



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 06:04 PM UTC

PDB ID : 4RR3 / pdb_00004rr3
Title : Crystal structure of a recombinant EV71 virus particle
Authors : Chen, R.; Lyu, K.
Deposited on : 2014-11-06
Resolution : 3.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

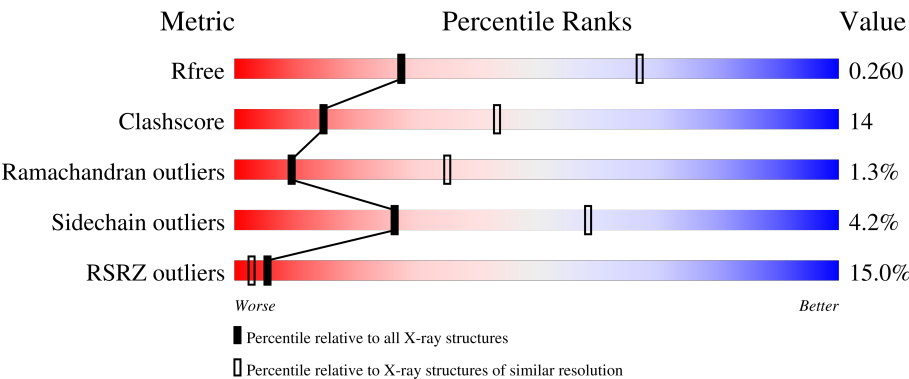
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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

Mol	Chain	Length	Quality of chain
1	A	303	13% 58% 14% • • 23%
1	E	303	12% 62% 12% • 23%
1	I	303	12% 57% 15% • • 23%
1	M	303	12% 59% 14% • 23%
1	Q	303	11% 57% 16% • • 23%

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Mol	Chain	Length	Quality of chain
2	B	242	11%63%29%5%
2	F	242	8%64%29%5%
2	J	242	11%67%24%5%
2	N	242	10%69%23%5%
2	R	242	11%66%24%5%5%
3	C	323	14%52%20%25%
3	G	323	12%53%20%25%
3	K	323	14%55%17%25%
3	O	323	14%52%20%25%
3	S	323	14%52%20%25%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 27390 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Capsid protein VP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	232	Total	C	N	O	S	0	0	0
			1844	1179	316	338	11			
1	Q	232	Total	C	N	O	S	0	0	0
			1844	1179	316	338	11			
1	I	232	Total	C	N	O	S	0	0	0
			1844	1179	316	338	11			
1	M	232	Total	C	N	O	S	0	0	0
			1844	1179	316	338	11			
1	A	232	Total	C	N	O	S	0	0	0
			1844	1179	316	338	11			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	101	GLU	-	expression tag	UNP F6KTB0
E	102	ARG	-	expression tag	UNP F6KTB0
E	103	LYS	-	expression tag	UNP F6KTB0
E	104	ARG	-	expression tag	UNP F6KTB0
E	105	ALA	-	expression tag	UNP F6KTB0
E	106	ARG	-	expression tag	UNP F6KTB0
E	107	LEU	-	expression tag	UNP F6KTB0
E	?	-	ASN	deletion	UNP F6KTB0
Q	101	GLU	-	expression tag	UNP F6KTB0
Q	102	ARG	-	expression tag	UNP F6KTB0
Q	103	LYS	-	expression tag	UNP F6KTB0
Q	104	ARG	-	expression tag	UNP F6KTB0
Q	105	ALA	-	expression tag	UNP F6KTB0
Q	106	ARG	-	expression tag	UNP F6KTB0
Q	107	LEU	-	expression tag	UNP F6KTB0
Q	?	-	ASN	deletion	UNP F6KTB0
I	101	GLU	-	expression tag	UNP F6KTB0
I	102	ARG	-	expression tag	UNP F6KTB0
I	103	LYS	-	expression tag	UNP F6KTB0

