.08	0.71
5:K:374:GLY:CA	5:K:378:GLY:O	2.39	0.71
5:L:408:MET:CA	5:L:688:LEU:HD12	2.21	0.71
3:I:70:CYS:SG	3:I:72:CYS:N	2.64	0.71
3:I:85:CYS:SG	3:I:86:GLU:N	2.61	0.71
5:K:52:ARG:CZ	5:K:54:MET:SD	2.79	0.71
5:K:185:ILE:HD12	5:K:185:ILE:N	2.04	0.71
5:K:61:ILE:HB	5:K:69:MET:CE	2.13	0.71
5:K:219:MET:HG3	5:K:227:PHE:HE1	1.56	0.71
5:L:408:MET:CE	5:L:691:ILE:HG22	2.21	0.71
5:L:580:MET:HE1	5:L:593:ARG:CD	2.20	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:185:ILE:HD12	5:L:185:ILE:N	2.06	0.70
5:L:408:MET:H	5:L:688:LEU:CD1	2.04	0.70
5:K:42:LEU:HG	5:K:242:ALA:CB	2.21	0.70
5:K:737:MET:CE	5:K:771:ARG:NH1	2.55	0.70
5:L:220:LEU:HA	5:L:224:ASN:HA	1.73	0.70
5:L:720:MET:CG	5:L:730:GLN:CD	2.65	0.70
5:K:54:MET:HG2	5:K:81:LEU:HD12	1.74	0.70
5:K:798:SER:O	5:K:865:LEU:HD12	1.91	0.70
5:L:215:TRP:O	5:L:219:MET:CG	2.40	0.70
5:L:359:LEU:H	5:L:359:LEU:CD2	2.03	0.70
5:L:433:LEU:HD23	5:L:433:LEU:C	2.17	0.70
5:L:725:ILE:N	5:L:725:ILE:HD12	2.06	0.70
5:K:372:MET:N	5:K:375:GLU:HG2	2.02	0.70
5:K:403:LEU:HB3	5:K:407:LEU:HD13	1.73	0.70
5:K:863:ARG:HE	5:K:961:ARG:CZ	2.05	0.70
2:C:790:ASP:O	2:C:792:GLY:N	2.25	0.70
5:L:42:LEU:HG	5:L:242:ALA:CB	2.22	0.70
3:I:70:CYS:SG	3:I:71:LEU:N	2.65	0.70
3:I:519:ASN:HD21	3:I:710:ASP:H	1.40	0.69
5:L:444:TYR:CE1	5:L:470:PRO:HB2	2.26	0.69
5:L:535:HIS:CE1	5:L:538:MET:N	2.59	0.69
5:K:162:ALA:HA	5:K:190:ILE:HD12	1.70	0.69
5:K:719:ALA:C	5:K:723:PHE:CZ	2.70	0.69
5:K:453:ILE:N	5:K:453:ILE:HD12	2.06	0.69
5:L:358:MET:HE2	5:L:358:MET:CA	2.15	0.69
3:I:43:THR:OG1	3:I:44:ILE:N	2.25	0.69
5:K:467:MET:O	5:K:467:MET:HE3	1.93	0.69
5:L:219:MET:HG2	5:L:227:PHE:HE1	0.83	0.69
5:L:220:LEU:HA	5:L:224:ASN:CA	2.22	0.69
5:L:494:LEU:CG	5:L:523:LEU:HD21	2.19	0.69
3:I:854:ALA:O	3:I:855:ASP:HB2	1.91	0.69
5:K:378:GLY:HA2	5:K:380:GLN:N	2.07	0.69
5:K:942:ASN:O	5:K:946:VAL:HG23	1.93	0.69
5:L:494:LEU:CG	5:L:523:LEU:CD2	2.70	0.69
5:L:852:LEU:O	5:L:852:LEU:CD1	2.32	0.69
5:L:219:MET:SD	5:L:227:PHE:HD1	2.07	0.69
5:L:219:MET:C	5:L:225:LEU:CB	2.66	0.69
2:H:790:ASP:O	2:H:792:GLY:N	2.25	0.69
5:K:318:GLN:O	5:K:319:LEU:CD2	2.38	0.69
5:K:722:LEU:CD1	5:K:726:ILE:HD11	2.23	0.69
5:L:61:ILE:CG2	5:L:70:GLN:HE22	1.96	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:69:MET:CB	5:L:86:THR:O	2.34	0.69
5:K:722:LEU:C	5:K:722:LEU:HD13	2.17	0.69
5:L:219:MET:HE2	5:L:227:PHE:CZ	2.26	0.69
5:L:843:MET:HA	5:L:850:ASN:HB2	1.74	0.69
5:L:911:ASP:OD1	5:L:947:MET:HE3	1.92	0.69
5:K:467:MET:SD	5:K:654:LEU:C	2.76	0.69
5:L:582:ASP:O	5:L:593:ARG:CZ	2.40	0.69
5:K:720:MET:HA	5:K:723:PHE:CZ	2.27	0.68
5:L:433:LEU:CD1	5:L:632:PHE:CG	2.76	0.68
5:L:720:MET:CG	5:L:730:GLN:NE2	2.54	0.68
5:K:320:GLY:HA2	5:K:321:MET:HB2	1.74	0.68
5:L:158:GLN:CD	5:L:186:GLU:HG2	2.19	0.68
5:L:165:VAL:HB	5:L:190:ILE:HG12	1.75	0.68
5:L:436:ILE:HD13	5:L:610:VAL:O	1.94	0.68
3:D:70:CYS:SG	3:D:71:LEU:N	2.66	0.68
3:D:1181:ASP:O	3:D:1183:SER:N	2.26	0.68
3:I:620:PHE:CZ	3:I:624:ILE:HD11	2.28	0.68
5:K:746:MET:HB3	5:K:747:LEU:CB	2.21	0.68
5:L:218:GLU:OE1	5:L:222:ARG:HG3	1.94	0.68
3:D:77:ARG:HD3	5:L:747:LEU:HD12	1.76	0.68
5:L:123:MET:HG3	5:L:865:LEU:CB	2.23	0.68
5:K:408:MET:HG3	5:K:692:HIS:HB2	1.74	0.68
5:K:818:LEU:CB	5:K:843:MET:HB3	2.24	0.68
5:L:158:GLN:HG2	5:L:186:GLU:CD	2.18	0.68
5:L:535:HIS:HE2	5:L:538:MET:HB2	1.58	0.68
5:L:728:ILE:HD12	5:L:747:LEU:HD21	1.69	0.68
3:D:77:ARG:HD2	5:L:747:LEU:CG	2.24	0.68
5:K:578:MET:HB3	5:K:607:GLN:C	2.19	0.68
5:L:141:ARG:CG	5:L:141:ARG:O	2.42	0.68
5:L:219:MET:CE	5:L:253:ILE:HG23	2.22	0.68
5:K:364:LYS:HE2	5:K:391:SER:HB2	1.75	0.68
3:I:396:ALA:HB2	5:K:733:ARG:NH1	2.04	0.68
5:L:162:ALA:HB2	5:L:189:MET:CB	2.23	0.68
5:L:494:LEU:HD11	5:L:523:LEU:CG	2.24	0.68
3:D:620:PHE:CZ	3:D:624:ILE:HD11	2.29	0.68
5:L:123:MET:HB3	5:L:865:LEU:HB2	1.74	0.68
5:L:775:GLN:O	5:L:777:ILE:N	2.27	0.68
5:K:406:MET:CG	5:K:410:ARG:HH21	2.07	0.67
5:L:455:GLY:O	5:L:456:ALA:CB	2.41	0.67
5:L:720:MET:HE2	5:L:730:GLN:HB2	1.76	0.67
5:L:737:MET:CE	5:L:761:ILE:HG22	2.22	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:662:SER:OG	2:C:663:VAL:N	2.27	0.67
2:H:813:GLU:O	3:I:461:PHE:O	2.11	0.67
5:L:448:ILE:HD13	5:L:467:MET:HA	1.76	0.67
3:I:773:PHE:O	3:I:776:THR:OG1	2.10	0.67
5:K:737:MET:HE1	5:K:771:ARG:HH11	1.59	0.67
5:L:272:ALA:O	5:L:273:GLU:HG2	1.95	0.67
5:L:578:MET:CB	5:L:607:GLN:O	2.42	0.67
5:K:322:GLU:HG2	5:K:323:SER:H	1.60	0.67
5:K:377:ILE:C	5:K:379:GLU:HB3	2.20	0.67
5:K:727:GLY:CA	5:K:746:MET:HB2	2.23	0.67
5:L:843:MET:HA	5:L:850:ASN:HD22	1.58	0.67
2:H:524:ILE:HD11	2:H:712:SER:HB3	1.77	0.67
5:K:863:ARG:CD	5:K:961:ARG:NE	2.57	0.67
5:L:469:TYR:O	5:L:473:ILE:HB	1.94	0.67
3:D:43:THR:OG1	3:D:44:ILE:N	2.24	0.67
3:I:396:ALA:HB1	5:K:733:ARG:HH11	1.42	0.67
5:K:360:LEU:HD12	5:K:360:LEU:N	2.10	0.67
2:H:662:SER:OG	2:H:663:VAL:N	2.27	0.67
5:K:147:LEU:HD22	5:K:189:MET:HE3	1.76	0.67
5:L:453:ILE:HD12	5:L:453:ILE:H	1.58	0.67
5:K:736:ASN:HD22	5:K:765:ARG:NH2	1.93	0.66
5:K:467:MET:HE2	5:K:654:LEU:CB	2.15	0.66
5:L:185:ILE:HD12	5:L:185:ILE:H	1.60	0.66
5:L:185:ILE:HG12	5:L:222:ARG:CZ	2.23	0.66
5:L:583:LEU:HD11	5:L:622:VAL:CG2	2.25	0.66
5:K:52:ARG:HG3	5:K:54:MET:HE1	1.77	0.66
5:K:464:ALA:O	5:K:467:MET:HG3	1.95	0.66
5:L:716:ILE:HG13	5:L:761:ILE:HG21	1.76	0.66
3:D:88:CYS:SG	8:D:1501:ZN:ZN	1.83	0.66
5:K:406:MET:HB3	5:K:410:ARG:HG3	1.75	0.66
5:L:376:MET:HG3	5:L:410:ARG:CG	2.26	0.66
5:L:495:MET:HE3	5:L:499:THR:HG22	1.77	0.66
5:K:433:LEU:HD23	5:K:433:LEU:C	2.20	0.66
5:K:467:MET:HE1	5:K:654:LEU:HD22	1.78	0.66
5:K:494:LEU:O	5:K:498:LEU:CB	2.43	0.66
3:D:773:PHE:O	3:D:776:THR:OG1	2.10	0.66
5:K:52:ARG:C	5:K:54:MET:CE	2.68	0.66
5:K:225:LEU:HD12	5:K:225:LEU:N	2.11	0.66
5:L:220:LEU:CA	5:L:224:ASN:HA	2.25	0.66
5:L:61:ILE:H	5:L:70:GLN:HG3	1.59	0.66
5:K:219:MET:CG	5:K:227:PHE:HE1	2.08	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:K:433:LEU:HD23	5:K:434:HIS:N	2.11	0.66
3:D:290:ILE:HB	2:H:352:ARG:O	1.96	0.65
5:K:69:MET:CE	5:K:83:TYR:CG	2.76	0.65
5:K:371:ASN:O	5:K:372:MET:CB	2.44	0.65
5:L:244:ASN:CB	5:L:245:PRO:CD	2.36	0.65
5:L:448:ILE:HG21	5:L:467:MET:HG2	1.77	0.65
2:C:524:ILE:HD11	2:C:712:SER:HB3	1.78	0.65
3:I:501:VAL:HG12	3:I:502:PRO:CD	2.26	0.65
5:L:217:VAL:O	5:L:218:GLU:CG	2.44	0.65
5:L:219:MET:H	5:L:225:LEU:HD12	1.58	0.65
5:L:373:LEU:O	5:L:373:LEU:HD13	1.96	0.65
7:P:1:A:H8	7:P:1:A:O5'	1.80	0.65
5:K:123:MET:H	5:K:865:LEU:HD11	1.57	0.65
5:K:151:ARG:NH1	5:K:221:ARG:O	2.28	0.65
5:L:54:MET:SD	5:L:81:LEU:HD11	2.31	0.65
5:L:70:GLN:HB3	5:L:71:VAL:HB	0.83	0.65
5:L:376:MET:CB	5:L:410:ARG:CD	2.72	0.65
5:K:123:MET:HB3	5:K:865:LEU:HD12	1.78	0.65
5:K:222:ARG:HG3	5:K:222:ARG:NH1	2.11	0.65
5:K:863:ARG:HB2	5:K:961:ARG:NH2	2.12	0.65
5:L:737:MET:CB	5:L:738:ILE:HB	2.22	0.65
5:K:775:GLN:O	5:K:777:ILE:N	2.28	0.65
5:L:465:ARG:O	5:L:469:TYR:CD2	2.42	0.65
5:L:493:TRP:CZ2	5:L:609:HIS:CD2	2.84	0.65
5:L:370:LEU:HD23	5:L:370:LEU:C	2.22	0.65
5:K:377:ILE:HG21	5:K:410:ARG:HD2	1.79	0.65
5:K:743:SER:HA	5:K:744:ASP:HB2	1.79	0.65
5:K:843:MET:SD	5:K:845:LEU:HD22	2.37	0.65
5:L:373:LEU:O	5:L:373:LEU:HD22	1.97	0.65
2:H:625:GLU:HG2	2:H:626:GLU:H	1.62	0.64
5:K:61:ILE:HG23	5:K:102:LEU:CD1	2.28	0.64
5:K:372:MET:N	5:K:375:GLU:HG3	2.07	0.64
5:L:494:LEU:CD1	5:L:523:LEU:HD11	2.17	0.64
5:L:842:ARG:O	5:L:850:ASN:ND2	2.30	0.64
5:K:69:MET:CE	5:K:83:TYR:HB2	2.26	0.64
5:K:722:LEU:CD1	5:K:726:ILE:CD1	2.75	0.64
5:L:538:MET:HG2	5:L:542:GLU:CG	2.26	0.64
2:C:625:GLU:HG2	2:C:626:GLU:H	1.62	0.64
5:K:52:ARG:CG	5:K:54:MET:CE	2.69	0.64
5:K:580:MET:HB3	5:K:610:VAL:HG12	1.79	0.64
5:L:582:ASP:HB2	5:L:593:ARG:HH22	1.60	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:737:MET:CG	5:L:738:ILE:CG2	2.70	0.64
5:L:818:LEU:HB2	5:L:843:MET:HB3	1.79	0.64
2:H:1065:LYS:NZ	7:N:8:C:O2'	2.30	0.64
3:I:393:THR:OG1	5:K:733:ARG:CG	2.45	0.64
5:K:863:ARG:NE	5:K:961:ARG:NE	2.46	0.64
5:L:436:ILE:CD1	5:L:609:HIS:CE1	2.81	0.64
5:K:466:ASP:CA	5:K:467:MET:HB3	2.27	0.64
5:L:719:ALA:O	5:L:723:PHE:CE1	2.50	0.64
5:K:61:ILE:HD12	5:K:83:TYR:CD1	2.33	0.63
5:L:123:MET:HG3	5:L:865:LEU:HD22	1.80	0.63
5:L:535:HIS:CE1	5:L:538:MET:CB	2.80	0.63
5:K:407:LEU:CG	5:K:408:MET:HG2	2.25	0.63
5:K:842:ARG:O	5:K:850:ASN:ND2	2.32	0.63
7:P:2:U:H6	7:P:2:U:O5'	1.81	0.63
5:K:123:MET:CB	5:K:865:LEU:HD12	2.28	0.63
5:K:53:VAL:O	5:K:54:MET:HG3	1.98	0.63
5:L:726:ILE:C	5:L:746:MET:HG2	2.22	0.63
1:B:44:ARG:CZ	3:D:538:ARG:HD2	2.29	0.63
3:D:501:VAL:HG12	3:D:502:PRO:CD	2.27	0.63
5:K:726:ILE:O	5:K:746:MET:CB	2.47	0.63
2:H:1273:MET:HA	2:H:1276:TRP:CD1	2.34	0.63
3:I:520:ALA:O	3:I:521:LYS:C	2.41	0.63
5:K:364:LYS:HG2	5:K:391:SER:CB	2.28	0.63
5:L:468:LEU:HD23	5:L:468:LEU:C	2.23	0.63
5:L:538:MET:CG	5:L:542:GLU:CB	2.77	0.63
3:I:1279:GLN:HB2	3:I:1282:TYR:HB2	1.81	0.63
5:L:357:ALA:HB1	5:L:362:GLY:N	2.13	0.63
2:C:1273:MET:HA	2:C:1276:TRP:CD1	2.34	0.62
7:P:2:U:H2'	7:P:3:C:C6	2.34	0.62
5:K:720:MET:SD	5:K:730:GLN:HG3	2.39	0.62
5:K:189:MET:N	5:K:223:PHE:CZ	2.68	0.62
5:K:219:MET:HG3	5:K:227:PHE:CE1	2.34	0.62
5:K:224:ASN:C	5:K:225:LEU:HD12	2.24	0.62
5:L:493:TRP:CE2	5:L:609:HIS:NE2	2.66	0.62
5:L:720:MET:SD	5:L:730:GLN:CD	2.82	0.62
5:L:407:LEU:HG	5:L:408:MET:N	2.13	0.62
5:K:42:LEU:HD11	5:K:242:ALA:HB2	1.82	0.62
5:L:185:ILE:CG1	5:L:222:ARG:NH2	2.62	0.62
5:L:318:GLN:O	5:L:319:LEU:HD23	1.99	0.62
2:C:689:ALA:HA	2:C:1235:LEU:HA	1.81	0.62
5:L:218:GLU:OE2	5:L:221:ARG:HB3	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:495:MET:CE	5:L:499:THR:HG22	2.29	0.62
5:K:185:ILE:H	5:K:185:ILE:CD1	2.12	0.62
5:K:357:ALA:O	5:K:359:LEU:N	2.32	0.62
5:K:61:ILE:HD12	5:K:83:TYR:CE1	2.33	0.62
5:K:222:ARG:HH11	5:K:222:ARG:CG	2.12	0.62
5:L:377:ILE:HG22	5:L:377:ILE:O	1.98	0.62
5:K:494:LEU:HD13	5:K:523:LEU:HD21	1.82	0.62
5:K:537:GLY:H	5:K:543:ARG:HH21	1.47	0.62
5:K:863:ARG:HB3	5:K:961:ARG:NH2	2.07	0.62
5:L:219:MET:HE3	5:L:253:ILE:HG21	1.80	0.62
5:L:220:LEU:N	5:L:225:LEU:H	1.98	0.62
3:D:77:ARG:CD	5:L:747:LEU:CD1	2.78	0.62
5:K:377:ILE:O	5:K:379:GLU:CB	2.43	0.62
5:L:42:LEU:HD11	5:L:242:ALA:HB2	1.82	0.62
5:K:123:MET:O	5:K:126:PHE:HB3	1.99	0.61
5:L:219:MET:HE1	5:L:253:ILE:HG23	1.80	0.61
5:K:405:SER:HB3	5:K:406:MET:SD	2.40	0.61
5:L:468:LEU:CB	5:L:617:ALA:HB1	2.30	0.61
5:L:725:ILE:HD12	5:L:725:ILE:H	1.63	0.61
2:H:689:ALA:HA	2:H:1235:LEU:HA	1.81	0.61
5:K:490:ARG:O	5:K:494:LEU:HG	2.00	0.61
2:H:841:ARG:CZ	3:I:257:GLY:HA2	2.30	0.61
5:K:403:LEU:CB	5:K:407:LEU:HD13	2.29	0.61
5:K:843:MET:HA	5:K:850:ASN:HB2	1.81	0.61
5:K:863:ARG:NE	5:K:961:ARG:CZ	2.64	0.61
5:L:270:CYS:O	5:L:272:ALA:N	2.32	0.61
5:L:433:LEU:HD12	5:L:632:PHE:HB2	1.83	0.61
5:L:468:LEU:HD22	5:L:469:TYR:CD2	2.36	0.61
5:L:578:MET:HG2	5:L:579:VAL:N	2.15	0.61
3:D:267:ASP:OD1	6:O:15:DG:O3'	2.17	0.61
3:D:1279:GLN:HB2	3:D:1282:TYR:HB2	1.82	0.61
2:H:912:ASP:CA	2:H:913:VAL:HG13	2.31	0.61
5:K:61:ILE:HB	5:K:69:MET:CB	2.23	0.61
5:K:403:LEU:CA	5:K:407:LEU:HB2	2.30	0.61
5:L:468:LEU:CG	5:L:617:ALA:CB	2.72	0.61
5:L:469:TYR:O	5:L:473:ILE:CG1	2.49	0.61
5:L:720:MET:HG3	5:L:730:GLN:CD	2.24	0.61
5:K:578:MET:SD	5:K:608:ILE:CD1	2.89	0.61
5:L:436:ILE:CG1	5:L:609:HIS:CE1	2.84	0.61
5:L:185:ILE:HD11	5:L:222:ARG:CZ	2.29	0.61
5:L:123:MET:HG3	5:L:865:LEU:HB2	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:407:LEU:HA	5:L:410:ARG:HB3	1.82	0.61
3:D:366:CYS:SG	3:D:367:GLY:N	2.74	0.61
3:I:366:CYS:SG	3:I:367:GLY:N	2.73	0.61
5:L:433:LEU:HD23	5:L:434:HIS:C	2.26	0.61
5:L:737:MET:CA	5:L:738:ILE:HG22	2.25	0.61
5:K:69:MET:CG	5:K:97:LEU:HB2	2.28	0.61
5:K:454:MET:HE1	5:K:457:ARG:HH21	1.66	0.61
5:L:59:ASP:O	5:L:70:GLN:CB	2.48	0.61
5:L:538:MET:CE	5:L:542:GLU:OE1	2.48	0.61
2:C:698:PRO:O	2:C:699:LEU:C	2.44	0.60
3:I:393:THR:OG1	5:K:733:ARG:CD	2.49	0.60
5:K:322:GLU:HG2	5:K:323:SER:N	2.16	0.60
5:L:579:VAL:HA	5:L:609:HIS:HB3	1.83	0.60
5:K:185:ILE:O	5:K:189:MET:HG2	2.01	0.60
5:L:217:VAL:O	5:L:218:GLU:HG3	2.00	0.60
5:L:436:ILE:HD11	5:L:609:HIS:CE1	2.36	0.60
5:L:738:ILE:HG23	5:L:759:ILE:CG2	2.29	0.60
2:H:887:VAL:HB	2:H:913:VAL:HG21	1.84	0.60
5:K:219:MET:HB2	5:K:227:PHE:CE1	2.36	0.60
2:C:912:ASP:CB	2:C:913:VAL:HG12	2.30	0.60
2:H:850:ILE:HA	2:H:885:GLY:O	2.01	0.60
5:K:140:PHE:O	5:K:142:MET:HG3	2.00	0.60
2:C:850:ILE:HA	2:C:885:GLY:O	2.01	0.60
2:H:698:PRO:O	2:H:699:LEU:C	2.43	0.60
5:K:226:ARG:HH22	5:K:752:PRO:HB3	1.67	0.60
5:K:495:MET:O	5:K:499:THR:HG22	2.01	0.60
5:L:469:TYR:O	5:L:473:ILE:HG13	2.01	0.60
2:C:799:ASN:HA	2:C:1230:MET:O	2.01	0.60
3:D:644:MET:O	3:D:764:ARG:NH1	2.35	0.60
5:K:59:ASP:C	5:K:71:VAL:HG23	2.26	0.60
5:K:374:GLY:HA3	5:K:378:GLY:O	2.01	0.60
5:L:726:ILE:HG22	5:L:747:LEU:HD23	1.84	0.60
5:L:737:MET:CB	5:L:738:ILE:HG21	1.95	0.60
5:K:617:ALA:O	5:K:620:VAL:HG22	2.02	0.60
5:K:843:MET:HE1	5:K:850:ASN:CG	2.21	0.60
5:L:123:MET:C	5:L:123:MET:SD	2.85	0.60
3:I:644:MET:O	3:I:764:ARG:NH1	2.35	0.60
5:L:62:THR:CB	5:L:68:GLN:OE1	2.50	0.60
3:D:584:PRO:O	3:D:586:GLY:N	2.35	0.60
5:K:52:ARG:CG	5:K:54:MET:HE1	2.31	0.60
5:K:377:ILE:C	5:K:379:GLU:CB	2.75	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:617:ALA:O	5:L:620:VAL:HG22	2.02	0.60
3:I:925:GLU:HB3	3:I:926:PRO:HD3	1.83	0.59
1:B:193:GLU:OE1	3:D:409:TRP:HB2	2.02	0.59
2:H:799:ASN:HA	2:H:1230:MET:O	2.01	0.59
5:K:70:GLN:HB2	5:K:86:THR:HB	1.82	0.59
5:K:453:ILE:HD12	5:K:453:ILE:H	1.67	0.59
2:C:1061:GLN:HB2	2:C:1062:PRO:CD	2.32	0.59
3:D:925:GLU:HB3	3:D:926:PRO:HD3	1.83	0.59
2:H:1061:GLN:HB2	2:H:1062:PRO:CD	2.32	0.59
5:K:433:LEU:HD12	5:K:632:PHE:CB	2.32	0.59
5:K:841:VAL:HG22	5:K:842:ARG:O	2.02	0.59
5:L:435:THR:CG2	5:L:437:LYS:HZ2	2.14	0.59
5:L:535:HIS:NE2	5:L:542:GLU:OE2	2.35	0.59
5:K:52:ARG:NH1	5:K:54:MET:SD	2.75	0.59
5:K:272:ALA:O	5:K:273:GLU:C	2.46	0.59
5:L:68:GLN:C	5:L:69:MET:HG2	2.13	0.59
5:L:185:ILE:HG13	5:L:222:ARG:CD	2.32	0.59
5:L:185:ILE:CD1	5:L:222:ARG:NH2	2.64	0.59
5:L:720:MET:HA	5:L:723:PHE:CZ	2.37	0.59
3:D:532:GLU:HA	3:D:535:ARG:HD3	1.85	0.59
5:K:406:MET:O	5:K:407:LEU:HB3	2.03	0.59
5:K:578:MET:HB3	5:K:608:ILE:HA	1.83	0.59
5:K:580:MET:CB	5:K:610:VAL:HG13	2.24	0.59
5:L:185:ILE:HD11	5:L:222:ARG:HH22	1.68	0.59
5:L:510:CYS:HA	5:L:581:PHE:HB3	1.84	0.59
5:L:737:MET:HB3	5:L:738:ILE:HG22	0.59	0.59
5:K:57:PRO:HA	5:K:71:VAL:CG1	2.31	0.59
5:K:719:ALA:O	5:K:723:PHE:CE1	2.55	0.59
2:C:490:GLN:O	2:C:492:MET:N	2.36	0.59
3:D:1179:PRO:HD2	3:D:1183:SER:O	2.02	0.59
3:D:1323:ALA:HB1	3:D:1328:THR:HG22	1.85	0.59
3:I:584:PRO:O	3:I:586:GLY:N	2.36	0.59
5:K:185:ILE:CG1	5:K:222:ARG:HD3	2.27	0.59
5:K:407:LEU:CG	5:K:408:MET:H	2.14	0.59
5:K:843:MET:CE	5:K:850:ASN:CB	2.80	0.59
5:K:726:ILE:O	5:K:746:MET:HB2	2.02	0.59
5:K:433:LEU:HD12	5:K:632:PHE:CG	2.38	0.58
5:L:162:ALA:HA	5:L:190:ILE:CD1	2.32	0.58
5:K:124:ASP:OD1	5:K:125:ARG:N	2.35	0.58
5:K:726:ILE:O	5:K:747:LEU:HB2	2.02	0.58
5:L:371:ASN:HD22	5:L:371:ASN:N	1.99	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1215:GLY:O	2:C:1217:THR:N	2.35	0.58
3:D:77:ARG:NE	5:L:747:LEU:CD1	2.66	0.58
3:D:1248:ILE:O	3:D:1249:ASN:C	2.46	0.58
2:H:490:GLN:O	2:H:492:MET:N	2.36	0.58
5:K:720:MET:CA	5:K:723:PHE:CZ	2.85	0.58
5:L:184:THR:OG1	5:L:185:ILE:HD12	2.03	0.58
5:L:736:ASN:HD22	5:L:736:ASN:N	1.99	0.58
2:H:1215:GLY:O	2:H:1217:THR:N	2.36	0.58
5:K:451:SER:O	5:K:455:GLY:N	2.37	0.58
2:C:553:THR:O	2:C:554:HIS:C	2.46	0.58
5:L:123:MET:SD	5:L:961:ARG:NH2	2.77	0.58
5:L:359:LEU:HD23	5:L:359:LEU:N	2.11	0.58
3:I:78:LEU:CD1	5:K:746:MET:SD	2.78	0.58
5:L:61:ILE:HG12	5:L:70:GLN:HE21	1.66	0.58
5:L:773:ASP:O	5:L:778:THR:HG21	2.04	0.58
3:I:164:GLN:O	3:I:166:LEU:N	2.37	0.58
3:I:1323:ALA:HB1	3:I:1328:THR:HG22	1.85	0.58
5:K:520:GLU:HG3	5:K:533:VAL:HG22	1.85	0.58
1:F:50:SER:O	1:F:51:MET:HB2	2.04	0.58
5:K:218:GLU:O	5:K:222:ARG:HB3	2.03	0.58
5:L:218:GLU:HG2	5:L:221:ARG:CA	2.34	0.58
5:L:277:LEU:HB3	5:L:309:VAL:HG12	1.86	0.58
5:L:727:GLY:HA3	5:L:746:MET:O	2.03	0.58
3:D:164:GLN:O	3:D:166:LEU:N	2.37	0.58
5:K:83:TYR:HB2	5:K:97:LEU:O	2.04	0.58
5:L:184:THR:CB	5:L:312:LEU:HD21	2.32	0.58
1:F:231:PHE:HB2	1:G:221:ALA:HB3	1.85	0.57
2:H:81:ASP:O	2:H:85:CYS:N	2.36	0.57
5:K:54:MET:HG2	5:K:81:LEU:CD1	2.34	0.57
5:L:185:ILE:CD1	5:L:222:ARG:NH1	2.67	0.57
5:L:444:TYR:CD1	5:L:470:PRO:HB2	2.38	0.57
3:D:208:THR:HG22	3:I:196:GLN:HB3	1.86	0.57
5:L:141:ARG:O	5:L:141:ARG:HG3	2.04	0.57
5:K:185:ILE:HA	5:K:222:ARG:HD3	1.86	0.57
5:K:377:ILE:HB	5:K:410:ARG:HD2	1.85	0.57
5:L:469:TYR:O	5:L:473:ILE:CB	2.53	0.57
3:D:338:PHE:CZ	3:D:1323:ALA:HB3	2.39	0.57
5:K:61:ILE:CD1	5:K:83:TYR:CD1	2.87	0.57
5:K:364:LYS:NZ	5:K:392:ASP:CG	2.62	0.57
5:K:403:LEU:HB2	5:K:407:LEU:HD22	1.86	0.57
5:K:720:MET:SD	5:K:730:GLN:CG	2.92	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:K:720:MET:N	5:K:723:PHE:CZ	2.73	0.57
5:L:577:HIS:O	5:L:578:MET:CB	2.40	0.57
5:K:726:ILE:CG2	5:K:747:LEU:HD23	2.34	0.57
5:L:83:TYR:HB2	5:L:97:LEU:O	2.04	0.57
5:L:139:GLN:HG3	5:L:142:MET:HE1	1.82	0.57
2:H:553:THR:O	2:H:554:HIS:C	2.47	0.57
5:K:357:ALA:C	5:K:359:LEU:N	2.54	0.57
3:D:78:LEU:CB	5:L:746:MET:HA	2.32	0.57
3:I:520:ALA:O	3:I:522:GLY:N	2.36	0.57
5:K:143:PRO:HD2	5:K:148:ARG:HH21	1.67	0.57
5:K:358:MET:HB3	5:K:365:LEU:HB2	1.87	0.57
5:L:520:GLU:HG3	5:L:533:VAL:HG22	1.85	0.57
2:H:807:TRP:O	2:H:809:GLY:N	2.38	0.57
2:H:912:ASP:CB	2:H:913:VAL:HG12	2.31	0.57
5:K:355:ALA:HA	5:K:358:MET:CG	2.26	0.57
5:K:743:SER:CA	5:K:744:ASP:HB2	2.34	0.57
5:K:773:ASP:O	5:K:778:THR:HG21	2.04	0.57
5:L:316:PRO:O	5:L:318:GLN:N	2.37	0.57
5:L:453:ILE:H	5:L:453:ILE:CD1	2.17	0.57
2:C:807:TRP:O	2:C:809:GLY:N	2.38	0.57