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Chain	Residue	Modelled	Actual	Comment	Reference
I	104	ARG	-	expression tag	UNP F6KTB0
I	105	ALA	-	expression tag	UNP F6KTB0
I	106	ARG	-	expression tag	UNP F6KTB0
I	107	LEU	-	expression tag	UNP F6KTB0
I	?	-	ASN	deletion	UNP F6KTB0
M	101	GLU	-	expression tag	UNP F6KTB0
M	102	ARG	-	expression tag	UNP F6KTB0
M	103	LYS	-	expression tag	UNP F6KTB0
M	104	ARG	-	expression tag	UNP F6KTB0
M	105	ALA	-	expression tag	UNP F6KTB0
M	106	ARG	-	expression tag	UNP F6KTB0
M	107	LEU	-	expression tag	UNP F6KTB0
M	?	-	ASN	deletion	UNP F6KTB0
A	101	GLU	-	expression tag	UNP F6KTB0
A	102	ARG	-	expression tag	UNP F6KTB0
A	103	LYS	-	expression tag	UNP F6KTB0
A	104	ARG	-	expression tag	UNP F6KTB0
A	105	ALA	-	expression tag	UNP F6KTB0
A	106	ARG	-	expression tag	UNP F6KTB0
A	107	LEU	-	expression tag	UNP F6KTB0
A	?	-	ASN	deletion	UNP F6KTB0

- Molecule 2 is a protein called Capsid protein VP3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	230	Total	C	N	O	S	0	0	0
			1762	1133	291	327	11			
2	R	230	Total	C	N	O	S	0	0	0
			1762	1133	291	327	11			
2	J	230	Total	C	N	O	S	0	0	0
			1762	1133	291	327	11			
2	N	230	Total	C	N	O	S	0	0	0
			1762	1133	291	327	11			
2	B	230	Total	C	N	O	S	0	0	0
			1762	1133	291	327	11			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	227	GLN	LYS	engineered mutation	UNP F6KTB0
R	227	GLN	LYS	engineered mutation	UNP F6KTB0
J	227	GLN	LYS	engineered mutation	UNP F6KTB0

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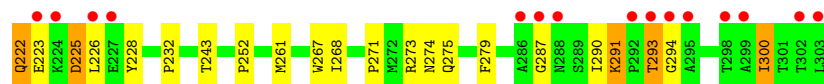
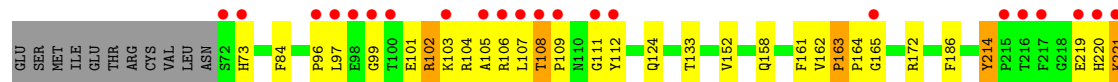
Chain	Residue	Modelled	Actual	Comment	Reference
N	227	GLN	LYS	engineered mutation	UNP F6KTB0
B	227	GLN	LYS	engineered mutation	UNP F6KTB0

- Molecule 3 is a protein called Capsid protein VP0.

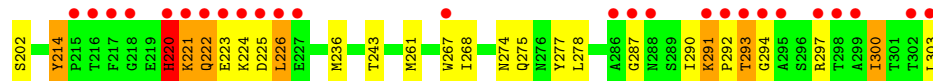
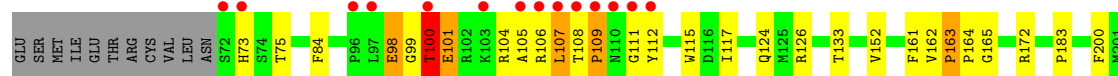
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	242	Total 1872	C 1201	N 310	O 353	S 8	0	0	0
3	S	242	Total 1872	C 1201	N 310	O 353	S 8	0	0	0
3	K	242	Total 1872	C 1201	N 310	O 353	S 8	0	0	0
3	O	242	Total 1872	C 1201	N 310	O 353	S 8	0	0	0
3	C	242	Total 1872	C 1201	N 310	O 353	S 8	0	0	0



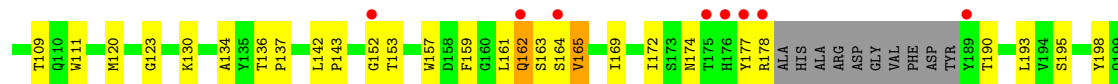
• Molecule 1: Capsid protein VP1



• Molecule 1: Capsid protein VP1

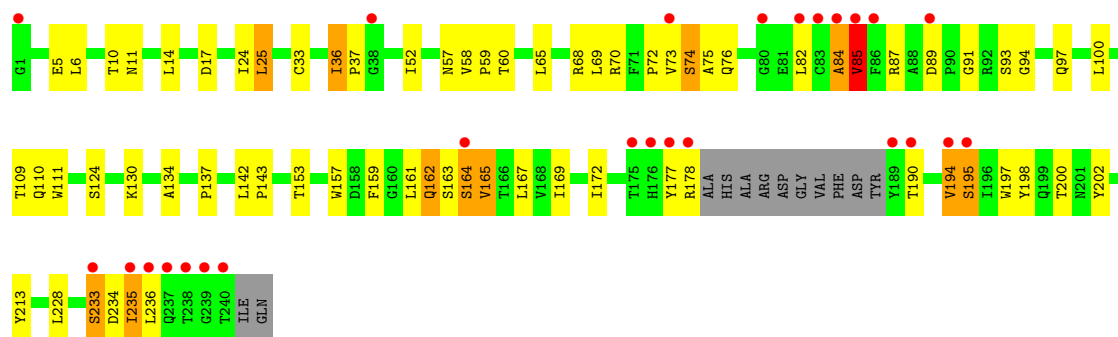


• Molecule 2: Capsid protein VP3

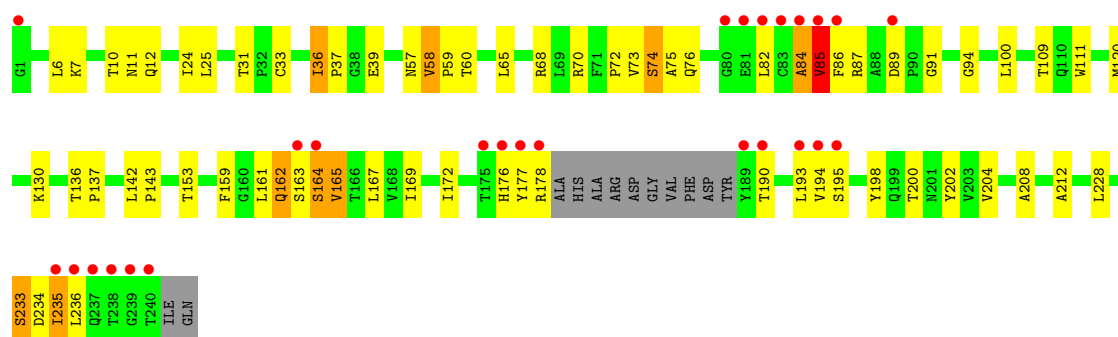


• Molecule 2: Capsid protein VP3

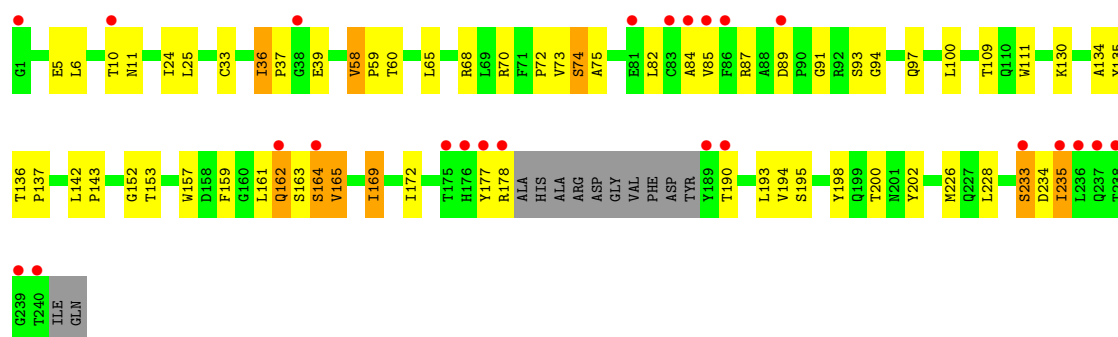




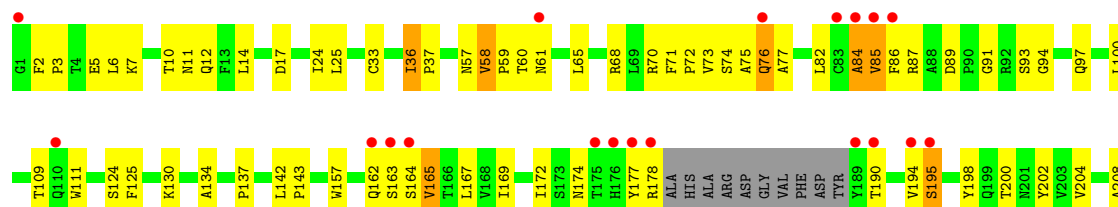
• Molecule 2: Capsid protein VP3

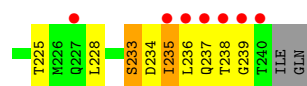


• Molecule 2: Capsid protein VP3

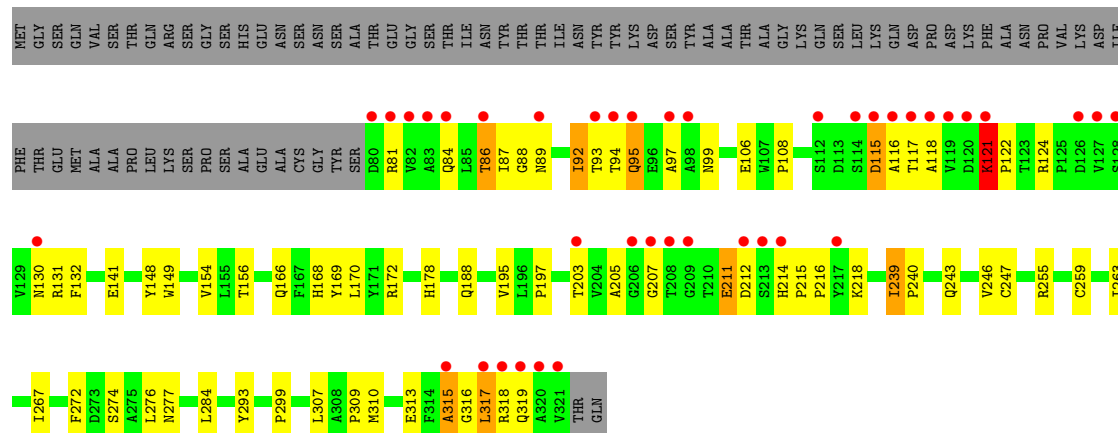


• Molecule 2: Capsid protein VP3

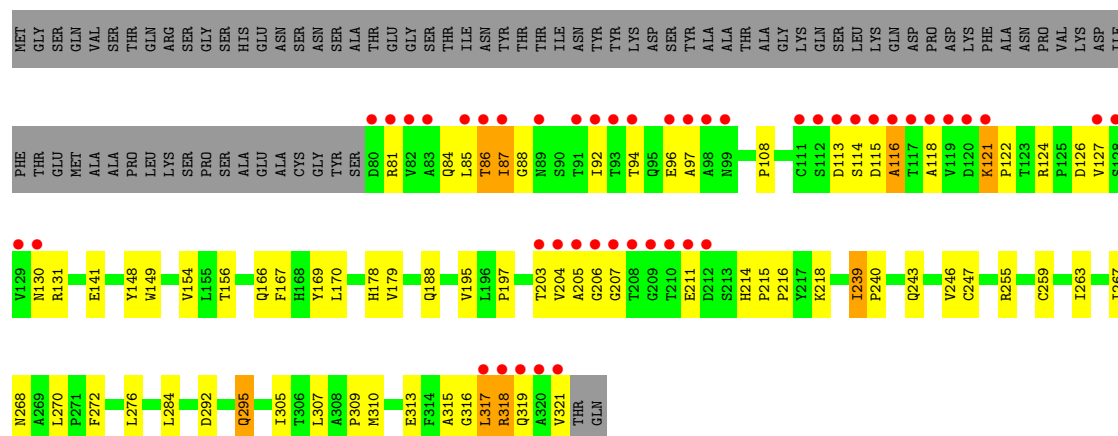




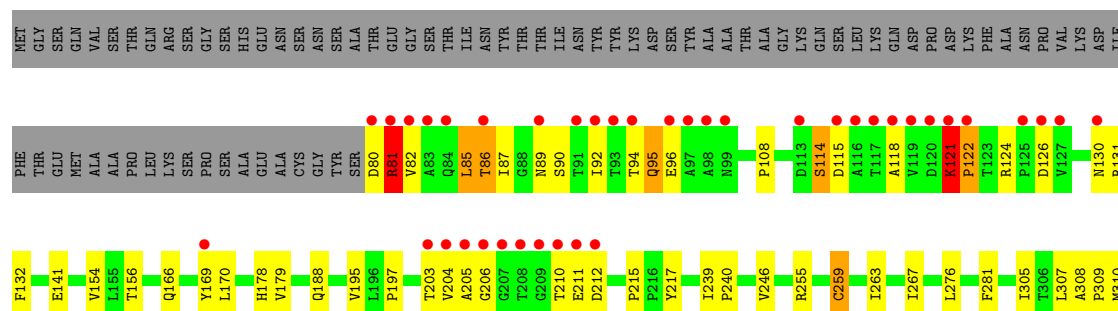
• Molecule 3: Capsid protein VP0



• Molecule 3: Capsid protein VP0

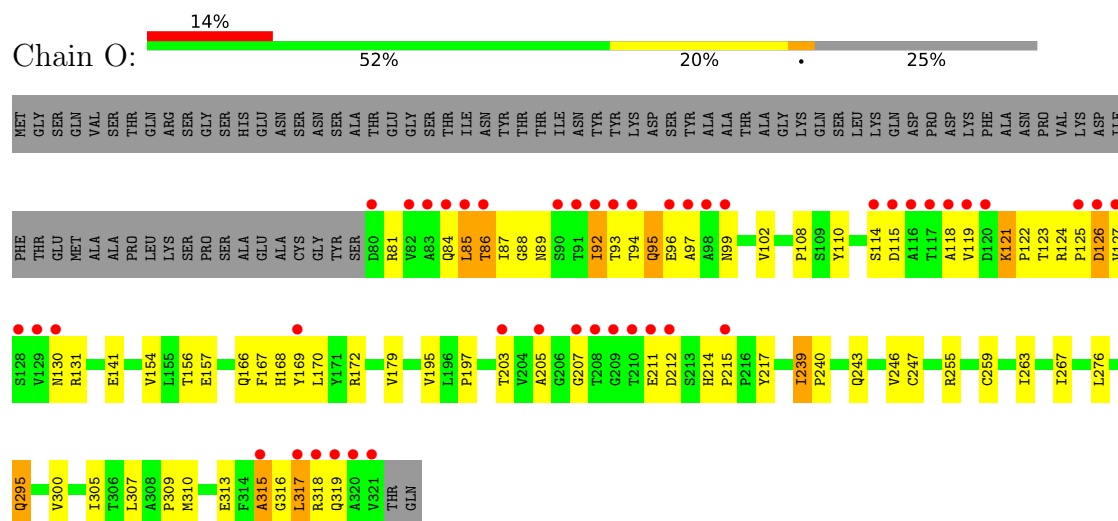


• Molecule 3: Capsid protein VP0

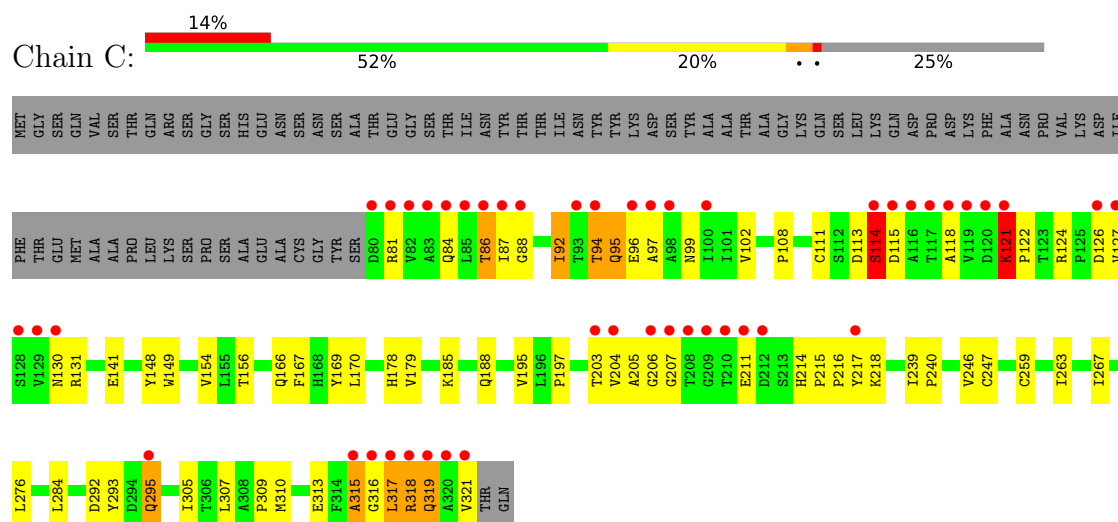




- Molecule 3: Capsid protein VP0