3:I:1248:ILE:O	3:I:1249:ASN:C	2.48	0.57
3:I:1264:ALA:HB2	3:I:1280:VAL:HG22	1.86	0.57
5:K:219:MET:HB2	5:K:227:PHE:HE1	1.69	0.57
5:L:407:LEU:HD13	5:L:410:ARG:HH21	1.65	0.57
2:C:561:ILE:O	2:C:680:LEU:HD13	2.05	0.57
2:C:912:ASP:CA	2:C:913:VAL:HG13	2.35	0.57
5:K:70:GLN:O	5:K:85:GLY:HA2	2.04	0.57
5:K:277:LEU:HB3	5:K:309:VAL:HG12	1.86	0.57
5:K:720:MET:CE	5:K:738:ILE:CD1	2.65	0.57
5:K:185:ILE:HG13	5:K:222:ARG:CZ	2.35	0.56
5:K:341:GLN:O	5:K:343:VAL:N	2.38	0.56
5:K:538:MET:O	5:K:539:SER:CB	2.53	0.56
2:H:906:PHE:HA	5:K:540:ILE:HD13	1.86	0.56
3:I:338:PHE:CZ	3:I:1323:ALA:HB3	2.40	0.56
5:K:162:ALA:CA	5:K:190:ILE:HD11	2.31	0.56
5:K:335:ARG:NH1	5:K:928:ASN:OD1	2.38	0.56
5:L:185:ILE:CD1	5:L:185:ILE:H	2.18	0.56
2:C:81:ASP:O	2:C:85:CYS:N	2.37	0.56
2:C:887:VAL:HB	2:C:913:VAL:HG21	1.86	0.56
5:K:407:LEU:CG	5:K:408:MET:N	2.68	0.56
5:L:123:MET:HG3	5:L:865:LEU:CD2	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:218:GLU:HA	5:L:219:MET:C	2.29	0.56
5:L:335:ARG:NH1	5:L:928:ASN:OD1	2.38	0.56
5:L:434:HIS:HB3	5:L:609:HIS:HA	1.85	0.56
1:A:50:SER:O	1:A:51:MET:HB2	2.04	0.56
4:E:6:VAL:HG13	4:E:6:VAL:O	2.06	0.56
2:H:912:ASP:CA	2:H:913:VAL:CG1	2.84	0.56
5:L:341:GLN:O	5:L:343:VAL:N	2.38	0.56
4:J:6:VAL:O	4:J:6:VAL:HG13	2.06	0.56
5:K:225:LEU:HB3	5:K:251:LEU:CD1	2.36	0.56
5:L:123:MET:SD	5:L:123:MET:O	2.64	0.56
5:L:174:LEU:HD12	5:L:328:LEU:HD21	1.87	0.56
3:I:854:ALA:O	3:I:855:ASP:CB	2.54	0.56
3:I:1181:ASP:O	3:I:1183:SER:N	2.38	0.56
5:K:60:THR:HB	5:K:69:MET:O	2.05	0.56
5:K:463:ARG:O	5:K:466:ASP:HB2	2.06	0.56
5:L:433:LEU:HD12	5:L:632:PHE:CD2	2.39	0.56
5:L:535:HIS:NE2	5:L:538:MET:CB	2.66	0.56
2:C:914:LYS:O	2:C:916:SER:N	2.38	0.56
3:D:1264:ALA:HB2	3:D:1280:VAL:HG22	1.87	0.56
5:K:217:VAL:O	5:K:221:ARG:N	2.39	0.56
5:K:466:ASP:CB	5:K:467:MET:CB	2.84	0.56
2:C:94:ALA:HB2	2:C:129:LEU:HD11	1.87	0.56
2:H:561:ILE:O	2:H:680:LEU:HD13	2.06	0.56
2:H:1126:ASP:HA	2:H:1129:ASN:HB3	1.87	0.56
3:I:519:ASN:ND2	3:I:710:ASP:H	2.03	0.56
3:I:532:GLU:HA	3:I:535:ARG:HD3	1.86	0.56
2:C:637:ARG:O	2:C:638:SER:HB3	2.06	0.56
2:C:907:GLY:HA3	5:L:539:SER:OG	2.07	0.56
3:D:78:LEU:HD12	5:L:746:MET:CE	2.25	0.56
2:H:637:ARG:O	2:H:638:SER:HB3	2.06	0.56
5:L:219:MET:HE2	5:L:227:PHE:CE1	2.41	0.56
5:L:540:ILE:HD12	5:L:540:ILE:H	1.70	0.56
3:D:270:ARG:O	3:D:273:ILE:N	2.39	0.55
5:K:437:LYS:HG3	5:K:612:TYR:CE1	2.42	0.55
5:K:535:HIS:CE1	5:K:538:MET:HG2	2.32	0.55
2:C:788:SER:O	2:C:795:ALA:N	2.36	0.55
2:H:94:ALA:HB2	2:H:129:LEU:HD11	1.87	0.55
5:K:174:LEU:HD12	5:K:328:LEU:HD21	1.87	0.55
5:K:405:SER:CB	5:K:406:MET:SD	2.94	0.55
5:K:539:SER:HB3	5:K:542:GLU:OE2	2.05	0.55
5:L:60:THR:HA	5:L:70:GLN:CG	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:498:LEU:HD21	5:L:529:ILE:CD1	2.36	0.55
5:L:761:ILE:O	5:L:761:ILE:HG12	2.06	0.55
1:G:44:ARG:CZ	3:I:538:ARG:HD2	2.36	0.55
5:L:61:ILE:HG12	5:L:70:GLN:NE2	2.21	0.55
5:L:911:ASP:CG	5:L:947:MET:CE	2.67	0.55
5:K:376:MET:O	5:K:377:ILE:HG13	1.98	0.55
5:L:69:MET:O	5:L:70:GLN:CG	2.54	0.55
5:L:139:GLN:CG	5:L:142:MET:SD	2.94	0.55
3:I:270:ARG:O	3:I:273:ILE:N	2.39	0.55
5:K:70:GLN:HB3	5:K:86:THR:OG1	2.07	0.55
5:K:377:ILE:CB	5:K:410:ARG:HD2	2.37	0.55
5:L:583:LEU:CD1	5:L:622:VAL:CG2	2.84	0.55
5:K:123:MET:CB	5:K:865:LEU:HD13	2.30	0.55
5:K:316:PRO:O	5:K:318:GLN:N	2.38	0.55
5:L:219:MET:C	5:L:225:LEU:CG	2.80	0.55
5:L:538:MET:CG	5:L:542:GLU:OE1	2.51	0.55
2:C:488:MET:HB2	2:C:489:PRO:HD3	1.89	0.55
2:C:698:PRO:HA	2:C:1231:TYR:CE1	2.41	0.55
3:D:212:THR:OG1	3:I:150:GLY:O	2.21	0.55
5:K:464:ALA:O	5:K:467:MET:CG	2.55	0.55
5:K:498:LEU:HD21	5:K:529:ILE:CD1	2.37	0.55
5:K:843:MET:SD	5:K:850:ASN:CG	2.88	0.55
5:K:408:MET:CG	5:K:692:HIS:HB2	2.37	0.55
5:L:721:ASN:C	5:L:725:ILE:HD13	2.31	0.55
2:C:1126:ASP:HA	2:C:1129:ASN:HB3	1.87	0.55
3:D:268:LEU:HD13	3:D:306:LEU:HA	1.89	0.55
3:I:268:LEU:HD13	3:I:306:LEU:HA	1.89	0.55
5:K:812:GLY:O	5:K:813:THR:C	2.49	0.55
5:L:376:MET:HG3	5:L:410:ARG:HH11	1.70	0.55
5:L:470:PRO:HD2	5:L:471:GLU:H	1.72	0.55
2:C:625:GLU:HG2	2:C:626:GLU:N	2.22	0.55
2:H:625:GLU:HG2	2:H:626:GLU:N	2.22	0.55
3:I:520:ALA:HB2	3:I:545:HIS:HB2	1.89	0.55
5:K:454:MET:HE1	5:K:457:ARG:NH2	2.21	0.55
5:K:946:VAL:C	5:K:949:SER:H	2.14	0.55
5:L:434:HIS:HD2	5:L:436:ILE:HD11	0.55	0.55
5:L:435:THR:HG22	5:L:437:LYS:NZ	2.22	0.55
2:H:488:MET:HB2	2:H:489:PRO:HD3	1.89	0.54
5:K:189:MET:N	5:K:223:PHE:HE1	2.01	0.54
5:K:737:MET:CE	5:K:771:ARG:HH11	2.19	0.54
5:K:843:MET:SD	5:K:850:ASN:ND2	2.80	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:153:VAL:O	1:B:158:ARG:NH1	2.40	0.54
1:G:153:VAL:O	1:G:158:ARG:NH1	2.40	0.54
5:K:226:ARG:NH2	5:K:752:PRO:HB3	2.21	0.54
5:K:431:ARG:NH2	5:K:635:THR:HG23	2.22	0.54
5:L:434:HIS:CD2	5:L:609:HIS:CE1	2.95	0.54
6:M:2:DC:C2'	6:M:3:DG:C8	2.86	0.54
5:K:466:ASP:CA	5:K:467:MET:CB	2.85	0.54
5:L:431:ARG:NH2	5:L:635:THR:HG23	2.23	0.54
5:L:493:TRP:HZ2	5:L:609:HIS:NE2	1.91	0.54
2:H:788:SER:O	2:H:795:ALA:N	2.36	0.54
5:K:341:GLN:O	5:K:342:PHE:C	2.51	0.54
5:L:198:GLY:O	5:L:200:ALA:N	2.37	0.54
5:L:216:LEU:O	5:L:219:MET:HB2	2.08	0.54
5:K:125:ARG:HG3	5:K:794:GLY:HA2	1.89	0.54
5:K:467:MET:HE2	5:K:654:LEU:HD13	1.90	0.54
5:L:357:ALA:O	5:L:358:MET:HB2	2.07	0.54
5:L:493:TRP:HZ2	5:L:609:HIS:CD2	2.26	0.54
5:K:374:GLY:C	5:K:378:GLY:O	2.50	0.54
5:L:437:LYS:HG3	5:L:612:TYR:CE1	2.41	0.54
5:L:538:MET:HB3	5:L:542:GLU:OE2	2.08	0.54
5:L:812:GLY:O	5:L:813:THR:C	2.50	0.54
2:H:914:LYS:O	2:H:916:SER:N	2.41	0.54
5:K:189:MET:CA	5:K:223:PHE:HE1	2.21	0.54
5:L:276:LEU:HA	5:L:308:GLY:O	2.08	0.54
5:L:405:SER:O	5:L:406:MET:C	2.48	0.54
5:L:736:ASN:O	5:L:760:THR:CB	2.56	0.54
3:D:1178:THR:HG22	3:D:1184:ASP:O	2.08	0.54
5:K:369:GLU:HG3	5:K:373:LEU:HD11	1.90	0.54
5:K:722:LEU:HD13	5:K:726:ILE:CD1	2.37	0.54
3:D:270:ARG:O	3:D:271:ARG:C	2.51	0.53
3:I:270:ARG:O	3:I:271:ARG:C	2.51	0.53
5:K:52:ARG:NH1	5:K:54:MET:CG	2.71	0.53
5:K:198:GLY:O	5:K:200:ALA:N	2.37	0.53
5:L:123:MET:HB2	5:L:961:ARG:CZ	2.38	0.53
5:L:139:GLN:CA	5:L:142:MET:HB2	2.38	0.53
5:K:188:GLY:O	5:K:192:HIS:N	2.32	0.53
5:K:453:ILE:O	5:K:453:ILE:HG22	2.08	0.53
5:K:467:MET:SD	5:K:654:LEU:HB3	2.48	0.53
5:K:533:VAL:HG12	5:K:535:HIS:HD2	1.72	0.53
5:L:242:ALA:O	5:L:243:TYR:HB2	2.08	0.53
5:L:725:ILE:CD1	5:L:725:ILE:H	2.20	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1132:LEU:O	2:C:1135:GLN:N	2.40	0.53
2:H:1185:PRO:O	2:H:1186:VAL:C	2.51	0.53
3:I:51:PRO:HB2	3:I:57:PHE:C	2.33	0.53
5:K:720:MET:HG2	5:K:723:PHE:HZ	1.74	0.53
5:L:69:MET:O	5:L:70:GLN:HG3	2.07	0.53
5:L:747:LEU:CD2	5:L:751:PHE:HE2	2.10	0.53
3:D:363:LEU:HA	3:D:450:HIS:NE2	2.24	0.53
5:L:194:GLN:HG3	5:L:200:ALA:HB3	1.89	0.53
5:L:358:MET:HB2	5:L:360:LEU:CD2	2.38	0.53
2:C:811:ASN:HB3	2:C:815:SER:O	2.08	0.53
2:C:912:ASP:CA	2:C:913:VAL:CG1	2.87	0.53
5:L:217:VAL:C	5:L:218:GLU:HG3	2.33	0.53
3:I:77:ARG:HB3	5:K:747:LEU:N	2.23	0.53
5:K:372:MET:H	5:K:375:GLU:CB	2.19	0.53
2:C:676:ALA:O	2:C:677:ASN:C	2.51	0.53
2:H:698:PRO:HA	2:H:1231:TYR:CE1	2.44	0.53
5:K:128:LEU:HD21	5:K:721:ASN:ND2	2.23	0.53
5:K:946:VAL:C	5:K:948:GLU:N	2.65	0.53
5:L:218:GLU:HG2	5:L:221:ARG:N	2.24	0.53
5:L:509:ILE:O	5:L:581:PHE:HB2	2.06	0.53
2:C:1061:GLN:HB2	2:C:1062:PRO:HD2	1.91	0.53
2:H:559:CYS:HB2	2:H:662:SER:HB2	1.91	0.53
5:L:219:MET:C	5:L:225:LEU:HG	2.34	0.53
5:L:408:MET:HE3	5:L:691:ILE:HG22	1.91	0.53
5:L:436:ILE:HG22	5:L:438:LEU:HD22	1.90	0.53
5:L:341:GLN:O	5:L:342:PHE:C	2.51	0.53
2:C:1072:ASN:OD1	2:C:1072:ASN:N	2.41	0.53
2:H:676:ALA:O	2:H:677:ASN:C	2.50	0.53
3:I:393:THR:OG1	5:K:733:ARG:HD2	2.09	0.53
5:L:123:MET:CB	5:L:865:LEU:HD13	2.25	0.53
5:L:352:VAL:O	5:L:356:VAL:N	2.42	0.53
5:L:407:LEU:CG	5:L:408:MET:H	2.20	0.53
2:C:114:VAL:O	2:C:115:LYS:C	2.52	0.52
3:D:334:LYS:HA	3:D:339:ARG:NE	2.24	0.52
5:K:61:ILE:HD11	5:K:83:TYR:CE2	2.40	0.52
5:K:488:ASP:C	5:K:488:ASP:OD1	2.52	0.52
5:L:74:VAL:HG13	5:L:81:LEU:CG	2.39	0.52
5:L:376:MET:HB2	5:L:410:ARG:CD	2.37	0.52
5:L:538:MET:CG	5:L:542:GLU:HB2	2.38	0.52
6:M:2:DC:H6	6:M:2:DC:O5'	1.92	0.52
1:B:159:ILE:HG22	1:B:159:ILE:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:51:PRO:HB2	3:D:57:PHE:C	2.34	0.52
3:I:363:LEU:HA	3:I:450:HIS:NE2	2.24	0.52
5:K:219:MET:CB	5:K:227:PHE:CE1	2.88	0.52
5:K:356:VAL:O	5:K:357:ALA:C	2.52	0.52
5:K:378:GLY:CA	5:K:379:GLU:HB2	2.36	0.52
5:L:736:ASN:O	5:L:760:THR:HB	2.09	0.52
3:D:290:ILE:HD13	2:H:353:VAL:HA	1.90	0.52
2:H:811:ASN:HB3	2:H:815:SER:O	2.09	0.52
5:K:189:MET:HA	5:K:223:PHE:HE1	1.75	0.52
5:K:454:MET:CE	5:K:457:ARG:NH2	2.72	0.52
2:C:61:SER:HB3	2:C:479:LEU:HD13	1.91	0.52
2:H:1215:GLY:O	2:H:1216:ARG:C	2.52	0.52
3:I:334:LYS:HA	3:I:339:ARG:NE	2.24	0.52
5:K:726:ILE:O	5:K:746:MET:HB3	2.09	0.52
5:L:61:ILE:N	5:L:70:GLN:HG3	2.23	0.52
5:L:353:ALA:N	5:L:356:VAL:HG23	2.23	0.52
5:L:408:MET:N	5:L:688:LEU:HD12	2.24	0.52
5:L:620:VAL:HG21	5:L:654:LEU:HD23	1.91	0.52
5:L:716:ILE:CD1	5:L:761:ILE:HG21	2.39	0.52
2:H:1061:GLN:HB2	2:H:1062:PRO:HD2	1.91	0.52
2:C:516:ASP:HA	2:C:761:GLN:HE22	1.74	0.52
1:G:159:ILE:O	1:G:159:ILE:HG22	2.10	0.52
2:H:114:VAL:O	2:H:115:LYS:C	2.53	0.52
3:I:140:TYR:O	3:I:141:PHE:HB2	2.09	0.52
4:J:20:VAL:O	4:J:24:ALA:N	2.35	0.52
5:L:189:MET:CB	5:L:190:ILE:HD12	2.39	0.52
3:D:814:CYS:CB	3:D:895:CYS:SG	2.98	0.52
2:H:61:SER:HB3	2:H:479:LEU:HD13	1.91	0.52
3:D:112:ALA:HA	3:D:238:ILE:HG23	1.92	0.52
3:I:112:ALA:HA	3:I:238:ILE:HG23	1.92	0.52
5:K:61:ILE:CB	5:K:69:MET:CE	2.66	0.52
5:K:242:ALA:O	5:K:243:TYR:HB2	2.08	0.52
5:K:748:VAL:HG13	5:K:749:PRO:HD2	1.92	0.52
5:L:408:MET:H	5:L:688:LEU:HD13	1.75	0.52
5:L:843:MET:CG	5:L:850:ASN:ND2	2.54	0.52
5:K:225:LEU:CD1	5:K:225:LEU:N	2.73	0.52
5:K:244:ASN:CB	5:K:245:PRO:CD	2.86	0.52
5:K:276:LEU:HA	5:K:308:GLY:O	2.08	0.52
5:K:539:SER:O	5:K:543:ARG:HG3	2.10	0.52
5:K:620:VAL:HG21	5:K:654:LEU:HD23	1.91	0.52
5:L:511:ALA:HB2	5:L:582:ASP:OD2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:716:ILE:CG1	5:L:761:ILE:HG21	2.40	0.52
5:L:738:ILE:CG2	5:L:759:ILE:CG2	2.88	0.52
2:C:674:ASP:N	2:C:674:ASP:OD1	2.43	0.52
5:L:538:MET:CB	5:L:542:GLU:OE2	2.58	0.52
5:L:433:LEU:CD1	5:L:632:PHE:CD2	2.93	0.51
2:C:144:VAL:HG11	2:C:527:LYS:HG2	1.91	0.51
2:H:822:VAL:O	2:H:825:GLU:O	2.28	0.51
5:K:195:LEU:HD11	5:K:225:LEU:CD2	2.39	0.51
5:K:360:LEU:N	5:K:360:LEU:CD1	2.73	0.51
5:K:745:HIS:O	5:K:746:MET:HB2	2.10	0.51
2:C:822:VAL:O	2:C:825:GLU:O	2.28	0.51
3:D:140:TYR:O	3:D:141:PHE:HB2	2.10	0.51
5:K:54:MET:CE	5:K:54:MET:N	2.73	0.51
5:K:75:LYS:HB2	5:K:82:THR:HB	1.92	0.51
5:K:128:LEU:HD21	5:K:721:ASN:CG	2.35	0.51
5:K:364:LYS:HZ1	5:K:392:ASP:CG	2.17	0.51
5:K:495:MET:O	5:K:499:THR:N	2.36	0.51
5:L:205:ILE:HB	5:L:253:ILE:HG22	1.91	0.51
5:L:488:ASP:C	5:L:488:ASP:OD1	2.52	0.51
2:C:559:CYS:HB2	2:C:662:SER:HB2	1.92	0.51
2:C:907:GLY:CA	5:L:539:SER:OG	2.59	0.51
5:L:406:MET:O	5:L:410:ARG:HB2	2.11	0.51
5:L:408:MET:H	5:L:688:LEU:HD12	1.76	0.51
5:L:436:ILE:CD1	5:L:436:ILE:N	2.73	0.51
2:C:436:ARG:HG2	2:C:436:ARG:HH11	1.74	0.51
2:C:1215:GLY:O	2:C:1216:ARG:C	2.52	0.51
1:F:159:ILE:O	1:F:159:ILE:HG22	2.11	0.51
2:H:820:GLU:HB2	2:H:1081:PRO:HA	1.93	0.51
5:K:123:MET:SD	5:K:123:MET:C	2.94	0.51
5:K:408:MET:C	5:K:688:LEU:HD12	2.34	0.51
5:K:620:VAL:HG21	5:K:654:LEU:CD2	2.41	0.51
5:L:216:LEU:O	5:L:219:MET:CB	2.59	0.51
5:L:582:ASP:O	5:L:593:ARG:NH2	2.43	0.51
5:L:843:MET:CA	5:L:850:ASN:HD22	2.21	0.51
2:H:144:VAL:HG11	2:H:527:LYS:HG2	1.91	0.51
2:H:436:ARG:HG2	2:H:436:ARG:HH11	1.74	0.51
5:K:123:MET:HB3	5:K:865:LEU:CD1	2.36	0.51
5:K:396:ALA:O	5:K:398:SER:N	2.43	0.51
5:K:408:MET:O	5:K:411:HIS:HB2	2.11	0.51
5:K:493:TRP:C	5:K:495:MET:H	2.18	0.51
5:L:68:GLN:O	5:L:69:MET:CB	2.58	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:620:VAL:HG21	5:L:654:LEU:CD2	2.41	0.51
5:L:737:MET:CB	5:L:760:THR:HA	2.34	0.51
3:D:369:PRO:O	3:D:372:MET:N	2.44	0.51
5:K:52:ARG:NH1	5:K:54:MET:HG3	2.26	0.51
5:K:52:ARG:HG2	5:K:54:MET:SD	2.46	0.51
5:K:342:PHE:O	5:K:343:VAL:C	2.53	0.51
5:K:372:MET:O	5:K:376:MET:HG2	2.10	0.51
5:K:453:ILE:N	5:K:453:ILE:CD1	2.73	0.51
5:L:407:LEU:CD1	5:L:688:LEU:CD1	2.88	0.51
5:L:510:CYS:HA	5:L:581:PHE:CD2	2.46	0.51
5:K:205:ILE:HB	5:K:253:ILE:HG22	1.91	0.51
5:L:219:MET:CB	5:L:225:LEU:HB2	2.41	0.51
5:L:716:ILE:CD1	5:L:761:ILE:HD13	2.28	0.51
5:L:746:MET:O	5:L:747:LEU:HD23	2.11	0.51
2:C:149:LEU:HD23	2:C:150:HIS:N	2.26	0.51
3:D:436:ALA:HB3	3:D:485:MET:HA	1.93	0.51
5:K:453:ILE:H	5:K:453:ILE:CD1	2.23	0.51
5:K:470:PRO:HA	5:K:473:ILE:HB	1.92	0.51
5:K:844:LEU:H	5:K:850:ASN:HB2	1.74	0.51
5:L:75:LYS:HB2	5:L:82:THR:HB	1.92	0.51
5:L:122:ARG:CB	5:L:124:ASP:OD1	2.55	0.51
1:A:159:ILE:O	1:A:159:ILE:HG22	2.10	0.51
2:C:1185:PRO:O	2:C:1186:VAL:C	2.53	0.51
2:H:516:ASP:HA	2:H:761:GLN:HE22	1.75	0.51
2:H:577:VAL:HG23	2:H:661:VAL:O	2.11	0.51
5:K:194:GLN:HG3	5:K:200:ALA:HB3	1.92	0.51
5:K:372:MET:CA	5:K:375:GLU:HB2	2.36	0.51
5:K:405:SER:C	5:K:406:MET:SD	2.94	0.51
5:L:218:GLU:HG2	5:L:221:ARG:H	1.76	0.51
5:L:577:HIS:CD2	5:L:607:GLN:OE1	2.63	0.51
5:L:719:ALA:O	5:L:723:PHE:CZ	2.64	0.51
5:K:69:MET:HE1	5:K:83:TYR:HB2	1.83	0.50
5:K:194:GLN:CG	5:K:200:ALA:HB3	2.40	0.50
5:L:342:PHE:O	5:L:343:VAL:C	2.53	0.50
5:L:356:VAL:C	5:L:358:MET:H	2.08	0.50
5:L:372:MET:HA	5:L:375:GLU:HG2	1.91	0.50
5:L:433:LEU:HD23	5:L:434:HIS:CA	2.41	0.50
6:O:15:DG:O6	7:P:1:A:H2	1.93	0.50
2:C:135:THR:HG22	2:C:144:VAL:HG22	1.93	0.50
2:C:820:GLU:HB2	2:C:1081:PRO:HA	1.92	0.50
2:H:149:LEU:HD23	2:H:150:HIS:N	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:K:722:LEU:HD11	5:K:726:ILE:CD1	2.39	0.50
5:L:219:MET:O	5:L:225:LEU:CG	2.56	0.50
2:C:842:ASP:HB2	2:C:1047:LEU:HG	1.93	0.50
3:I:814:CYS:CB	3:I:895:CYS:SG	2.99	0.50
5:K:722:LEU:HD13	5:K:722:LEU:O	2.10	0.50
5:L:322:GLU:HA	5:L:324:HIS:CD2	2.46	0.50
2:H:135:THR:HG22	2:H:144:VAL:HG22	1.94	0.50
2:H:842:ASP:HB2	2:H:1047:LEU:HG	1.94	0.50
2:C:577:VAL:HG23	2:C:661:VAL:O	2.11	0.50
3:D:86:GLU:N	3:D:86:GLU:CD	2.70	0.50
1:G:193:GLU:OE1	3:I:409:TRP:HB2	2.11	0.50
3:I:791:ALA:HB2	6:M:5:DC:C5	2.47	0.50
5:L:435:THR:HG22	5:L:437:LYS:HZ2	1.76	0.50
5:L:538:MET:HG2	5:L:542:GLU:HB2	1.91	0.50
5:K:743:SER:HB2	5:K:744:ASP:HB2	1.93	0.50
5:L:218:GLU:HG2	5:L:221:ARG:CB	2.42	0.50
5:L:561:LEU:HD13	5:L:562:CYS:N	2.27	0.50
5:L:578:MET:O	5:L:609:HIS:CB	2.57	0.50
5:L:725:ILE:CD1	5:L:725:ILE:N	2.73	0.50
2:C:496:LYS:HB3	2:C:497:PRO:HD3	1.94	0.50
2:H:674:ASP:N	2:H:674:ASP:OD1	2.44	0.50
2:H:1073:LYS:NZ	7:N:9:A:OP1	2.32	0.50
5:K:123:MET:HB3	5:K:798:SER:O	2.12	0.50
5:K:546:ALA:O	5:K:550:PHE:N	2.39	0.50
5:L:187:ALA:O	5:L:188:GLY:C	2.52	0.50
5:L:818:LEU:O	5:L:843:MET:CB	2.57	0.50
2:C:359:ARG:NE	2:C:363:LEU:HD11	2.27	0.50
3:D:78:LEU:CG	5:L:746:MET:CB	2.89	0.50
2:C:798:GLN:O	2:C:1231:TYR:HA	2.12	0.50
3:D:814:CYS:HB3	3:D:895:CYS:SG	2.51	0.50
2:H:704:MET:O	2:H:708:VAL:HG23	2.12	0.50
5:K:151:ARG:HB2	5:K:221:ARG:O	2.12	0.50
5:K:374:GLY:O	5:K:378:GLY:N	2.44	0.50
5:L:128:LEU:CD2	5:L:721:ASN:O	2.60	0.50
2:C:194:LEU:O	2:C:206:ALA:HB2	2.11	0.49
2:C:704:MET:O	2:C:708:VAL:HG23	2.12	0.49
3:I:436:ALA:HB3	3:I:485:MET:HA	1.94	0.49
5:K:318:GLN:O	5:K:319:LEU:CG	2.59	0.49
5:K:466:ASP:CB	5:K:467:MET:HB3	2.42	0.49
5:L:219:MET:CE	5:L:253:ILE:HD12	2.36	0.49
5:K:123:MET:HG3	5:K:865:LEU:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:K:468:LEU:CD2	5:K:468:LEU:C	2.85	0.49
5:K:491:VAL:HA	5:K:494:LEU:HD12	1.93	0.49
5:K:719:ALA:HB1	5:K:723:PHE:HE1	1.77	0.49
5:L:433:LEU:C	5:L:433:LEU:CD2	2.86	0.49
3:D:80:HIS:CE1	5:L:54:MET:CE	2.95	0.49
1:G:131:CYS:SG	1:G:132:HIS:N	2.85	0.49
2:H:359:ARG:NE	2:H:363:LEU:HD11	2.27	0.49
3:I:814:CYS:HB3	3:I:895:CYS:SG	2.52	0.49
5:L:122:ARG:C	5:L:124:ASP:H	2.19	0.49
5:L:219:MET:CE	5:L:227:PHE:CE1	2.95	0.49
5:L:468:LEU:C	5:L:468:LEU:CD2	2.86	0.49
1:F:131:CYS:SG	1:F:132:HIS:N	2.84	0.49
2:H:194:LEU:O	2:H:206:ALA:HB2	2.11	0.49
2:H:798:GLN:O	2:H:1231:TYR:HA	2.12	0.49
5:K:19:LEU:CD1	5:K:102:LEU:CD2	2.88	0.49
5:K:321:MET:O	5:K:323:SER:N	2.45	0.49
5:K:410:ARG:HG2	5:K:927:VAL:HG13	1.95	0.49
5:K:433:LEU:C	5:K:433:LEU:CD2	2.86	0.49
5:L:374:GLY:C	5:L:376:MET:N	2.71	0.49
5:L:448:ILE:HG23	5:L:467:MET:HG3	1.93	0.49
5:K:61:ILE:CG2	5:K:69:MET:HE2	2.40	0.49
1:A:131:CYS:SG	1:A:132:HIS:N	2.85	0.49
2:C:475:VAL:HG12	2:C:479:LEU:HD12	1.95	0.49
2:H:672:GLU:O	3:I:767:LEU:HD13	2.11	0.49
3:I:392:THR:HB	5:K:733:ARG:NH2	2.28	0.49
5:K:190:ILE:HD12	5:K:190:ILE:N	2.28	0.49
5:K:433:LEU:HD12	5:K:632:PHE:HB2	1.95	0.49
5:K:843:MET:HA	5:K:850:ASN:CB	2.40	0.49
3:D:78:LEU:HB2	5:L:746:MET:CA	2.34	0.49
5:L:219:MET:HE2	5:L:227:PHE:CE2	2.48	0.49
2:C:1065:LYS:NZ	7:P:8:C:O2'	2.46	0.49
2:H:1072:ASN:OD1	2:H:1072:ASN:N	2.41	0.49
3:I:369:PRO:O	3:I:372:MET:N	2.45	0.49
3:I:506:VAL:HG13	3:I:628:GLY:HA3	1.95	0.49
5:K:356:VAL:O	5:K:359:LEU:N	2.43	0.49
5:K:561:LEU:HD13	5:K:562:CYS:N	2.27	0.49
5:L:349:TYR:OH	5:L:376:MET:HE3	2.12	0.49
5:L:433:LEU:HA	5:L:608:ILE:HB	1.94	0.49
5:L:436:ILE:HG22	5:L:438:LEU:CD2	2.42	0.49
2:C:692:THR:HG21	2:C:798:GLN:OE1	2.12	0.49
3:I:848:VAL:HG13	3:I:850:LYS:HG2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:890:THR:O	3:I:891:ASP:C	2.56	0.49
5:K:408:MET:SD	5:K:691:ILE:CB	3.01	0.49
5:K:748:VAL:HG12	5:K:749:PRO:N	2.26	0.49
5:L:219:MET:HE2	5:L:253:ILE:HG23	1.95	0.49
5:L:243:TYR:O	5:L:244:ASN:HB2	2.13	0.49
2:H:1132:LEU:O	2:H:1135:GLN:N	2.39	0.49
2:H:1255:THR:O	2:H:1257:GLN:N	2.46	0.49
2:H:1336:ASN:HB2	3:I:29:MET:SD	2.53	0.49
4:J:30:MET:HG2	4:J:35:LYS:HB3	1.95	0.49
5:K:143:PRO:CD	5:K:148:ARG:HH22	2.23	0.49
5:K:377:ILE:HB	5:K:410:ARG:CD	2.42	0.49