- Molecule 3: Capsid protein VP0



4 Data and refinement statistics

Property	Value	Source
Space group	P 4 ₂ 3 2	Depositor
Cell constants a, b, c, α , β , γ	350.60Å 350.60Å 350.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.44 – 3.10 46.44 – 3.10	Depositor EDS
% Data completeness (in resolution range)	(Not available) (46.44-3.10) 90.5 (46.44-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.66 (at 3.12Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.235 , 0.265 0.235 , 0.260	Depositor DCC
R_{free} test set	2000 reflections (1.52%)	wwPDB-VP
Wilson B-factor (Å ²)	59.5	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 29.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	27390	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.18% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.47	0/1899	1.05	15/2584 (0.6%)
1	E	0.53	3/1899 (0.2%)	0.95	3/2584 (0.1%)
1	I	0.45	0/1899	1.01	11/2584 (0.4%)
1	M	0.43	0/1899	0.95	9/2584 (0.3%)
1	Q	0.49	0/1899	0.98	14/2584 (0.5%)
2	B	0.45	0/1810	0.96	14/2477 (0.6%)
2	F	0.40	0/1810	0.90	5/2477 (0.2%)
2	J	0.45	0/1810	0.96	13/2477 (0.5%)
2	N	0.39	0/1810	0.89	9/2477 (0.4%)
2	R	0.45	1/1810 (0.1%)	0.95	13/2477 (0.5%)
3	C	0.46	0/1927	0.89	4/2644 (0.2%)
3	G	0.38	0/1927	0.87	2/2644 (0.1%)
3	K	0.41	0/1927	0.89	4/2644 (0.2%)
3	O	0.40	0/1927	0.89	3/2644 (0.1%)
3	S	0.42	1/1927 (0.1%)	0.87	2/2644 (0.1%)
All	All	0.44	5/28180 (0.0%)	0.94	121/38525 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	I	0	1
1	Q	0	2
3	C	0	2
3	G	0	2
3	K	0	2
3	O	0	1
All	All	0	10

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	220	HIS	ND1-CE1	-8.79	1.23	1.32
1	E	220	HIS	CE1-NE2	8.13	1.40	1.32
1	E	220	HIS	CG-ND1	6.54	1.45	1.38
2	R	194	VAL	CA-C	5.47	1.59	1.52
3	S	178	HIS	CD2-NE2	5.40	1.43	1.37