5:L:370:LEU:C	5:L:370:LEU:CD2	2.86	0.49
5:L:720:MET:CE	5:L:720:MET:CA	2.66	0.49
5:K:144:TYR:CG	5:K:706:ILE:HD11	2.48	0.48
5:K:190:ILE:CD1	5:K:190:ILE:N	2.76	0.48
5:K:843:MET:CE	5:K:850:ASN:HB3	2.39	0.48
5:L:184:THR:HA	5:L:312:LEU:HD21	1.94	0.48
5:L:735:ASP:C	5:L:737:MET:H	2.19	0.48
5:L:737:MET:HE3	5:L:761:ILE:HG21	1.93	0.48
2:H:692:THR:HG21	2:H:798:GLN:OE1	2.13	0.48
5:K:192:HIS:HB2	5:K:223:PHE:HD1	1.78	0.48
5:K:539:SER:O	5:K:543:ARG:CZ	2.61	0.48
5:K:722:LEU:CD1	5:K:722:LEU:C	2.85	0.48
5:L:190:ILE:N	5:L:190:ILE:CD1	2.73	0.48
2:C:700:VAL:HG21	2:C:1114:GLU:HG3	1.95	0.48
3:D:87:LYS:HD2	5:L:78:ASN:HA	1.94	0.48
3:D:488:ASN:OD1	4:E:16:ARG:NE	2.46	0.48
2:H:496:LYS:HB3	2:H:497:PRO:HD3	1.94	0.48
5:K:195:LEU:HD11	5:K:225:LEU:HD23	1.95	0.48
5:L:546:ALA:O	5:L:550:PHE:N	2.38	0.48
5:L:578:MET:CG	5:L:579:VAL:N	2.76	0.48
5:L:736:ASN:O	5:L:737:MET:HB2	2.13	0.48
1:B:131:CYS:SG	1:B:132:HIS:N	2.86	0.48
4:E:30:MET:HG2	4:E:35:LYS:HB3	1.95	0.48
2:H:1120:ALA:HB1	2:H:1198:LEU:CD2	2.44	0.48
5:K:495:MET:O	5:K:499:THR:CB	2.61	0.48
2:C:185:ASP:HB2	2:C:197:ARG:HB2	1.96	0.48
5:K:815:LEU:O	5:K:962:LEU:HB3	2.13	0.48
5:L:523:LEU:O	5:L:524:ARG:C	2.57	0.48
5:L:578:MET:N	5:L:607:GLN:O	2.47	0.48
5:L:785:ARG:O	5:L:789:ASP:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:810:PRO:O	5:L:811:VAL:C	2.56	0.48
2:C:813:GLU:O	3:D:461:PHE:O	2.30	0.48
2:H:475:VAL:HG12	2:H:479:LEU:HD12	1.94	0.48
2:H:638:SER:O	2:H:639:LYS:C	2.57	0.48
2:H:1269:ARG:HA	3:I:346:ARG:HA	1.95	0.48
5:L:737:MET:CE	5:L:761:ILE:HG21	2.41	0.48
2:C:433:ILE:O	2:C:434:ASP:C	2.57	0.48
2:C:1120:ALA:HB1	2:C:1198:LEU:CD2	2.44	0.48
2:C:1255:THR:O	2:C:1257:GLN:N	2.47	0.48
2:H:1329:GLU:O	2:H:1333:LEU:HB2	2.14	0.48
5:K:121:ASP:HB2	5:K:125:ARG:HD2	1.95	0.48
5:L:188:GLY:O	5:L:191:LEU:N	2.43	0.48
5:L:342:PHE:O	5:L:345:GLU:N	2.47	0.48
5:L:535:HIS:HE1	5:L:538:MET:N	2.09	0.48
5:L:738:ILE:CG2	5:L:759:ILE:HG22	2.39	0.48
2:C:193:ASN:OD1	2:C:194:LEU:N	2.47	0.48
2:C:458:GLU:O	2:C:461:GLU:HB3	2.13	0.48
5:K:369:GLU:HG2	5:K:373:LEU:CD1	2.42	0.48
5:K:450:VAL:HA	5:K:453:ILE:HD13	1.96	0.48
5:K:826:ALA:HB3	5:K:832:LEU:HD13	1.95	0.48
5:L:665:ASP:O	5:L:669:ASN:N	2.47	0.48
5:L:715:LEU:HB3	5:L:761:ILE:HD11	1.95	0.48
5:L:826:ALA:HB3	5:L:832:LEU:HD13	1.94	0.48
2:H:455:SER:O	2:H:456:VAL:C	2.57	0.48
3:I:77:ARG:HD2	5:K:746:MET:O	2.14	0.48
5:K:719:ALA:HB1	5:K:723:PHE:CE1	2.49	0.48
5:K:737:MET:HE1	5:K:771:ARG:NH1	2.22	0.48
5:K:810:PRO:O	5:K:811:VAL:C	2.56	0.48
3:D:67:ASP:O	3:D:68:TYR:C	2.56	0.48
3:D:365:GLN:HA	3:D:438:GLU:O	2.14	0.48
1:F:66:HIS:CE1	1:F:69:SER:HB3	2.49	0.48
2:H:458:GLU:O	2:H:461:GLU:HB3	2.13	0.48
5:K:53:VAL:C	5:K:54:MET:CE	2.86	0.48
5:K:217:VAL:O	5:K:220:LEU:N	2.47	0.48
5:K:539:SER:OG	5:K:540:ILE:N	2.47	0.48
5:K:796:THR:HG22	5:K:960:LEU:HB2	1.96	0.48
5:K:907:ARG:HH21	5:K:947:MET:CE	2.17	0.48
5:L:818:LEU:C	5:L:843:MET:HB2	2.38	0.48
6:M:3:DG:C2'	6:M:4:DA:C5'	2.86	0.48
3:D:77:ARG:C	5:L:744:ASP:O	2.57	0.47
2:H:21:VAL:HG21	2:H:592:ARG:NH1	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:K:373:LEU:O	5:K:377:ILE:HG12	2.13	0.47
5:L:189:MET:HB2	5:L:190:ILE:HD12	1.96	0.47
5:L:353:ALA:CA	5:L:356:VAL:CG2	2.55	0.47
5:L:407:LEU:C	5:L:409:ASP:N	2.72	0.47
2:C:1329:GLU:O	2:C:1333:LEU:HB2	2.14	0.47
3:D:78:LEU:CB	5:L:746:MET:CA	2.91	0.47
2:H:700:VAL:HG21	2:H:1114:GLU:HG3	1.96	0.47
5:K:358:MET:HA	5:K:362:GLY:HA3	1.95	0.47
5:K:362:GLY:O	5:K:363:ASN:HB2	2.14	0.47
5:K:372:MET:O	5:K:376:MET:CG	2.62	0.47
5:K:409:ASP:C	5:K:411:HIS:H	2.22	0.47
5:K:495:MET:O	5:K:499:THR:CG2	2.61	0.47
5:K:495:MET:O	5:K:499:THR:HB	2.14	0.47
5:L:63:SER:H	5:L:68:GLN:HB3	1.79	0.47
5:L:436:ILE:HD11	5:L:609:HIS:ND1	2.28	0.47
5:L:737:MET:HE1	5:L:761:ILE:CG2	2.44	0.47
1:A:67:GLU:O	1:A:78:ILE:HB	2.14	0.47
2:H:193:ASN:OD1	2:H:194:LEU:N	2.47	0.47
3:I:86:GLU:N	3:I:86:GLU:CD	2.72	0.47
3:I:136:GLU:HA	3:I:139:LEU:HD22	1.96	0.47
5:K:123:MET:N	5:K:865:LEU:HD11	2.25	0.47
5:K:243:TYR:O	5:K:244:ASN:HB2	2.14	0.47
5:K:843:MET:SD	5:K:845:LEU:CD2	3.01	0.47
2:H:912:ASP:HB3	2:H:913:VAL:CG1	2.37	0.47
3:I:365:GLN:HA	3:I:438:GLU:O	2.13	0.47
5:K:374:GLY:O	5:K:378:GLY:CA	2.63	0.47
5:K:467:MET:CE	5:K:654:LEU:CB	2.75	0.47
2:C:832:HIS:CG	2:C:1058:ARG:HE	2.33	0.47
3:D:136:GLU:HA	3:D:139:LEU:HD22	1.96	0.47
3:D:814:CYS:SG	3:D:898:CYS:HB3	2.48	0.47
2:H:1118:GLY:C	2:H:1229:TYR:HB2	2.40	0.47
5:K:355:ALA:C	5:K:358:MET:HG2	2.38	0.47
5:L:188:GLY:C	5:L:190:ILE:N	2.72	0.47
5:L:220:LEU:HD12	5:L:224:ASN:CB	2.44	0.47
5:L:422:ARG:HG3	5:L:428:PHE:CZ	2.49	0.47
1:F:67:GLU:O	1:F:78:ILE:HB	2.14	0.47
5:K:342:PHE:O	5:K:345:GLU:N	2.47	0.47
5:K:422:ARG:HG3	5:K:428:PHE:CZ	2.49	0.47
5:K:523:LEU:O	5:K:524:ARG:C	2.58	0.47
5:L:61:ILE:O	5:L:68:GLN:HB2	2.14	0.47
5:L:580:MET:CE	5:L:593:ARG:HD3	2.33	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:735:ASP:C	5:L:737:MET:N	2.73	0.47
5:L:818:LEU:HB2	5:L:843:MET:CB	2.44	0.47
2:C:21:VAL:HG21	2:C:592:ARG:NH1	2.29	0.47
2:C:1118:GLY:C	2:C:1229:TYR:HB2	2.40	0.47
3:D:78:LEU:CG	5:L:746:MET:HB3	2.43	0.47
3:D:369:PRO:O	3:D:370:LYS:C	2.58	0.47
3:D:814:CYS:HB3	3:D:895:CYS:CB	2.45	0.47
2:H:206:ALA:HB3	2:H:350:THR:HG21	1.97	0.47
3:I:1256:ILE:O	3:I:1259:GLN:N	2.48	0.47
5:K:397:GLN:O	5:K:401:GLN:NE2	2.48	0.47
5:K:433:LEU:HD21	5:K:435:THR:HG23	1.96	0.47
5:K:506:VAL:HG12	5:K:579:VAL:HG23	1.97	0.47
5:L:186:GLU:O	5:L:189:MET:HB2	2.15	0.47
5:L:186:GLU:O	5:L:189:MET:CB	2.62	0.47
5:L:448:ILE:CG2	5:L:467:MET:CG	2.93	0.47
5:L:583:LEU:CD1	5:L:622:VAL:HG23	2.44	0.47
5:L:636:CYS:SG	5:L:639:GLY:N	2.88	0.47
5:L:815:LEU:O	5:L:962:LEU:HB3	2.15	0.47
1:B:67:GLU:O	1:B:78:ILE:HB	2.14	0.47
4:J:39:VAL:O	4:J:40:PRO:C	2.58	0.47
3:D:80:HIS:HB3	3:D:83:VAL:CG2	2.45	0.47
3:D:334:LYS:HG2	3:D:339:ARG:HD2	1.97	0.47
3:D:506:VAL:HG13	3:D:628:GLY:HA3	1.95	0.47
3:I:67:ASP:O	3:I:68:TYR:C	2.57	0.47
3:I:895:CYS:O	3:I:896:ALA:HB3	2.15	0.47
5:K:665:ASP:O	5:K:669:ASN:N	2.47	0.47
5:L:184:THR:HG23	5:L:312:LEU:HD23	1.88	0.47
5:L:720:MET:HE1	5:L:740:LEU:CD2	2.39	0.47
2:C:206:ALA:HB3	2:C:350:THR:HG21	1.97	0.47
3:I:292:VAL:O	3:I:295:GLU:N	2.38	0.47
3:I:1259:GLN:HA	3:I:1262:ARG:HG2	1.97	0.47
5:K:151:ARG:HD2	5:K:221:ARG:O	2.15	0.47
5:K:736:ASN:HD22	5:K:765:ARG:CZ	2.27	0.47
5:L:358:MET:CE	5:L:358:MET:CA	2.86	0.47
5:L:796:THR:HG22	5:L:960:LEU:HB2	1.96	0.47
2:C:18:ARG:NH1	2:C:621:SER:O	2.47	0.46
5:K:69:MET:SD	5:K:97:LEU:O	2.74	0.46
5:K:70:GLN:HB3	5:K:86:THR:N	2.30	0.46
5:K:74:VAL:HG12	5:K:81:LEU:HD22	1.96	0.46
5:K:223:PHE:C	5:K:225:LEU:CD1	2.86	0.46
5:K:375:GLU:OE1	5:K:375:GLU:HA	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:K:785:ARG:O	5:K:789:ASP:N	2.45	0.46
2:C:906:PHE:HA	5:L:540:ILE:HD13	1.96	0.46
2:C:1329:GLU:O	2:C:1333:LEU:N	2.48	0.46
3:D:78:LEU:HG	5:L:746:MET:CB	2.40	0.46
2:H:551:HIS:O	2:H:553:THR:N	2.48	0.46
3:I:334:LYS:HG2	3:I:339:ARG:HD2	1.97	0.46
3:I:369:PRO:O	3:I:370:LYS:C	2.58	0.46
3:I:1266:ILE:HG21	3:I:1300:ALA:HB1	1.97	0.46
5:K:629:LEU:O	5:K:630:ASP:C	2.59	0.46
5:K:640:ARG:C	5:K:642:ILE:H	2.23	0.46
5:L:356:VAL:C	5:L:358:MET:N	2.70	0.46
5:L:843:MET:HA	5:L:850:ASN:ND2	2.27	0.46
2:C:634:VAL:N	2:C:645:PHE:O	2.44	0.46
3:D:890:THR:O	3:D:891:ASP:C	2.58	0.46
2:H:185:ASP:HB2	2:H:197:ARG:HB2	1.97	0.46
2:H:433:ILE:O	2:H:434:ASP:C	2.57	0.46
3:I:80:HIS:HB3	3:I:83:VAL:CG2	2.45	0.46
3:I:165:TYR:OH	3:I:178:ALA:HB3	2.15	0.46
5:K:222:ARG:NH1	5:K:222:ARG:CG	2.73	0.46
5:L:68:GLN:C	5:L:69:MET:CG	2.82	0.46
5:L:123:MET:HB3	5:L:865:LEU:CB	2.42	0.46
5:L:185:ILE:HG12	5:L:222:ARG:NE	2.28	0.46
5:L:407:LEU:HD11	5:L:688:LEU:HD13	1.93	0.46
2:C:455:SER:O	2:C:456:VAL:C	2.58	0.46
3:D:77:ARG:CD	5:L:747:LEU:CG	2.87	0.46
4:E:39:VAL:O	4:E:40:PRO:C	2.58	0.46
5:K:636:CYS:SG	5:K:639:GLY:N	2.88	0.46
5:L:299:ILE:O	5:L:300:GLU:C	2.58	0.46
5:L:311:LEU:HD21	5:L:331:LEU:HD21	1.98	0.46
5:L:640:ARG:C	5:L:642:ILE:H	2.24	0.46
1:A:66:HIS:CE1	1:A:69:SER:HB3	2.51	0.46
3:D:165:TYR:OH	3:D:178:ALA:HB3	2.15	0.46
3:I:139:LEU:C	3:I:139:LEU:HD23	2.41	0.46
5:K:102:LEU:HG	5:K:103:ASP:N	2.31	0.46
5:L:149:GLY:H	5:L:777:ILE:HD11	1.79	0.46
5:L:220:LEU:O	5:L:224:ASN:N	2.48	0.46
5:L:939:ILE:HA	5:L:942:ASN:HB3	1.98	0.46
3:D:1266:ILE:HG21	3:D:1300:ALA:HB1	1.97	0.46
5:K:192:HIS:HB2	5:K:223:PHE:CD1	2.50	0.46
5:K:561:LEU:HD11	5:K:565:ILE:HD11	1.97	0.46
5:L:74:VAL:HG11	5:L:81:LEU:CD1	2.26	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:244:ASN:HB3	5:L:245:PRO:HD3	1.78	0.46
5:L:454:MET:HG3	5:L:454:MET:O	2.16	0.46
2:C:638:SER:O	2:C:639:LYS:C	2.58	0.46
5:K:378:GLY:N	5:K:379:GLU:HB2	2.30	0.46
5:L:375:GLU:OE1	5:L:375:GLU:HA	2.16	0.46
3:D:474:LEU:HD21	4:E:31:GLN:OE1	2.16	0.46
2:H:6:THR:O	2:H:6:THR:HG22	2.15	0.46
2:H:832:HIS:CG	2:H:1058:ARG:HE	2.34	0.46
2:H:1112:ILE:HG22	2:H:1116:HIS:CD2	2.51	0.46
2:H:1156:ARG:O	2:H:1158:LYS:N	2.49	0.46
5:K:378:GLY:CA	5:K:379:GLU:HB3	2.31	0.46
5:K:509:ILE:HG23	5:K:561:LEU:HD12	1.97	0.46
5:K:533:VAL:CG1	5:K:535:HIS:HD2	2.29	0.46
5:K:939:ILE:HA	5:K:942:ASN:HB3	1.98	0.46
5:L:407:LEU:CG	5:L:408:MET:N	2.78	0.46
5:L:407:LEU:HD21	5:L:688:LEU:HD22	1.98	0.46
5:L:561:LEU:HD11	5:L:565:ILE:HD11	1.97	0.46
2:C:170:VAL:O	2:C:170:VAL:HG13	2.16	0.46
3:D:80:HIS:HE1	5:L:54:MET:CE	2.28	0.46
5:K:270:CYS:O	5:K:272:ALA:N	2.49	0.46
5:K:404:VAL:HG23	5:K:405:SER:N	2.31	0.46
5:K:468:LEU:HD23	5:K:469:TYR:N	2.30	0.46
5:L:122:ARG:C	5:L:124:ASP:N	2.74	0.46
5:L:522:VAL:O	5:L:526:ARG:N	2.49	0.46
1:A:67:GLU:HA	1:A:78:ILE:HG21	1.98	0.45
2:C:14:ASP:HA	2:C:1183:ALA:HB3	1.98	0.45
2:C:551:HIS:O	2:C:553:THR:N	2.48	0.45
3:D:77:ARG:O	5:L:744:ASP:O	2.32	0.45
1:G:67:GLU:O	1:G:78:ILE:HB	2.15	0.45
2:H:90:VAL:O	2:H:140:GLY:N	2.49	0.45
3:I:519:ASN:HD21	3:I:710:ASP:N	2.11	0.45
5:K:315:THR:H	5:K:316:PRO:HD3	1.81	0.45
5:L:732:ASP:O	5:L:738:ILE:HA	2.16	0.45
5:L:801:ILE:O	5:L:803:LEU:N	2.48	0.45
3:D:1256:ILE:O	3:D:1259:GLN:N	2.49	0.45
1:F:67:GLU:HA	1:F:78:ILE:HG21	1.98	0.45
2:H:213:LEU:HD21	2:H:390:PHE:CZ	2.50	0.45
5:L:326:ALA:O	5:L:330:LEU:HD13	2.16	0.45
5:L:509:ILE:HG23	5:L:561:LEU:HD12	1.97	0.45
5:L:928:ASN:N	5:L:929:PRO:CD	2.79	0.45
2:C:6:THR:O	2:C:6:THR:HG22	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1072:ASN:ND2	2:C:1111:GLN:OE1	2.49	0.45
2:C:1274:GLU:OE1	2:C:1274:GLU:N	2.50	0.45
2:H:14:ASP:HA	2:H:1183:ALA:HB3	1.99	0.45
2:H:1121:ALA:C	2:H:1123:GLY:H	2.24	0.45
5:K:320:GLY:CA	5:K:321:MET:CB	2.84	0.45
5:K:726:ILE:C	5:K:746:MET:HB2	2.41	0.45
5:L:448:ILE:CG2	5:L:467:MET:HG2	2.44	0.45
5:L:580:MET:HB3	5:L:610:VAL:HB	1.98	0.45
2:C:213:LEU:HD21	2:C:390:PHE:CZ	2.51	0.45
2:C:1156:ARG:O	2:C:1158:LYS:N	2.50	0.45
3:D:775:SER:O	3:D:776:THR:C	2.58	0.45
3:D:895:CYS:O	3:D:896:ALA:HB3	2.16	0.45
3:I:392:THR:O	3:I:392:THR:HG22	2.16	0.45
3:I:814:CYS:HB3	3:I:895:CYS:CB	2.45	0.45
5:K:125:ARG:HG3	5:K:794:GLY:CA	2.46	0.45
5:K:245:PRO:O	5:K:246:PHE:C	2.58	0.45
5:K:326:ALA:O	5:K:330:LEU:HD13	2.16	0.45
5:K:368:ASP:O	5:K:371:ASN:O	2.34	0.45
5:L:321:MET:O	5:L:322:GLU:HG3	2.16	0.45
5:L:509:ILE:HD12	5:L:578:MET:HE3	1.97	0.45
5:L:629:LEU:O	5:L:630:ASP:C	2.59	0.45
5:L:722:LEU:O	5:L:726:ILE:HG13	2.16	0.45
2:C:514:PHE:CD1	2:C:760:ASN:HB3	2.52	0.45
2:C:1112:ILE:HG22	2:C:1116:HIS:CD2	2.52	0.45
3:I:139:LEU:HD23	3:I:140:TYR:N	2.31	0.45
5:L:165:VAL:HG13	5:L:168:ARG:HD2	1.98	0.45
5:L:720:MET:CE	5:L:723:PHE:CZ	2.85	0.45
2:C:90:VAL:O	2:C:140:GLY:N	2.48	0.45
2:C:557:ARG:NE	2:C:608:ALA:HB2	2.32	0.45
3:D:307:LEU:O	3:D:328:ALA:HB2	2.16	0.45
3:D:350:SER:HA	3:D:468:VAL:O	2.17	0.45
2:H:12:ARG:NH1	2:H:698:PRO:O	2.50	0.45
2:H:488:MET:CB	2:H:489:PRO:HD3	2.46	0.45
2:H:1072:ASN:ND2	2:H:1111:GLN:OE1	2.49	0.45
3:I:77:ARG:HD2	5:K:743:SER:O	2.16	0.45
3:I:77:ARG:CD	5:K:743:SER:O	2.65	0.45
4:J:10:VAL:HG22	4:J:19:LEU:HD22	1.99	0.45
5:L:746:MET:O	5:L:747:LEU:HG	2.17	0.45
2:C:488:MET:CB	2:C:489:PRO:HD3	2.46	0.45
2:C:692:THR:OG1	2:C:693:LEU:N	2.48	0.45
3:D:80:HIS:HE1	5:L:54:MET:HE3	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:363:LEU:HA	3:D:450:HIS:CE1	2.52	0.45
2:H:170:VAL:O	2:H:170:VAL:HG13	2.17	0.45
2:H:634:VAL:N	2:H:645:PHE:O	2.44	0.45
2:H:1274:GLU:OE1	2:H:1274:GLU:N	2.50	0.45
5:K:522:VAL:O	5:K:526:ARG:N	2.49	0.45
5:L:162:ALA:HA	5:L:190:ILE:HD11	1.98	0.45
5:L:315:THR:H	5:L:316:PRO:HD3	1.81	0.45
5:L:807:LYS:HB3	5:L:808:ALA:HA	1.99	0.45
2:C:624:ASP:O	2:C:625:GLU:HB3	2.17	0.45
3:D:57:PHE:CE1	3:D:252:LEU:HD12	2.52	0.45
3:D:1144:LEU:HD13	3:D:1237:VAL:HG22	1.98	0.45
3:D:1259:GLN:HA	3:D:1262:ARG:HG2	1.97	0.45
4:E:10:VAL:HG22	4:E:19:LEU:HD22	1.99	0.45
1:G:67:GLU:HA	1:G:78:ILE:HG21	1.99	0.45
2:H:1329:GLU:O	2:H:1333:LEU:N	2.49	0.45
3:I:77:ARG:CB	5:K:747:LEU:N	2.80	0.45
3:I:372:MET:HG2	3:I:376:LEU:HD11	1.99	0.45
3:I:1144:LEU:HD13	3:I:1237:VAL:HG22	1.98	0.45
5:K:52:ARG:C	5:K:54:MET:HE1	2.42	0.45
5:K:843:MET:HE2	5:K:850:ASN:HD21	1.64	0.45
5:L:817:GLU:HA	5:L:844:LEU:HD23	1.97	0.45
3:D:1145:PHE:HB3	3:D:1309:ILE:HD11	1.99	0.45
2:H:557:ARG:NE	2:H:608:ALA:HB2	2.32	0.45
3:I:57:PHE:CE1	3:I:252:LEU:HD12	2.51	0.45
3:I:775:SER:O	3:I:776:THR:C	2.59	0.45
5:K:397:GLN:HB3	5:K:400:ARG:HB2	1.97	0.45
5:L:124:ASP:O	5:L:125:ARG:HB3	2.17	0.45
5:L:371:ASN:N	5:L:371:ASN:ND2	2.65	0.45
5:L:372:MET:C	5:L:374:GLY:CA	2.55	0.45
3:D:139:LEU:HD23	3:D:140:TYR:N	2.32	0.45
2:H:464:PHE:O	2:H:468:LEU:HG	2.16	0.45
3:I:303:VAL:C	3:I:305:ALA:H	2.24	0.45
5:K:217:VAL:O	5:K:220:LEU:C	2.60	0.45
5:K:722:LEU:CD1	5:K:726:ILE:HD12	2.45	0.45
3:D:139:LEU:HD23	3:D:139:LEU:C	2.41	0.44
2:H:673:HIS:CE1	3:I:765:GLU:C	2.95	0.44
5:K:222:ARG:HD2	5:K:223:PHE:CE2	2.53	0.44
5:K:408:MET:HB3	5:K:688:LEU:CB	2.45	0.44
2:C:94:ALA:CB	2:C:129:LEU:HD11	2.47	0.44
3:I:363:LEU:HA	3:I:450:HIS:CE1	2.52	0.44
4:J:63:ILE:HG22	4:J:63:ILE:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:K:219:MET:O	5:K:225:LEU:N	2.32	0.44
5:K:311:LEU:HD21	5:K:331:LEU:HD21	1.98	0.44
5:K:539:SER:HB3	5:K:542:GLU:CD	2.42	0.44
5:K:721:ASN:O	5:K:725:ILE:HD13	2.17	0.44
5:L:59:ASP:C	5:L:70:GLN:HB2	2.41	0.44
5:L:204:LEU:HD22	5:L:269:LEU:HD22	1.99	0.44
5:L:272:ALA:C	5:L:273:GLU:CG	2.90	0.44
5:L:769:LEU:HD13	5:L:771:ARG:CZ	2.47	0.44
2:C:12:ARG:NH1	2:C:698:PRO:O	2.50	0.44
2:H:30:ILE:HG23	2:H:581:THR:OG1	2.18	0.44
2:H:624:ASP:O	2:H:625:GLU:HB3	2.17	0.44
5:K:353:ALA:O	5:K:356:VAL:HB	2.17	0.44
5:K:580:MET:HG2	5:K:608:ILE:HG23	2.00	0.44
5:L:185:ILE:CG1	5:L:222:ARG:NH1	2.57	0.44
5:L:246:PHE:CD2	5:L:246:PHE:O	2.70	0.44
6:O:2:DC:O5'	6:O:2:DC:C6	2.71	0.44
2:C:464:PHE:O	2:C:468:LEU:HG	2.17	0.44
3:D:364:HIS:O	3:D:438:GLU:N	2.51	0.44
3:D:372:MET:HG2	3:D:376:LEU:HD11	2.00	0.44
1:F:162:GLU:OE2	1:F:166:ARG:NH2	2.51	0.44
2:H:94:ALA:CB	2:H:129:LEU:HD11	2.47	0.44
5:K:165:VAL:HG13	5:K:168:ARG:HD2	1.98	0.44
5:K:212:GLN:O	5:K:213:HIS:C	2.60	0.44
5:K:464:ALA:HB2	5:K:651:ILE:HD11	2.00	0.44
5:K:466:ASP:HB3	5:K:467:MET:HB3	1.94	0.44
5:L:372:MET:O	5:L:373:LEU:HB3	2.17	0.44
2:C:558:VAL:HG13	2:C:573:ASN:HB3	2.00	0.44
2:H:591:TYR:CE2	2:H:616:ILE:HD13	2.53	0.44
2:H:887:VAL:HB	2:H:913:VAL:CG2	2.46	0.44
3:I:1145:PHE:HB3	3:I:1309:ILE:HD11	1.99	0.44
5:K:407:LEU:HD11	5:K:408:MET:HE3	0.62	0.44
5:L:60:THR:C	5:L:70:GLN:OE1	2.60	0.44
7:N:2:U:C6	7:N:2:U:O5'	2.70	0.44
6:O:15:DG:O6	7:P:1:A:C2	2.70	0.44
2:C:812:PHE:CE2	3:D:451:PRO:O	2.70	0.44
2:C:887:VAL:HB	2:C:913:VAL:CG2	2.47	0.44
2:H:786:GLY:N	2:H:789:THR:OG1	2.46	0.44
2:H:803:ALA:HB3	2:H:1097:VAL:HA	2.00	0.44
3:I:350:SER:HA	3:I:468:VAL:O	2.16	0.44
5:K:907:ARG:NH2	5:K:947:MET:CE	2.77	0.44
6:M:2:DC:H4'	6:M:3:DG:OP1	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:67:GLU:HA	1:B:78:ILE:HG21	1.99	0.44
2:C:519:ASN:ND2	2:C:689:ALA:O	2.51	0.44
2:C:1330:ILE:HG22	2:C:1335:ILE:HB	2.00	0.44
3:D:475:GLU:OE2	4:E:24:ALA:HB1	2.18	0.44
3:D:746:LEU:HA	3:D:758:PRO:HB3	2.00	0.44
4:E:63:ILE:HG22	4:E:63:ILE:O	2.17	0.44
2:H:502:VAL:O	2:H:503:LYS:C	2.61	0.44
2:H:811:ASN:HA	2:H:815:SER:HB2	2.00	0.44
5:K:299:ILE:O	5:K:300:GLU:C	2.58	0.44
5:K:314:ALA:O	5:K:315:THR:CB	2.66	0.44
5:K:688:LEU:O	5:K:692:HIS:N	2.48	0.44
5:K:946:VAL:C	5:K:948:GLU:H	2.26	0.44
5:L:60:THR:C	5:L:70:GLN:CD	2.85	0.44
5:L:538:MET:HG3	5:L:542:GLU:CB	2.46	0.44
2:C:661:VAL:HG12	2:C:662:SER:N	2.33	0.44
3:D:303:VAL:C	3:D:305:ALA:H	2.26	0.44
2:H:18:ARG:NH1	2:H:621:SER:O	2.47	0.44
2:H:166:SER:OG	2:H:167:SER:N	2.51	0.44
2:H:454:ARG:HD3	2:H:462:ASN:ND2	2.33	0.44
3:I:368:LEU:HD23	3:I:369:PRO:HD2	2.00	0.44
5:K:53:VAL:C	5:K:54:MET:HG3	2.43	0.44
5:K:61:ILE:HG23	5:K:102:LEU:HD13	1.98	0.44
5:K:222:ARG:HD2	5:K:223:PHE:HE2	1.83	0.44
5:K:580:MET:N	5:K:609:HIS:O	2.34	0.44
5:L:212:GLN:O	5:L:213:HIS:C	2.60	0.44
5:L:255:SER:O	5:L:258:PHE:HB3	2.18	0.44
5:L:376:MET:CG	5:L:410:ARG:CD	2.70	0.44
5:L:495:MET:O	5:L:498:LEU:N	2.50	0.44
5:L:535:HIS:CD2	5:L:542:GLU:OE2	2.71	0.44
5:L:540:ILE:HD12	5:L:540:ILE:N	2.33	0.44
7:N:2:U:O5'	7:N:2:U:H6	2.00	0.44
2:C:1121:ALA:C	2:C:1123:GLY:H	2.25	0.44
2:H:668:ILE:HB	2:H:671:LEU:HD13	2.00	0.44
3:I:59:ALA:CB	3:I:71:LEU:HD21	2.48	0.44
3:I:145:VAL:CG1	3:I:184:ALA:HB1	2.48	0.44
3:I:307:LEU:O	3:I:328:ALA:HB2	2.16	0.44
5:K:70:GLN:HB3	5:K:86:THR:CA	2.46	0.44
5:K:122:ARG:HB3	5:K:124:ASP:OD1	2.18	0.44
5:K:373:LEU:O	5:K:376:MET:HB2	2.18	0.44
5:K:769:LEU:HD13	5:K:771:ARG:CZ	2.47	0.44
5:L:155:ILE:CG2	5:L:600:ILE:HG21	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:175:LEU:O	5:L:313:THR:N	2.51	0.44
5:L:720:MET:CG	5:L:730:GLN:OE1	2.63	0.44
3:D:356:THR:HG22	3:D:357:VAL:N	2.34	0.43
2:H:131:THR:OG1	2:H:135:THR:N	2.50	0.43
2:H:672:GLU:HB3	3:I:767:LEU:H	1.82	0.43
2:H:1066:MET:HA	2:H:1233:LEU:O	2.18	0.43
5:L:60:THR:HG23	5:L:69:MET:CA	2.45	0.43
5:L:185:ILE:CD1	5:L:185:ILE:N	2.73	0.43
5:L:219:MET:CA	5:L:225:LEU:CG	2.90	0.43
5:L:219:MET:HB3	5:L:227:PHE:HD1	1.83	0.43
2:C:666:SER:HA	2:C:1186:VAL:HG22	2.00	0.43
3:D:504:GLN:O	3:D:507:VAL:HB	2.18	0.43
3:D:842:ARG:NH1	3:D:884:SER:OG	2.51	0.43
1:G:91:ARG:HB2	1:G:122:GLU:O	2.18	0.43
2:H:36:GLN:O	2:H:40:GLU:HB2	2.18	0.43
2:H:964:LEU:O	2:H:968:GLU:HB2	2.18	0.43
3:I:504:GLN:O	3:I:507:VAL:HB	2.18	0.43
5:K:123:MET:HG2	5:K:799:SER:OG	2.18	0.43
5:K:494:LEU:O	5:K:498:LEU:HB2	2.16	0.43
5:K:818:LEU:O	5:K:843:MET:CG	2.65	0.43
5:L:218:GLU:HB3	5:L:222:ARG:HB2	2.00	0.43
5:L:748:VAL:HG13	5:L:749:PRO:HD2	2.01	0.43
5:L:775:GLN:C	5:L:777:ILE:H	2.24	0.43
2:C:93:SER:OG	2:C:94:ALA:N	2.51	0.43
2:C:454:ARG:HD3	2:C:462:ASN:ND2	2.33	0.43
3:D:77:ARG:HB3	5:L:747:LEU:N	2.34	0.43
2:H:395:TYR:CE2	2:H:420:LEU:HG	2.54	0.43
2:H:1330:ILE:HG22	2:H:1335:ILE:HB	2.00	0.43
5:K:255:SER:O	5:K:258:PHE:HB3	2.18	0.43
5:K:352:VAL:O	5:K:356:VAL:N	2.50	0.43
5:K:365:LEU:HD12	5:K:366:SER:H	1.82	0.43
5:K:408:MET:HB3	5:K:688:LEU:O	2.18	0.43
5:K:540:ILE:N	5:K:540:ILE:HD12	2.33	0.43
5:L:538:MET:CB	5:L:542:GLU:CD	2.90	0.43
2:C:591:TYR:CE2	2:C:616:ILE:HD13	2.54	0.43
2:C:964:LEU:HD12	2:C:1025:PHE:CE2	2.53	0.43
3:D:80:HIS:CE1	5:L:54:MET:HE3	2.53	0.43
3:D:292:VAL:O	3:D:295:GLU:N	2.39	0.43
2:H:692:THR:OG1	2:H:693:LEU:N	2.48	0.43
2:H:789:THR:HA	2:H:793:GLU:O	2.18	0.43
3:I:746:LEU:HA	3:I:758:PRO:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:K:123:MET:CG	5:K:865:LEU:HB2	2.48	0.43
5:L:142:MET:CG	5:L:143:PRO:CD	2.96	0.43
2:C:131:THR:OG1	2:C:135:THR:N	2.50	0.43
3:D:77:ARG:HB3	5:L:747:LEU:H	1.83	0.43
3:D:615:LYS:N	3:D:616:PRO:CD	2.82	0.43
3:D:1257:VAL:HG22	3:D:1260:MET:HE2	2.00	0.43
2:H:509:SER:OG	2:H:510:GLN:N	2.52	0.43
2:H:514:PHE:CD1	2:H:760:ASN:HB3	2.53	0.43
2:H:661:VAL:HG12	2:H:662:SER:N	2.34	0.43
3:I:78:LEU:HB3	5:K:746:MET:SD	2.59	0.43
5:K:155:ILE:CG2	5:K:600:ILE:HG21	2.48	0.43
5:K:536:GLU:OE1	5:K:536:GLU:HA	2.19	0.43
5:K:807:LYS:HB3	5:K:808:ALA:HA	2.00	0.43
5:L:810:PRO:O	5:L:812:GLY:N	2.52	0.43
2:C:395:TYR:CE2	2:C:420:LEU:HG	2.54	0.43
2:C:660:VAL:HG23	2:C:661:VAL:HG23	2.00	0.43
2:H:161:LYS:O	2:H:162:GLY:C	2.62	0.43
2:H:519:ASN:ND2	2:H:689:ALA:O	2.52	0.43
2:H:964:LEU:HD12	2:H:1025:PHE:CE2	2.53	0.43
3:I:356:THR:HG22	3:I:357:VAL:N	2.34	0.43
3:I:364:HIS:O	3:I:438:GLU:N	2.51	0.43
3:I:842:ARG:NH1	3:I:884:SER:OG	2.52	0.43
5:K:801:ILE:O	5:K:803:LEU:N	2.50	0.43
3:D:1262:ARG:O	3:D:1263:LYS:HB2	2.19	0.43
2:H:937:ASP:HA	2:H:1039:GLY:HA2	2.01	0.43
2:H:1191:LYS:O	2:H:1192:GLU:C	2.61	0.43
3:I:776:THR:O	3:I:780:ARG:HB2	2.18	0.43
5:K:928:ASN:N	5:K:929:PRO:CD	2.81	0.43
5:L:188:GLY:C	5:L:190:ILE:H	2.24	0.43
5:L:272:ALA:C	5:L:273:GLU:CD	2.86	0.43
5:L:407:LEU:O	5:L:408:MET:HB2	2.18	0.43
5:L:719:ALA:C	5:L:723:PHE:CZ	2.96	0.43
2:C:161:LYS:O	2:C:162:GLY:C	2.62	0.43
2:C:1191:LYS:O	2:C:1192:GLU:C	2.62	0.43
3:D:145:VAL:CG1	3:D:184:ALA:HB1	2.48	0.43
3:I:80:HIS:HB3	3:I:83:VAL:HB	2.01	0.43
5:K:175:LEU:O	5:K:313:THR:N	2.52	0.43
5:K:438:LEU:HD22	5:K:438:LEU:N	2.34	0.43
5:K:612:TYR:CD2	5:K:619:SER:HA	2.54	0.43
5:L:184:THR:HG21	5:L:215:TRP:CZ2	2.53	0.43
6:M:2:DC:H2"	6:M:3:DG:OP1	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:ARG:HD2	1:B:197:ASP:HB3	2.01	0.43
2:C:803:ALA:HB3	2:C:1097:VAL:HA	1.99	0.43
2:C:1066:MET:HA	2:C:1233:LEU:O	2.19	0.43
3:D:80:HIS:HB3	3:D:83:VAL:HB	2.01	0.43
2:H:93:SER:OG	2:H:94:ALA:N	2.51	0.43
3:I:1257:VAL:HG22	3:I:1260:MET:HE2	2.00	0.43
3:I:1262:ARG:O	3:I:1263:LYS:HB2	2.19	0.43
5:K:318:GLN:C	5:K:319:LEU:HG	2.44	0.43
5:K:493:TRP:C	5:K:495:MET:N	2.72	0.43
5:K:720:MET:CG	5:K:730:GLN:NE2	2.82	0.43
2:C:30:ILE:HG23	2:C:581:THR:OG1	2.19	0.43
2:C:36:GLN:O	2:C:40:GLU:HB2	2.18	0.43
2:C:937:ASP:HA	2:C:1039:GLY:HA2	2.01	0.43
2:C:964:LEU:O	2:C:968:GLU:HB2	2.19	0.43
3:D:84:ILE:HB	5:L:73:GLU:HB2	2.01	0.43
3:D:616:PRO:O	3:D:620:PHE:HB3	2.19	0.43
3:D:801:VAL:HG22	3:D:920:ALA:HB3	2.00	0.43
2:H:431:LYS:O	2:H:432:LEU:C	2.62	0.43
2:H:839:VAL:HG11	2:H:841:ARG:NH2	2.34	0.43
3:I:519:ASN:HD22	3:I:709:ARG:HB2	1.80	0.43
3:I:615:LYS:N	3:I:616:PRO:CD	2.82	0.43
3:I:801:VAL:HG22	3:I:920:ALA:HB3	2.00	0.43
5:K:140:PHE:C	5:K:142:MET:HG3	2.43	0.43
5:K:176:ALA:O	5:K:177:ASP:C	2.62	0.43
5:K:194:GLN:O	5:K:194:GLN:NE2	2.52	0.43
5:K:204:LEU:HD22	5:K:269:LEU:HD22	2.00	0.43
5:K:219:MET:O	5:K:224:ASN:N	2.51	0.43
5:K:810:PRO:O	5:K:812:GLY:N	2.52	0.43
5:L:184:THR:CA	5:L:312:LEU:HD21	2.49	0.43
5:L:538:MET:HG3	5:L:542:GLU:HB3	1.99	0.43
5:L:736:ASN:N	5:L:736:ASN:ND2	2.66	0.43
2:C:1138:VAL:HG13	2:C:1141:LEU:HD23	2.00	0.42
3:D:59:ALA:CB	3:D:71:LEU:HD21	2.49	0.42
5:K:72:GLU:O	5:K:73:GLU:CB	2.63	0.42
5:K:179:VAL:HG12	5:K:180:GLY:N	2.34	0.42
5:L:374:GLY:O	5:L:375:GLU:HB2	2.19	0.42
5:L:716:ILE:HD11	5:L:761:ILE:CG2	2.48	0.42
1:A:162:GLU:OE2	1:A:166:ARG:NH2	2.52	0.42
3:D:57:PHE:CD1	3:D:252:LEU:HD12	2.54	0.42
3:D:127:LEU:HD13	3:D:223:LEU:HD12	2.02	0.42
3:D:368:LEU:HD23	3:D:369:PRO:HD2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1347:LEU:O	3:D:1351:VAL:HG23	2.19	0.42
3:I:57:PHE:CD1	3:I:252:LEU:HD12	2.54	0.42
5:K:272:ALA:O	5:K:274:TRP:N	2.52	0.42
5:K:722:LEU:O	5:K:726:ILE:HG13	2.20	0.42
5:K:844:LEU:O	5:K:850:ASN:HA	2.18	0.42
5:K:863:ARG:CD	5:K:961:ARG:CZ	2.97	0.42
5:L:314:ALA:O	5:L:315:THR:CB	2.66	0.42
5:L:321:MET:HE3	5:L:684:GLY:O	2.19	0.42
5:L:434:HIS:N	5:L:608:ILE:O	2.52	0.42
5:L:538:MET:CG	5:L:542:GLU:HB3	2.49	0.42
2:C:912:ASP:HB3	2:C:913:VAL:CG1	2.40	0.42
3:D:67:ASP:O	3:D:69:GLU:N	2.52	0.42
2:H:501:ALA:O	2:H:502:VAL:C	2.61	0.42
1:A:207:THR:OG1	1:A:208:ASN:N	2.52	0.42
1:B:91:ARG:HB2	1:B:122:GLU:O	2.18	0.42
2:C:389:PHE:HB2	2:C:390:PHE:CD2	2.54	0.42
2:C:502:VAL:O	2:C:503:LYS:C	2.61	0.42
2:C:509:SER:OG	2:C:510:GLN:N	2.52	0.42
2:C:577:VAL:HG21	2:C:658:GLN:HG2	2.02	0.42
2:C:878:THR:HG22	2:C:879:GLY:N	2.34	0.42
3:D:161:THR:O	3:D:163:GLU:N	2.52	0.42
3:I:79:LYS:HB2	5:K:747:LEU:O	2.19	0.42
3:I:127:LEU:HD13	3:I:223:LEU:HD12	2.01	0.42
5:K:223:PHE:O	5:K:225:LEU:HD11	2.15	0.42
5:L:240:HIS:O	5:L:241:ASP:C	2.62	0.42
5:L:946:VAL:C	5:L:949:SER:H	2.27	0.42
2:C:176:ILE:HD11	2:C:428:VAL:HG11	2.02	0.42
2:C:1227:VAL:HG12	2:C:1228:GLY:N	2.34	0.42
3:D:362:ARG:O	3:D:363:LEU:C	2.62	0.42
2:H:1138:VAL:HG13	2:H:1141:LEU:HD23	2.01	0.42
3:I:616:PRO:O	3:I:620:PHE:HB3	2.19	0.42
5:K:506:VAL:CG1	5:K:579:VAL:HG23	2.50	0.42
5:L:438:LEU:HD22	5:L:438:LEU:N	2.33	0.42
5:L:612:TYR:CD2	5:L:619:SER:HA	2.54	0.42
5:L:720:MET:O	5:L:724:ASP:HB2	2.19	0.42
3:I:161:THR:O	3:I:163:GLU:N	2.52	0.42
5:K:139:GLN:O	5:K:142:MET:N	2.52	0.42
5:L:42:LEU:CG	5:L:242:ALA:CB	2.97	0.42
5:L:165:VAL:HG21	5:L:173:VAL:HG11	2.01	0.42
5:L:219:MET:CE	5:L:227:PHE:CD1	2.99	0.42
6:M:2:DC:O5'	6:M:2:DC:C6	2.71	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:568:ASN:HA	2:C:571:LEU:HD12	2.01	0.42
2:C:789:THR:HA	2:C:793:GLU:O	2.20	0.42
2:C:811:ASN:HA	2:C:815:SER:HB2	2.01	0.42
3:D:580:TRP:CZ3	3:D:583:VAL:HG11	2.55	0.42
4:E:20:VAL:O	4:E:24:ALA:N	2.36	0.42
5:K:359:LEU:C	5:K:360:LEU:HD12	2.44	0.42
5:K:378:GLY:N	5:K:379:GLU:CB	2.83	0.42
5:K:726:ILE:O	5:K:726:ILE:HG22	2.20	0.42
5:L:495:MET:O	5:L:496:GLY:C	2.62	0.42
5:L:737:MET:HE1	5:L:761:ILE:HB	2.00	0.42
2:C:795:ALA:HA	2:C:1231:TYR:OH	2.20	0.42
2:C:1088:ASP:N	2:C:1091:GLY:O	2.52	0.42
2:C:1149:TYR:HB3	2:C:1159:VAL:HG21	2.02	0.42
3:D:353:SER:OG	3:D:354:VAL:N	2.52	0.42
3:I:66:LYS:NZ	3:I:70:CYS:O	2.49	0.42
5:K:720:MET:HE1	5:K:738:ILE:HG21	2.02	0.42
5:K:818:LEU:CA	5:K:843:MET:HB3	2.50	0.42
5:L:444:TYR:HE1	5:L:470:PRO:HB2	1.80	0.42
5:L:578:MET:HB3	5:L:608:ILE:HA	2.02	0.42
2:C:668:ILE:HB	2:C:671:LEU:HD13	2.00	0.42
3:D:35:PHE:O	3:D:61:ILE:HG23	2.20	0.42
3:D:77:ARG:HB2	5:L:747:LEU:O	2.20	0.42
3:I:35:PHE:O	3:I:61:ILE:HG23	2.20	0.42
5:K:318:GLN:O	5:K:319:LEU:HG	2.19	0.42
5:K:371:ASN:HA	5:K:375:GLU:CG	2.50	0.42
5:K:377:ILE:C	5:K:379:GLU:HB2	2.45	0.42
5:K:843:MET:CE	5:K:894:GLN:HG3	2.49	0.42
5:L:176:ALA:O	5:L:177:ASP:C	2.62	0.42
5:L:218:GLU:N	5:L:219:MET:HB2	2.35	0.42
2:C:370:MET:HE2	2:C:388:LEU:HD21	2.01	0.42
2:C:1131:MET:O	2:C:1133:LYS:N	2.53	0.42
2:H:666:SER:HA	2:H:1186:VAL:HG22	2.00	0.42
2:H:1172:LEU:O	2:H:1173:ALA:C	2.63	0.42
3:I:786:THR:HA	3:I:789:LYS:HB2	2.02	0.42
3:I:1347:LEU:O	3:I:1351:VAL:HG23	2.19	0.42
5:L:372:MET:HG2	5:L:375:GLU:OE2	2.19	0.42
2:C:501:ALA:O	2:C:502:VAL:C	2.62	0.41
2:C:782:VAL:HG11	2:C:792:GLY:N	2.35	0.41
2:H:795:ALA:HA	2:H:1231:TYR:OH	2.20	0.41
2:H:812:PHE:O	3:I:504:GLN:NE2	2.52	0.41
2:H:878:THR:HG22	2:H:879:GLY:N	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1227:VAL:HG12	2:H:1228:GLY:N	2.35	0.41
5:K:70:GLN:H	5:K:85:GLY:C	2.28	0.41
5:K:165:VAL:HG21	5:K:173:VAL:HG11	2.02	0.41
5:L:260:ARG:O	5:L:261:ARG:C	2.63	0.41
5:L:540:ILE:H	5:L:540:ILE:CD1	2.32	0.41
5:L:887:ILE:HG22	5:L:887:ILE:O	2.21	0.41
2:C:431:LYS:O	2:C:432:LEU:C	2.62	0.41
2:H:429:MET:HA	2:H:432:LEU:HB3	2.02	0.41
2:H:519:ASN:HB2	2:H:520:PRO:HD2	2.03	0.41
2:H:660:VAL:HG23	2:H:661:VAL:HG23	2.01	0.41
2:H:782:VAL:HG11	2:H:792:GLY:N	2.35	0.41
2:H:1088:ASP:N	2:H:1091:GLY:O	2.54	0.41
5:K:467:MET:CA	5:K:617:ALA:HB2	2.41	0.41
5:L:436:ILE:HG22	5:L:437:LYS:N	2.34	0.41
5:L:736:ASN:OD1	5:L:765:ARG:HG2	2.20	0.41
7:N:7:U:H2'	7:N:8:C:C6	2.55	0.41
2:C:839:VAL:HG11	2:C:841:ARG:NH2	2.35	0.41
2:C:912:ASP:HB3	2:C:913:VAL:HG12	2.02	0.41
1:F:11:PRO:HB3	1:F:31:LEU:HG	2.01	0.41
1:F:207:THR:OG1	1:F:208:ASN:N	2.53	0.41
2:H:15:PHE:CE2	2:H:1182:ILE:HG23	2.55	0.41
3:I:67:ASP:O	3:I:69:GLU:N	2.53	0.41
5:K:677:LEU:HA	5:K:680:GLN:HB3	2.02	0.41
5:L:179:VAL:HG12	5:L:180:GLY:N	2.34	0.41
5:L:220:LEU:O	5:L:224:ASN:OD1	2.38	0.41
5:L:371:ASN:O	5:L:372:MET:HB2	2.19	0.41
5:L:410:ARG:HG2	5:L:410:ARG:O	2.20	0.41
5:L:770:ALA:C	5:L:771:ARG:HG3	2.45	0.41
2:C:429:MET:HA	2:C:432:LEU:HB3	2.02	0.41
2:C:847:PRO:HB3	2:C:1047:LEU:HD11	2.03	0.41
2:C:1254:VAL:HG13	2:C:1255:THR:H	1.85	0.41
2:H:370:MET:HE2	2:H:388:LEU:HD21	2.01	0.41
2:H:389:PHE:HB2	2:H:390:PHE:CD2	2.55	0.41
2:H:558:VAL:HG13	2:H:573:ASN:HB3	2.01	0.41
2:H:1269:ARG:HE	3:I:344:GLY:HA2	1.85	0.41
5:K:409:ASP:C	5:K:411:HIS:N	2.79	0.41
5:K:422:ARG:HG3	5:K:428:PHE:CE2	2.56	0.41
5:K:887:ILE:HG22	5:K:887:ILE:O	2.21	0.41
5:L:122:ARG:HA	5:L:865:LEU:HD21	2.03	0.41
5:L:512:LYS:O	5:L:513:ALA:C	2.63	0.41
2:C:15:PHE:CE2	2:C:1182:ILE:HG23	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:473:THR:O	3:D:474:LEU:C	2.63	0.41
3:D:1284:ARG:HA	3:D:1287:ILE:HG22	2.02	0.41
2:H:577:VAL:HG21	2:H:658:GLN:HG2	2.01	0.41
5:K:260:ARG:O	5:K:261:ARG:C	2.64	0.41
5:K:421:THR:O	5:K:425:VAL:HG12	2.21	0.41
5:K:491:VAL:HA	5:K:494:LEU:CD1	2.51	0.41
5:L:155:ILE:HG21	5:L:600:ILE:HG21	2.02	0.41
5:L:436:ILE:HG12	5:L:609:HIS:HE1	1.77	0.41
3:D:1184:ASP:OD1	3:D:1185:PRO:HD3	2.20	0.41
2:H:847:PRO:HB3	2:H:1047:LEU:HD11	2.03	0.41
5:K:225:LEU:HB3	5:K:251:LEU:HD11	2.03	0.41
5:K:468:LEU:HD23	5:K:469:TYR:CB	2.49	0.41
5:L:90:THR:O	5:L:91:GLU:HB2	2.21	0.41
5:L:190:ILE:HD12	5:L:190:ILE:H	1.82	0.41
1:B:11:PRO:HB3	1:B:31:LEU:HG	2.02	0.41
3:D:41:PRO:HB3	3:D:273:ILE:CG2	2.51	0.41
3:D:776:THR:O	3:D:780:ARG:HB2	2.20	0.41
1:F:167:PRO:HB3	5:K:528:GLY:CA	2.51	0.41
2:H:176:ILE:HD11	2:H:428:VAL:HG11	2.02	0.41
3:I:362:ARG:O	3:I:363:LEU:C	2.63	0.41
5:K:384:PRO:O	5:K:385:LEU:C	2.64	0.41
5:K:623:ARG:HG2	5:K:627:GLU:HB2	2.03	0.41
5:K:733:ARG:CD	5:K:733:ARG:C	2.86	0.41
5:K:844:LEU:N	5:K:850:ASN:HB2	2.35	0.41
5:L:183:LYS:O	5:L:187:ALA:HB2	2.20	0.41
5:L:701:ALA:O	5:L:702:LEU:C	2.64	0.41
5:L:737:MET:SD	5:L:738:ILE:HG21	2.59	0.41
5:L:842:ARG:O	5:L:843:MET:HG3	2.11	0.41
2:C:928:VAL:HG12	2:C:929:ILE:N	2.36	0.41
3:D:755:ILE:H	3:D:755:ILE:HD12	1.85	0.41
1:G:11:PRO:HB3	1:G:31:LEU:HG	2.02	0.41
2:H:1254:VAL:HG13	2:H:1255:THR:H	1.86	0.41
3:I:580:TRP:CZ3	3:I:583:VAL:HG11	2.56	0.41
5:K:231:ASP:OD1	5:K:231:ASP:N	2.54	0.41
5:K:374:GLY:C	5:K:378:GLY:C	2.84	0.41
5:L:422:ARG:HG3	5:L:428:PHE:CE2	2.56	0.41
5:L:748:VAL:CG1	5:L:749:PRO:HD2	2.51	0.41
1:A:11:PRO:HB3	1:A:31:LEU:HG	2.02	0.41
2:C:522:SER:O	2:C:523:GLU:C	2.63	0.41
2:C:947:GLU:O	2:C:951:MET:HG2	2.21	0.41
2:C:1325:VAL:HG22	3:D:249:LEU:HD22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:78:LEU:CG	5:L:746:MET:HB2	2.50	0.41
2:H:518:ASN:N	2:H:761:GLN:OE1	2.54	0.41
2:H:947:GLU:O	2:H:951:MET:HG2	2.21	0.41
2:H:1047:LEU:HB3	2:H:1048:LYS:HG3	2.03	0.41
2:H:1281:TYR:CD2	3:I:484:MET:HG2	2.55	0.41
3:I:41:PRO:HB3	3:I:273:ILE:CG2	2.51	0.41
3:I:42:GLU:O	3:I:56:LEU:N	2.54	0.41
3:I:473:THR:O	3:I:474:LEU:C	2.64	0.41
3:I:755:ILE:H	3:I:755:ILE:HD12	1.86	0.41
5:K:58:GLY:H	5:K:71:VAL:HB	1.86	0.41
5:K:240:HIS:O	5:K:241:ASP:C	2.63	0.41
5:K:721:ASN:OD1	5:K:725:ILE:HD13	2.21	0.41
5:L:74:VAL:HG12	5:L:81:LEU:CD1	2.40	0.41
5:L:123:MET:N	5:L:865:LEU:CD2	2.55	0.41
5:L:142:MET:CG	5:L:143:PRO:HD2	2.51	0.41
5:L:148:ARG:NH2	5:L:706:ILE:HG13	2.36	0.41
5:L:219:MET:CB	5:L:227:PHE:CD1	3.01	0.41
5:L:231:ASP:OD1	5:L:231:ASP:N	2.54	0.41
5:L:407:LEU:HD11	5:L:688:LEU:CD1	2.49	0.41
5:L:614:GLU:O	5:L:615:LYS:HB2	2.21	0.41
5:L:688:LEU:O	5:L:692:HIS:N	2.49	0.41
3:D:84:ILE:HB	5:L:73:GLU:CB	2.51	0.41
3:D:475:GLU:HG3	4:E:24:ALA:CB	2.50	0.41
2:H:551:HIS:C	2:H:553:THR:H	2.29	0.41
5:K:54:MET:N	5:K:54:MET:HE3	2.35	0.41
5:K:173:VAL:HG23	5:K:175:LEU:HD11	2.03	0.41
5:L:139:GLN:HA	5:L:142:MET:HB2	2.02	0.41
5:L:536:GLU:OE1	5:L:536:GLU:HA	2.21	0.41
2:C:786:GLY:N	2:C:789:THR:OG1	2.46	0.40
2:C:1172:LEU:O	2:C:1173:ALA:C	2.64	0.40
3:D:1184:ASP:OD1	3:D:1184:ASP:N	2.47	0.40
2:H:445:ILE:O	2:H:451:ARG:HD3	2.22	0.40
2:H:673:HIS:C	2:H:674:ASP:OD1	2.64	0.40
3:I:677:GLU:O	3:I:678:ARG:C	2.64	0.40
3:I:1284:ARG:HA	3:I:1287:ILE:HG22	2.02	0.40
5:K:225:LEU:HB3	5:K:251:LEU:HD13	2.03	0.40
5:K:512:LYS:O	5:K:513:ALA:C	2.64	0.40
5:K:612:TYR:CD2	5:K:612:TYR:C	3.00	0.40
5:K:701:ALA:O	5:K:702:LEU:C	2.65	0.40
5:K:720:MET:HG2	5:K:723:PHE:CZ	2.54	0.40
5:L:62:THR:HG21	5:L:107:VAL:HG23	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:468:LEU:HD22	5:L:469:TYR:CZ	2.54	0.40
5:L:677:LEU:HA	5:L:680:GLN:HB3	2.02	0.40
6:M:7:DG:O6	6:M:8:DA:N6	2.53	0.40
2:C:87:ILE:C	2:C:89:GLY:H	2.30	0.40
2:C:1204:LEU:O	2:C:1205:PRO:C	2.64	0.40
3:D:42:GLU:O	3:D:56:LEU:N	2.54	0.40
3:D:372:MET:O	3:D:376:LEU:HG	2.22	0.40
3:D:786:THR:HA	3:D:789:LYS:HB2	2.03	0.40
2:H:866:ASP:O	2:H:867:GLU:HG3	2.21	0.40
2:H:925:SER:O	2:H:926:GLY:C	2.64	0.40
2:H:1149:TYR:HB3	2:H:1159:VAL:HG21	2.02	0.40
3:I:701:LEU:O	3:I:701:LEU:HG	2.22	0.40
5:K:322:GLU:O	5:K:323:SER:CB	2.70	0.40
5:K:770:ALA:C	5:K:771:ARG:HG3	2.46	0.40
5:L:321:MET:C	5:L:322:GLU:HG3	2.46	0.40
5:L:769:LEU:HD13	5:L:771:ARG:NH2	2.36	0.40
1:A:150:ARG:NH1	1:B:6:THR:OG1	2.53	0.40
2:C:124:MET:HA	2:C:498:ILE:HD13	2.03	0.40
3:D:45:ASN:O	3:D:47:ARG:N	2.54	0.40
3:D:814:CYS:SG	3:D:814:CYS:O	2.79	0.40
1:G:33:ARG:HD2	1:G:197:ASP:HB3	2.02	0.40
2:H:1204:LEU:O	2:H:1205:PRO:C	2.64	0.40
5:K:743:SER:CB	5:K:744:ASP:HB2	2.51	0.40
5:L:173:VAL:HG23	5:L:175:LEU:HD11	2.02	0.40
5:L:217:VAL:C	5:L:218:GLU:CG	2.93	0.40
5:L:404:VAL:HB	5:L:408:MET:SD	2.61	0.40
5:L:852:LEU:HD12	5:L:852:LEU:C	2.35	0.40
2:C:502:VAL:HG12	2:C:503:LYS:N	2.37	0.40
2:C:518:ASN:N	2:C:761:GLN:OE1	2.55	0.40
2:C:1047:LEU:HB3	2:C:1048:LYS:HG3	2.03	0.40
3:D:305:ALA:HB1	3:D:316:ILE:HD11	2.03	0.40
2:H:61:SER:CB	2:H:479:LEU:HD13	2.51	0.40
2:H:709:ALA:HB3	2:H:792:GLY:O	2.21	0.40
2:H:1199:LEU:HB3	2:H:1204:LEU:O	2.22	0.40
5:K:299:ILE:O	5:K:302:LEU:HB2	2.21	0.40
5:K:314:ALA:C	5:K:315:THR:HG1	2.28	0.40
5:K:720:MET:CA	5:K:723:PHE:CE2	2.86	0.40
5:K:745:HIS:O	5:K:746:MET:CB	2.69	0.40
5:L:408:MET:HE3	5:L:691:ILE:C	2.46	0.40
5:L:421:THR:O	5:L:425:VAL:HG12	2.21	0.40
5:L:623:ARG:HG2	5:L:627:GLU:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:503:LYS:O	2:C:507:GLY:N	2.55	0.40
2:C:519:ASN:HB2	2:C:520:PRO:HD2	2.04	0.40
2:C:709:ALA:HB3	2:C:792:GLY:O	2.22	0.40
2:C:866:ASP:O	2:C:867:GLU:HG3	2.21	0.40
2:C:1199:LEU:HB3	2:C:1204:LEU:O	2.22	0.40
2:H:87:ILE:C	2:H:89:GLY:H	2.30	0.40
2:H:928:VAL:HG12	2:H:929:ILE:N	2.37	0.40
2:H:1120:ALA:HB1	2:H:1198:LEU:HD22	2.02	0.40
2:H:1131:MET:O	2:H:1133:LYS:N	2.54	0.40
2:H:1165:SER:O	2:H:1166:ASP:C	2.65	0.40
3:I:305:ALA:HB1	3:I:316:ILE:HD11	2.03	0.40
3:I:372:MET:O	3:I:376:LEU:HG	2.20	0.40
3:I:393:THR:HG1	5:K:733:ARG:HG3	1.83	0.40
3:I:1265:THR:HG21	3:I:1275:LEU:HG	2.03	0.40
5:K:19:LEU:CD1	5:K:102:LEU:HD23	2.39	0.40
5:K:368:ASP:C	5:K:371:ASN:O	2.65	0.40
5:K:614:GLU:O	5:K:615:LYS:HB2	2.21	0.40
5:L:141:ARG:O	5:L:141:ARG:HG2	2.19	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	225/329 (68%)	202 (90%)	19 (8%)	4 (2%)	6	33
1	B	225/329 (68%)	205 (91%)	20 (9%)	0	100	100
1	F	225/329 (68%)	202 (90%)	19 (8%)	4 (2%)	6	33
1	G	225/329 (68%)	205 (91%)	19 (8%)	1 (0%)	30	67
2	C	1171/1342 (87%)	894 (76%)	211 (18%)	66 (6%)	1	14
2	H	1165/1342 (87%)	889 (76%)	206 (18%)	70 (6%)	1	13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	D	1143/1416 (81%)	867 (76%)	235 (21%)	41 (4%)	2	20
3	I	1156/1416 (82%)	869 (75%)	240 (21%)	47 (4%)	2	18
4	E	73/90 (81%)	59 (81%)	8 (11%)	6 (8%)	0	9
4	J	73/90 (81%)	59 (81%)	8 (11%)	6 (8%)	0	9
5	K	959/974 (98%)	689 (72%)	201 (21%)	69 (7%)	1	11
5	L	959/974 (98%)	694 (72%)	200 (21%)	65 (7%)	1	12
All	All	7599/8960 (85%)	5834 (77%)	1386 (18%)	379 (5%)	1	16