All (121) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	214	TYR	CA-C-N	10.00	130.15	119.05
1	I	214	TYR	C-N-CA	10.00	130.15	119.05
2	B	85	VAL	N-CA-C	9.41	121.91	108.17
1	A	101	GLU	N-CA-C	9.38	123.12	109.14
2	R	85	VAL	N-CA-C	8.43	120.47	108.17
2	B	84	ALA	CA-C-N	-8.40	110.56	122.75
2	B	84	ALA	C-N-CA	-8.40	110.56	122.75
2	J	85	VAL	N-CA-C	8.35	122.34	108.81
3	C	92	ILE	N-CA-C	8.12	119.06	108.35
1	I	108	THR	CA-C-N	7.72	129.49	119.84
1	I	108	THR	C-N-CA	7.72	129.49	119.84
1	E	214	TYR	CA-C-N	7.67	126.95	118.97
1	E	214	TYR	C-N-CA	7.67	126.95	118.97
2	J	84	ALA	CA-C-N	-7.57	111.38	122.58
2	J	84	ALA	C-N-CA	-7.57	111.38	122.58
3	O	92	ILE	N-CA-C	7.52	118.27	108.35
3	K	114	SER	N-CA-C	7.35	121.36	110.48
3	G	92	ILE	N-CA-C	7.26	117.93	108.35
1	A	221	LYS	CA-C-N	7.02	131.15	119.35
1	A	221	LYS	C-N-CA	7.02	131.15	119.35
1	A	214	TYR	CA-C-N	6.97	126.78	119.05
1	A	214	TYR	C-N-CA	6.97	126.78	119.05
1	M	214	TYR	CA-C-N	6.96	126.21	118.97
1	M	214	TYR	C-N-CA	6.96	126.21	118.97
1	Q	100	THR	N-CA-C	6.91	119.98	109.62
2	R	195	SER	N-CA-C	6.89	120.23	110.23
1	M	225	ASP	CA-C-N	-6.81	112.81	122.41
1	M	225	ASP	C-N-CA	-6.81	112.81	122.41
2	F	233	SER	N-CA-C	6.79	119.08	108.96
3	S	116	ALA	N-CA-C	6.78	118.56	111.03
1	I	223	GLU	N-CA-C	6.76	121.17	110.70
2	R	233	SER	N-CA-C	6.74	118.04	108.74
1	A	222	GLN	N-CA-C	-6.57	104.01	113.21
1	Q	214	TYR	CA-C-N	6.51	126.28	119.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	214	TYR	C-N-CA	6.51	126.28	119.05
2	J	233	SER	N-CA-C	6.37	117.53	108.74
1	A	221	LYS	N-CA-C	6.36	119.19	107.99
1	Q	225	ASP	N-CA-C	6.31	118.71	107.80
3	G	97	ALA	N-CA-C	6.29	119.08	111.40
2	N	169	ILE	CA-C-N	6.26	125.75	119.24
2	N	169	ILE	C-N-CA	6.26	125.75	119.24
2	B	84	ALA	N-CA-C	-6.25	102.43	110.19
2	R	169	ILE	CA-C-N	6.25	125.74	119.24
2	R	169	ILE	C-N-CA	6.25	125.74	119.24
2	J	58	VAL	CA-C-N	-6.24	112.64	120.51
2	J	58	VAL	C-N-CA	-6.24	112.64	120.51
1	A	220	HIS	CA-C-N	-6.22	113.27	122.41
1	A	220	HIS	C-N-CA	-6.22	113.27	122.41
2	B	233	SER	N-CA-C	6.16	117.25	108.74
2	N	58	VAL	CA-C-N	-6.06	112.87	120.51
2	N	58	VAL	C-N-CA	-6.06	112.87	120.51
1	A	100	THR	N-CA-C	6.06	123.70	110.80
1	I	104	ARG	NE-CZ-NH1	-6.04	115.46	121.50
1	Q	108	THR	N-CA-C	6.01	123.09	109.81
2	J	169	ILE	CA-C-N	6.00	125.48	119.24
2	J	169	ILE	C-N-CA	6.00	125.48	119.24
3	K	85	LEU	N-CA-C	-5.94	105.28	113.18
1	M	108	THR	CA-C-N	5.93	127.26	119.84
1	M	108	THR	C-N-CA	5.93	127.26	119.84
2	F	36	ILE	CA-C-N	5.92	126.07	119.32