All (379) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	51	MET
2	C	43	PRO
2	C	63	SER
2	C	115	LYS
2	C	216	THR
2	C	488	MET
2	C	491	ASP
2	C	577	VAL
2	C	791	LEU
2	C	808	ASN
2	C	915	ASP
2	C	1216	ARG
2	C	1223	ARG
3	D	53	ARG
3	D	141	PHE
3	D	162	GLU
3	D	165	TYR
3	D	256	ASP
3	D	585	LYS
3	D	670	SER
3	D	706	VAL
3	D	834	PRO
3	D	891	ASP
3	D	1182	GLY
3	D	1186	TYR
4	E	44	ASP
1	F	51	MET
2	H	43	PRO
2	H	63	SER

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Mol	Chain	Res	Type
2	H	115	LYS
2	H	216	THR
2	H	488	MET
2	H	491	ASP
2	H	577	VAL
2	H	791	LEU
2	H	808	ASN
2	H	915	ASP
2	H	1216	ARG
2	H	1223	ARG
3	I	46	TYR
3	I	53	ARG
3	I	141	PHE
3	I	162	GLU
3	I	165	TYR
3	I	256	ASP
3	I	585	LYS
3	I	670	SER
3	I	706	VAL
3	I	834	PRO
3	I	855	ASP
3	I	891	ASP
3	I	1182	GLY
3	I	1185	PRO
4	J	44	ASP
5	K	92	GLU
5	K	199	ALA
5	K	244	ASN
5	K	273	GLU
5	K	315	THR
5	K	317	GLU
5	K	342	PHE
5	K	513	ALA
5	K	554	ASP
5	K	776	PHE
5	K	811	VAL
5	L	92	GLU
5	L	125	ARG
5	L	189	MET
5	L	199	ALA
5	L	244	ASN
5	L	315	THR

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Mol	Chain	Res	Type
5	L	317	GLU
5	L	342	PHE
5	L	357	ALA
5	L	382	ILE
5	L	456	ALA
5	L	513	ALA
5	L	554	ASP
5	L	584	PRO
5	L	611	PRO
5	L	738	ILE
5	L	776	PHE
5	L	811	VAL
2	C	456	VAL
2	C	502	VAL
2	C	552	PRO
2	C	677	ASN
2	C	692	THR
2	C	730	SER
2	C	844	LYS
2	C	926	GLY
2	C	1156	ARG
2	C	1157	GLN
2	C	1162	SER
2	C	1254	VAL
2	C	1297	ASP
3	D	68	TYR
3	D	79	LYS
3	D	155	GLU
3	D	711	GLY
3	D	1309	ILE
3	D	1311	LYS
2	H	456	VAL
2	H	502	VAL
2	H	552	PRO
2	H	677	ASN
2	H	692	THR
2	H	730	SER
2	H	844	LYS
2	H	926	GLY
2	H	1156	ARG
2	H	1157	GLN
2	H	1162	SER

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Mol	Chain	Res	Type
2	H	1254	VAL
2	H	1297	ASP
3	I	68	TYR
3	I	79	LYS
3	I	155	GLU
3	I	521	LYS
3	I	711	GLY
3	I	1183	SER
3	I	1309	ILE
3	I	1311	LYS
5	K	10	ILE
5	K	66	GLY
5	K	73	GLU
5	K	246	PHE
5	K	271	GLU
5	K	313	THR
5	K	316	PRO
5	K	323	SER
5	K	358	MET
5	K	379	GLU
5	K	397	GLN
5	K	478	GLU
5	K	511	ALA
5	K	584	PRO
5	K	595	GLY
5	K	813	THR
5	L	10	ILE
5	L	66	GLY
5	L	69	MET
5	L	313	THR
5	L	316	PRO
5	L	381	ASP
5	L	470	PRO
5	L	474	TYR
5	L	478	GLU
5	L	511	ALA
5	L	595	GLY
2	C	26	TYR
2	C	77	GLU
2	C	165	HIS
2	C	613	ASN
2	C	638	SER