2	F	36	ILE	C-N-CA	5.92	126.07	119.32
1	E	220	HIS	CG-CD2-NE2	5.91	113.11	107.20
3	C	114	SER	N-CA-C	5.88	118.48	110.55
2	B	94	GLY	CA-C-N	5.88	126.02	119.32
2	B	94	GLY	C-N-CA	5.88	126.02	119.32
1	Q	106	ARG	NE-CZ-NH2	5.86	124.47	119.20
2	R	94	GLY	CA-C-N	5.85	125.99	119.32
2	R	94	GLY	C-N-CA	5.85	125.99	119.32
2	N	233	SER	N-CA-C	5.84	116.81	108.74
1	A	108	THR	CA-C-N	5.83	127.13	119.84
1	A	108	THR	C-N-CA	5.83	127.13	119.84
2	R	84	ALA	CA-C-N	-5.82	114.31	122.75
2	R	84	ALA	C-N-CA	-5.82	114.31	122.75
1	Q	106	ARG	NE-CZ-NH1	-5.72	115.78	121.50
1	M	162	VAL	CA-C-N	5.71	123.83	119.66
1	M	162	VAL	C-N-CA	5.71	123.83	119.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	94	GLY	CA-C-N	5.68	125.80	119.32
2	N	94	GLY	C-N-CA	5.68	125.80	119.32
3	K	81	ARG	N-CA-C	5.59	117.62	108.52
2	N	36	ILE	CA-C-N	5.54	125.64	119.32
2	N	36	ILE	C-N-CA	5.54	125.64	119.32
2	R	36	ILE	CA-C-N	5.53	125.63	119.32
2	R	36	ILE	C-N-CA	5.53	125.63	119.32
2	B	36	ILE	CA-C-N	5.53	125.62	119.32
2	B	36	ILE	C-N-CA	5.53	125.62	119.32
1	I	223	GLU	CA-C-N	-5.53	114.40	122.86
1	I	223	GLU	C-N-CA	-5.53	114.40	122.86
3	C	113	ASP	N-CA-CB	-5.53	101.88	110.39
2	J	195	SER	N-CA-C	5.49	118.24	110.50
2	J	36	ILE	CA-C-N	5.47	125.55	119.32
2	J	36	ILE	C-N-CA	5.47	125.55	119.32
3	O	110	TYR	N-CA-C	-5.45	103.43	110.19
1	A	162	VAL	CA-C-N	5.43	123.62	119.66
1	A	162	VAL	C-N-CA	5.43	123.62	119.66
1	Q	108	THR	CA-C-N	5.43	126.62	119.84
1	Q	108	THR	C-N-CA	5.43	126.62	119.84
1	I	223	GLU	CB-CA-C	-5.42	103.68	111.91
1	A	163	PRO	O-C-N	5.41	123.80	121.31
3	C	318	ARG	CB-CG-CD	-5.41	98.86	111.30
2	J	94	GLY	CA-C-N	5.38	125.45	119.32
2	J	94	GLY	C-N-CA	5.38	125.45	119.32
2	F	169	ILE	CA-C-N	5.32	124.77	119.24
2	F	169	ILE	C-N-CA	5.32	124.77	119.24
2	R	25	LEU	CA-C-N	5.32	124.95	119.05
2	R	25	LEU	C-N-CA	5.32	124.95	119.05
2	B	195	SER	N-CA-C	5.26	118.27	110.48
1	Q	226	LEU	N-CA-C	5.25	121.97	110.80
3	K	122	PRO	N-CA-C	5.24	119.44	111.11
1	Q	219	GLU	N-CA-CB	-5.18	101.73	110.49
2	B	169	ILE	CA-C-N	5.18	124.63	119.24
2	B	169	ILE	C-N-CA	5.18	124.63	119.24
1	Q	218	GLY	CA-C-N	5.17	131.42	121.54
1	Q	218	GLY	C-N-CA	5.17	131.42	121.54
1	M	163	PRO	O-C-N	5.15	123.68	121.31
1	I	163	PRO	O-C-N	5.14	123.67	121.31
3	O	295	GLN	CA-CB-CG	-5.12	103.87	114.10
1	I	218	GLY	N-CA-C	-5.11	101.08	113.18
2	B	58	VAL	CA-C-N	-5.10	114.08	120.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	58	VAL	C-N-CA	-5.10	114.08	120.51
1	Q	163	PRO	O-C-N	5.07	123.64	121.31
3	S	116	ALA	CA-C-O	-5.03	115.72	120.90