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Mol	Chain	Res	Type
2	C	912	ASP
2	C	1047	LEU
2	C	1103	VAL
2	C	1132	LEU
2	C	1153	ALA
2	C	1237	HIS
2	C	1238	LEU
2	C	1256	GLN
3	D	77	ARG
3	D	131	PRO
3	D	270	ARG
3	D	679	TYR
3	D	1150	PRO
4	E	43	ASN
2	H	26	TYR
2	H	77	GLU
2	H	165	HIS
2	H	912	ASP
2	H	1047	LEU
2	H	1103	VAL
2	H	1132	LEU
2	H	1153	ALA
2	H	1237	HIS
2	H	1238	LEU
2	H	1256	GLN
3	I	77	ARG
3	I	131	PRO
3	I	270	ARG
3	I	679	TYR
3	I	857	LEU
3	I	1150	PRO
4	J	43	ASN
5	K	241	ASP
5	K	272	ALA
5	K	372	MET
5	K	467	MET
5	K	474	TYR
5	K	539	SER
5	K	585	PHE
5	K	721	ASN
5	L	241	ASP
5	L	585	PHE

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Mol	Chain	Res	Type
5	L	732	ASP
5	L	802	SER
5	L	813	THR
5	L	843	MET
2	C	27	LEU
2	C	88	ARG
2	C	698	PRO
2	C	866	ASP
2	C	939	VAL
2	C	1131	MET
2	C	1155	VAL
2	C	1317	PRO
3	D	46	TYR
3	D	47	ARG
3	D	286	ALA
3	D	1275	LEU
4	E	35	LYS
2	H	27	LEU
2	H	88	ARG
2	H	613	ASN
2	H	638	SER
2	H	866	ASP
2	H	939	VAL
2	H	1131	MET
2	H	1155	VAL
2	H	1317	PRO
3	I	47	ARG
3	I	286	ALA
3	I	1275	LEU
4	J	35	LYS
5	K	3	PHE
5	K	65	ASP
5	K	142	MET
5	K	177	ASP
5	K	261	ARG
5	K	322	GLU
5	K	343	VAL
5	K	394	GLU
5	K	458	LYS
5	K	604	HIS
5	K	630	ASP
5	K	657	PRO

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Mol	Chain	Res	Type
5	K	659	GLN
5	K	662	GLY
5	K	732	ASP
5	K	744	ASP
5	K	763	PHE
5	K	802	SER
5	K	812	GLY
5	K	823	GLU
5	L	3	PHE
5	L	65	ASP
5	L	177	ASP
5	L	261	ARG
5	L	343	VAL
5	L	358	MET
5	L	458	LYS
5	L	604	HIS
5	L	630	ASP
5	L	657	PRO
5	L	659	GLN
5	L	763	PHE
5	L	812	GLY
5	L	823	GLU
1	A	165	GLU
1	A	214	GLU
2	C	214	ASN
2	C	436	ARG
2	C	487	LEU
2	C	1313	HIS
3	D	86	GLU
3	D	174	ASP
3	D	546	ALA
3	D	593	ASN
3	D	776	THR
4	E	40	PRO
4	E	41	GLU
1	F	165	GLU
1	F	214	GLU
2	H	214	ASN
2	H	436	ARG
2	H	487	LEU
2	H	698	PRO
2	H	910	ALA

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Mol	Chain	Res	Type
2	H	1313	HIS
3	I	86	GLU
3	I	174	ASP
3	I	546	ALA
3	I	593	ASN
3	I	776	THR
3	I	851	PRO
3	I	1184	ASP
4	J	40	PRO
4	J	41	GLU
5	K	27	ALA
5	K	318	GLN
5	K	341	GLN
5	K	485	TRP
5	K	641	THR
5	K	746	MET
5	K	810	PRO
5	K	869	ASN
5	L	27	ALA
5	L	341	GLN
5	L	393	SER
5	L	394	GLU
5	L	485	TRP
5	L	641	THR
5	L	662	GLY
5	L	737	MET
5	L	810	PRO
5	L	869	ASN
2	C	489	PRO
2	C	910	ALA
2	C	1122	LYS
2	C	1186	VAL
2	C	1215	GLY
2	C	1318	GLY
3	D	122	SER
3	D	313	GLY
3	D	879	ALA
1	F	179	PRO
1	G	214	GLU
2	H	108	GLU
2	H	352	ARG
2	H	451	ARG

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Mol	Chain	Res	Type
2	H	489	PRO
2	H	498	ILE
2	H	1122	LYS
2	H	1186	VAL
2	H	1215	GLY
2	H	1318	GLY
3	I	122	SER
3	I	313	GLY
3	I	879	ALA
3	I	1179	PRO
5	K	46	SER
5	K	111	PRO
5	K	522	VAL
5	K	873	GLY
5	L	46	SER
5	L	522	VAL
5	L	873	GLY
1	A	179	PRO
2	C	498	ILE
5	L	111	PRO
2	C	134	GLY
2	C	1185	PRO
2	C	1205	PRO
2	C	1334	GLY
3	D	671	GLY
3	D	1191	PRO
2	H	134	GLY
2	H	1205	PRO
2	H	1334	GLY
3	I	586	GLY
3	I	671	GLY
3	I	1191	PRO
5	K	110	LYS
5	L	110	LYS
2	C	178	PRO
3	D	233	LYS
2	H	1185	PRO
3	I	233	LYS
2	C	79	VAL
2	C	153	PRO
2	C	168	GLY
2	C	669	PRO

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Mol	Chain	Res	Type
3	D	586	GLY
3	D	616	PRO
4	E	4	VAL
2	H	79	VAL
2	H	153	PRO
2	H	168	GLY
2	H	178	PRO
2	H	669	PRO
5	K	245	PRO
3	D	92	VAL
2	H	355	PRO
3	I	92	VAL
4	J	4	VAL
5	L	727	GLY

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	195/286 (68%)	191 (98%)	4 (2%)	47	65
1	B	195/286 (68%)	187 (96%)	8 (4%)	27	49
1	F	195/286 (68%)	191 (98%)	4 (2%)	47	65
1	G	195/286 (68%)	187 (96%)	8 (4%)	27	49
2	C	1016/1157 (88%)	937 (92%)	79 (8%)	11	32
2	H	1011/1157 (87%)	931 (92%)	80 (8%)	11	32
3	D	962/1177 (82%)	884 (92%)	78 (8%)	11	31
3	I	971/1177 (82%)	895 (92%)	76 (8%)	11	32
4	E	65/74 (88%)	62 (95%)	3 (5%)	24	46
4	J	65/74 (88%)	62 (95%)	3 (5%)	24	46
5	K	822/835 (98%)	720 (88%)	102 (12%)	4	18
5	L	822/835 (98%)	727 (88%)	95 (12%)	5	19
All	All	6514/7630 (85%)	5974 (92%)	540 (8%)	10	31

All (540) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	GLU
1	A	90	VAL
1	A	91	ARG
1	A	186	ASN
1	B	29	GLU
1	B	66	HIS
1	B	90	VAL
1	B	91	ARG
1	B	101	THR
1	B	134	THR
1	B	135	ASP
1	B	186	ASN
2	C	62	TYR
2	C	86	GLN
2	C	132	ASP
2	C	158	ASP
2	C	161	LYS
2	C	188	PHE
2	C	350	THR
2	C	365	GLU
2	C	379	GLU
2	C	397	LEU
2	C	403	MET
2	C	436	ARG
2	C	437	ASN
2	C	441	GLU
2	C	454	ARG
2	C	472	GLU
2	C	479	LEU
2	C	514	PHE
2	C	523	GLU
2	C	539	THR
2	C	541	GLU
2	C	545	PHE
2	C	561	ILE
2	C	581	THR
2	C	588	GLU
2	C	593	LYS
2	C	628	HIS
2	C	631	GLU
2	C	643	SER
2	C	657	THR

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Mol	Chain	Res	Type
2	C	674	ASP
2	C	680	LEU
2	C	699	LEU
2	C	702	THR
2	C	714	VAL
2	C	733	VAL
2	C	748	ILE
2	C	749	ASP
2	C	757	THR
2	C	789	THR
2	C	799	ASN
2	C	811	ASN
2	C	834	GLN
2	C	835	GLU
2	C	840	SER
2	C	894	GLN
2	C	912	ASP
2	C	933	VAL
2	C	944	ARG
2	C	947	GLU
2	C	948	ILE
2	C	964	LEU
2	C	971	LEU
2	C	1020	GLU
2	C	1034	ARG
2	C	1037	THR
2	C	1042	LEU
2	C	1049	ILE
2	C	1056	VAL
2	C	1058	ARG
2	C	1072	ASN
2	C	1075	VAL
2	C	1077	SER
2	C	1082	ILE
2	C	1085	MET
2	C	1087	TYR
2	C	1096	ILE
2	C	1098	LEU
2	C	1138	VAL
2	C	1145	ILE
2	C	1184	THR
2	C	1188	ASP

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Mol	Chain	Res	Type
2	C	1231	TYR
2	C	1235	LEU
2	C	1276	TRP
2	C	1306	LYS
2	C	1319	MET
2	C	1333	LEU
2	C	1335	ILE
3	D	21	LYS
3	D	42	GLU
3	D	58	CYS
3	D	70	CYS
3	D	78	LEU
3	D	86	GLU
3	D	88	CYS
3	D	93	THR
3	D	139	LEU
3	D	156	ARG
3	D	157	GLN
3	D	159	ILE
3	D	169	LEU
3	D	171	GLU
3	D	199	GLU
3	D	208	THR
3	D	212	THR
3	D	223	LEU
3	D	229	GLN
3	D	250	ARG
3	D	252	LEU
3	D	285	LEU
3	D	290	ILE
3	D	294	ASN
3	D	300	GLN
3	D	316	ILE
3	D	330	MET
3	D	331	ILE
3	D	335	GLN
3	D	338	PHE
3	D	342	LEU
3	D	368	LEU
3	D	378	LYS
3	D	393	THR
3	D	416	ILE

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Mol	Chain	Res	Type
3	D	440	VAL
3	D	450	HIS
3	D	454	CYS
3	D	465	GLN
3	D	501	VAL
3	D	503	SER
3	D	515	ARG
3	D	534	GLU
3	D	572	THR
3	D	644	MET
3	D	646	ILE
3	D	672	LEU
3	D	680	ASN
3	D	690	ASN
3	D	700	ASN
3	D	701	LEU
3	D	736	GLN
3	D	746	LEU
3	D	783	LEU
3	D	792	ASN
3	D	846	GLU
3	D	847	ASP
3	D	860	ARG
3	D	884	SER
3	D	889	ASP
3	D	891	ASP
3	D	898	CYS
3	D	1144	LEU
3	D	1155	ILE
3	D	1192	LYS
3	D	1198	VAL
3	D	1199	PHE
3	D	1231	ARG
3	D	1246	VAL
3	D	1262	ARG
3	D	1298	VAL
3	D	1305	ASP
3	D	1318	SER
3	D	1330	ARG
3	D	1345	ARG
3	D	1348	LYS
3	D	1366	HIS

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Mol	Chain	Res	Type
3	D	1369	ARG
4	E	44	ASP
4	E	67	ARG
4	E	70	GLN
1	F	29	GLU
1	F	90	VAL
1	F	91	ARG
1	F	186	ASN
1	G	29	GLU
1	G	66	HIS
1	G	90	VAL
1	G	91	ARG
1	G	101	THR
1	G	134	THR
1	G	135	ASP
1	G	186	ASN
2	H	62	TYR
2	H	86	GLN
2	H	132	ASP
2	H	158	ASP
2	H	161	LYS
2	H	188	PHE
2	H	350	THR
2	H	365	GLU
2	H	379	GLU
2	H	397	LEU
2	H	403	MET
2	H	436	ARG
2	H	437	ASN
2	H	441	GLU
2	H	454	ARG
2	H	472	GLU
2	H	479	LEU
2	H	514	PHE
2	H	523	GLU
2	H	539	THR
2	H	541	GLU
2	H	561	ILE
2	H	581	THR
2	H	588	GLU
2	H	593	LYS
2	H	628	HIS

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Mol	Chain	Res	Type
2	H	631	GLU
2	H	643	SER
2	H	657	THR
2	H	674	ASP
2	H	680	LEU
2	H	699	LEU
2	H	702	THR
2	H	714	VAL
2	H	733	VAL
2	H	748	ILE
2	H	749	ASP
2	H	757	THR
2	H	789	THR
2	H	799	ASN
2	H	811	ASN
2	H	834	GLN
2	H	835	GLU
2	H	840	SER
2	H	854	ILE
2	H	894	GLN
2	H	912	ASP
2	H	933	VAL
2	H	944	ARG
2	H	947	GLU
2	H	948	ILE
2	H	964	LEU
2	H	971	LEU
2	H	1020	GLU
2	H	1034	ARG
2	H	1037	THR
2	H	1042	LEU
2	H	1049	ILE
2	H	1056	VAL
2	H	1058	ARG
2	H	1072	ASN
2	H	1075	VAL
2	H	1077	SER
2	H	1082	ILE
2	H	1085	MET
2	H	1087	TYR
2	H	1096	ILE
2	H	1098	LEU

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Mol	Chain	Res	Type
2	H	1138	VAL
2	H	1145	ILE
2	H	1184	THR
2	H	1188	ASP
2	H	1231	TYR
2	H	1235	LEU
2	H	1276	TRP
2	H	1299	ASN
2	H	1306	LYS
2	H	1319	MET
2	H	1333	LEU
2	H	1335	ILE
3	I	21	LYS
3	I	42	GLU
3	I	58	CYS
3	I	70	CYS
3	I	78	LEU
3	I	86	GLU
3	I	88	CYS
3	I	93	THR
3	I	139	LEU
3	I	156	ARG
3	I	157	GLN
3	I	159	ILE
3	I	169	LEU
3	I	171	GLU
3	I	199	GLU
3	I	208	THR
3	I	212	THR
3	I	223	LEU
3	I	229	GLN
3	I	250	ARG
3	I	252	LEU
3	I	285	LEU
3	I	290	ILE
3	I	294	ASN
3	I	300	GLN
3	I	316	ILE
3	I	330	MET
3	I	331	ILE
3	I	335	GLN
3	I	338	PHE

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Mol	Chain	Res	Type
3	I	342	LEU
3	I	368	LEU
3	I	378	LYS
3	I	393	THR
3	I	416	ILE
3	I	440	VAL
3	I	450	HIS
3	I	454	CYS
3	I	465	GLN
3	I	501	VAL
3	I	503	SER
3	I	515	ARG
3	I	534	GLU
3	I	572	THR
3	I	644	MET
3	I	646	ILE
3	I	672	LEU
3	I	680	ASN
3	I	690	ASN
3	I	700	ASN
3	I	701	LEU
3	I	736	GLN
3	I	746	LEU
3	I	783	LEU
3	I	792	ASN
3	I	846	GLU
3	I	860	ARG
3	I	884	SER
3	I	889	ASP
3	I	898	CYS
3	I	1144	LEU
3	I	1155	ILE
3	I	1192	LYS
3	I	1198	VAL
3	I	1199	PHE
3	I	1231	ARG
3	I	1246	VAL
3	I	1262	ARG
3	I	1298	VAL
3	I	1305	ASP
3	I	1318	SER
3	I	1330	ARG

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Mol	Chain	Res	Type
3	I	1345	ARG
3	I	1348	LYS
3	I	1366	HIS
3	I	1369	ARG
4	J	44	ASP
4	J	67	ARG
4	J	70	GLN
5	K	13	THR
5	K	19	LEU
5	K	42	LEU
5	K	54	MET
5	K	61	ILE
5	K	67	TRP
5	K	90	THR
5	K	114	ARG
5	K	115	LEU
5	K	153	SER
5	K	155	ILE
5	K	174	LEU
5	K	178	GLU
5	K	183	LYS
5	K	185	ILE
5	K	190	ILE
5	K	191	LEU
5	K	193	GLN
5	K	196	LEU
5	K	225	LEU
5	K	248	THR
5	K	253	ILE
5	K	254	CYS
5	K	256	LEU
5	K	257	ASP
5	K	273	GLU
5	K	285	LEU
5	K	288	SER
5	K	310	LEU
5	K	311	LEU
5	K	313	THR
5	K	327	ARG
5	K	343	VAL
5	K	360	LEU
5	K	366	SER

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Mol	Chain	Res	Type
5	K	370	LEU
5	K	385	LEU
5	K	386	LEU
5	K	400	ARG
5	K	401	GLN
5	K	402	GLU
5	K	435	THR
5	K	440	LEU
5	K	445	GLN
5	K	453	ILE
5	K	476	GLU
5	K	488	ASP
5	K	504	GLN
5	K	510	CYS
5	K	512	LYS
5	K	515	THR
5	K	518	GLN
5	K	520	GLU
5	K	533	VAL
5	K	552	GLU
5	K	553	GLU
5	K	561	LEU
5	K	562	CYS
5	K	565	ILE
5	K	577	HIS
5	K	613	LEU
5	K	635	THR
5	K	641	THR
5	K	644	ASP
5	K	650	LEU
5	K	660	THR
5	K	675	GLU
5	K	688	LEU
5	K	690	GLU
5	K	706	ILE
5	K	710	ASP
5	K	720	MET
5	K	723	PHE
5	K	725	ILE
5	K	729	ASN
5	K	741	THR
5	K	744	ASP

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Mol	Chain	Res	Type
5	K	759	ILE
5	K	760	THR
5	K	761	ILE
5	K	762	THR
5	K	769	LEU
5	K	775	GLN
5	K	788	LEU
5	K	814	LEU
5	K	831	GLN
5	K	843	MET
5	K	845	LEU
5	K	847	LYS
5	K	862	ASN
5	K	865	LEU
5	K	868	VAL
5	K	872	THR
5	K	877	VAL
5	K	881	GLN
5	K	912	GLU
5	K	918	LEU
5	K	931	ILE
5	K	932	ARG
5	K	950	LEU
5	K	960	LEU
5	K	962	LEU
5	L	13	THR
5	L	19	LEU
5	L	42	LEU
5	L	67	TRP
5	L	90	THR
5	L	114	ARG
5	L	115	LEU
5	L	141	ARG
5	L	153	SER
5	L	155	ILE
5	L	174	LEU
5	L	178	GLU
5	L	185	ILE
5	L	190	ILE
5	L	191	LEU
5	L	193	GLN
5	L	196	LEU

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Mol	Chain	Res	Type
5	L	253	ILE
5	L	254	CYS
5	L	256	LEU
5	L	257	ASP
5	L	273	GLU
5	L	285	LEU
5	L	288	SER
5	L	310	LEU
5	L	311	LEU
5	L	313	THR
5	L	327	ARG
5	L	343	VAL
5	L	358	MET
5	L	359	LEU
5	L	360	LEU
5	L	366	SER
5	L	385	LEU
5	L	386	LEU
5	L	400	ARG
5	L	401	GLN
5	L	402	GLU
5	L	436	ILE
5	L	440	LEU
5	L	445	GLN
5	L	446	THR
5	L	453	ILE
5	L	476	GLU
5	L	488	ASP
5	L	504	GLN
5	L	510	CYS
5	L	512	LYS
5	L	515	THR
5	L	518	GLN
5	L	520	GLU
5	L	533	VAL
5	L	552	GLU
5	L	553	GLU
5	L	561	LEU
5	L	562	CYS
5	L	565	ILE
5	L	577	HIS
5	L	613	LEU

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Mol	Chain	Res	Type
5	L	635	THR
5	L	641	THR
5	L	644	ASP
5	L	650	LEU
5	L	660	THR
5	L	675	GLU
5	L	690	GLU
5	L	706	ILE
5	L	710	ASP
5	L	720	MET
5	L	725	ILE
5	L	729	ASN
5	L	741	THR
5	L	759	ILE
5	L	760	THR
5	L	762	THR
5	L	769	LEU
5	L	775	GLN
5	L	788	LEU
5	L	814	LEU
5	L	831	GLN
5	L	845	LEU
5	L	847	LYS
5	L	862	ASN
5	L	868	VAL
5	L	872	THR
5	L	877	VAL
5	L	881	GLN
5	L	912	GLU
5	L	918	LEU
5	L	931	ILE
5	L	932	ARG
5	L	947	MET
5	L	950	LEU
5	L	960	LEU
5	L	962	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (108) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	132	HIS
1	A	160	HIS

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Mol	Chain	Res	Type
1	A	186	ASN
1	B	132	HIS
1	B	186	ASN
2	C	31	GLN
2	C	41	GLN
2	C	387	ASN
2	C	462	ASN
2	C	673	HIS
2	C	688	GLN
2	C	725	GLN
2	C	737	ASN
2	C	752	ASN
2	C	766	ASN
2	C	1023	HIS
2	C	1116	HIS
2	C	1264	GLN
3	D	80	HIS
3	D	113	HIS
3	D	419	HIS
3	D	469	HIS
3	D	477	GLN
3	D	606	ASN
3	D	680	ASN
3	D	929	GLN
3	D	1326	GLN
4	E	29	GLN
1	F	66	HIS
1	F	132	HIS
1	F	186	ASN
1	G	132	HIS
1	G	186	ASN
2	H	31	GLN
2	H	41	GLN
2	H	387	ASN
2	H	573	ASN
2	H	673	HIS
2	H	725	GLN
2	H	752	ASN
2	H	766	ASN
2	H	1023	HIS
2	H	1116	HIS
2	H	1264	GLN

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Mol	Chain	Res	Type
2	H	1268	GLN
3	I	113	HIS
3	I	200	GLN
3	I	419	HIS
3	I	469	HIS
3	I	519	ASN
3	I	545	HIS
3	I	606	ASN
3	I	680	ASN
3	I	875	ASN
3	I	929	GLN
3	I	1326	GLN
4	J	29	GLN
5	K	70	GLN
5	K	194	GLN
5	K	212	GLN
5	K	239	GLN
5	K	244	ASN
5	K	283	HIS
5	K	324	HIS
5	K	341	GLN
5	K	348	ASN
5	K	367	ASN
5	K	371	ASN
5	K	401	GLN
5	K	535	HIS
5	K	577	HIS
5	K	592	GLN
5	K	602	GLN
5	K	669	ASN
5	K	709	GLN
5	K	714	ASN
5	K	729	ASN
5	K	736	ASN
5	K	829	GLN
5	K	831	GLN
5	K	833	ASN
5	K	850	ASN
5	K	851	ASN
5	K	944	GLN
5	L	70	GLN
5	L	239	GLN

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Mol	Chain	Res	Type
5	L	244	ASN
5	L	283	HIS
5	L	324	HIS
5	L	341	GLN
5	L	348	ASN
5	L	367	ASN
5	L	371	ASN
5	L	380	GLN
5	L	434	HIS
5	L	535	HIS
5	L	592	GLN
5	L	602	GLN
5	L	652	ASN
5	L	669	ASN
5	L	714	ASN
5	L	729	ASN
5	L	736	ASN
5	L	831	GLN
5	L	833	ASN
5	L	850	ASN
5	L	851	ASN
5	L	944	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
7	N	8/9 (88%)	3 (37%)	0
7	P	8/9 (88%)	1 (12%)	0
All	All	16/18 (88%)	4 (25%)	0

All (4) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
7	N	2	U
7	N	6	C
7	N	7	U
7	P	7	U

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	227/329 (68%)	-0.51	0 100 100	178, 268, 367, 400	0
1	B	227/329 (68%)	-0.45	0 100 100	237, 380, 491, 539	0
1	F	227/329 (68%)	-0.62	0 100 100	192, 268, 357, 401	0
1	G	227/329 (68%)	-0.47	0 100 100	256, 379, 484, 537	0
2	C	1179/1342 (87%)	-0.58	3 (0%) 90 80	126, 241, 378, 510	0
2	H	1173/1342 (87%)	-0.60	2 (0%) 91 82	143, 251, 375, 532	0
3	D	1149/1416 (81%)	-0.53	1 (0%) 92 86	181, 301, 441, 641	0
3	I	1160/1416 (81%)	-0.59	1 (0%) 92 86	175, 282, 433, 662	0
4	E	75/90 (83%)	-0.40	0 100 100	285, 343, 385, 396	0
4	J	75/90 (83%)	-0.50	0 100 100	329, 349, 365, 376	0
5	K	961/974 (98%)	-0.46	9 (0%) 81 66	178, 278, 461, 664	0
5	L	961/974 (98%)	-0.45	9 (0%) 81 66	169, 269, 469, 638	0
6	M	15/15 (100%)	-0.21	0 100 100	321, 353, 461, 465	0
6	O	15/15 (100%)	-0.13	0 100 100	331, 351, 543, 550	0
7	N	9/9 (100%)	-0.69	0 100 100	258, 268, 381, 391	0
7	P	9/9 (100%)	-0.73	0 100 100	236, 245, 375, 395	0
All	All	7689/9008 (85%)	-0.53	25 (0%) 90 80	126, 279, 441, 664	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	K	578	MET	5.8
5	K	580	MET	4.2
5	L	72	GLU	3.9
5	K	408	MET	3.3
5	K	54	MET	3.1

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Mol	Chain	Res	Type	RSRZ
2	C	208	ILE	3.1
3	I	854	ALA	3.0
5	L	578	MET	2.8
5	L	71	VAL	2.7
3	D	1190	ILE	2.7
5	L	746	MET	2.7
5	K	467	MET	2.6
2	C	967	LEU	2.6
5	L	358	MET	2.6
2	C	209	ILE	2.5
5	L	579	VAL	2.3
5	K	72	GLU	2.3
5	K	720	MET	2.3
5	K	746	MET	2.2
2	H	179	TYR	2.2
5	K	60	THR	2.2
2	H	796	LEU	2.1
5	L	189	MET	2.1
5	L	54	MET	2.1
5	L	69	MET	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	ZN	D	1501	1/1	0.79	0.17	106,106,106,106	0
8	ZN	I	1501	1/1	0.79	0.13	131,131,131,131	0
9	MG	I	1503	1/1	0.93	0.12	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	ZN	I	1502	1/1	0.97	0.12	117,117,117,117	0
8	ZN	D	1502	1/1	0.98	0.20	84,84,84,84	0
9	MG	D	1503	1/1	0.99	0.17	10,10,10,10	0

6.5 Other polymers [i](#)

There are no such residues in this entry.