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	121	LYS	Peptide
3	C	95	GLN	Peptide
3	G	121	LYS	Peptide
3	G	95	GLN	Peptide
1	I	219	GLU	Peptide
3	K	121	LYS	Peptide
3	K	95	GLN	Peptide
3	O	95	GLN	Peptide
1	Q	225	ASP	Peptide
1	Q	226	LEU	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1844	0	1803	61	0
1	E	1844	0	1803	47	0
1	I	1844	0	1803	56	0
1	M	1844	0	1803	69	0
1	Q	1844	0	1803	69	0
2	B	1762	0	1746	70	0
2	F	1762	0	1746	70	0
2	J	1762	0	1746	65	0
2	N	1762	0	1746	59	0
2	R	1762	0	1746	65	0
3	C	1872	0	1811	59	0
3	G	1872	0	1811	55	0
3	K	1872	0	1811	47	0
3	O	1872	0	1811	65	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	S	1872	0	1811	67	0
All	All	27390	0	26800	752	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 14.

All (752) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:98:GLU:HA	1:I:104:ARG:HH12	1.19	1.04
2:R:85:VAL:HG21	2:R:195:SER:HA	1.40	1.02
3:C:295:GLN:HE21	3:C:295:GLN:HA	1.19	1.00
1:M:105:ALA:HA	1:M:108:THR:HA	1.44	0.99
1:I:105:ALA:HA	1:I:108:THR:HA	1.43	0.98
3:G:95:GLN:HG3	3:G:99:ASN:HA	1.47	0.97
2:F:137:PRO:HG3	3:S:317:LEU:HB3	1.51	0.92
3:S:295:GLN:HE21	3:S:295:GLN:HA	1.35	0.92
2:J:137:PRO:HG3	3:O:317:LEU:HB3	1.51	0.91
1:M:291:LYS:H	1:M:291:LYS:HD2	1.35	0.90
1:M:226:LEU:HB3	3:O:214:HIS:HB2	1.53	0.89
1:Q:105:ALA:HA	1:Q:109:PRO:HD2	1.56	0.88
1:I:300:ILE:HA	2:J:84:ALA:H	1.40	0.86
3:K:86:THR:OG1	3:K:87:ILE:N	2.02	0.86
3:C:111:CYS:SG	3:C:114:SER:OG	2.36	0.82
1:Q:300:ILE:HA	2:R:84:ALA:H	1.44	0.82
3:G:317:LEU:HB3	2:B:137:PRO:HG3	1.60	0.82
3:S:263:ILE:HG23	3:S:310:MET:HE1	1.61	0.81
3:O:263:ILE:HG23	3:O:310:MET:HE1	1.64	0.80
3:C:95:GLN:HB2	3:C:99:ASN:HA	1.63	0.80
1:I:98:GLU:HA	1:I:104:ARG:NH1	1.97	0.80
3:G:81:ARG:NH1	3:G:94:THR:O	2.17	0.78
3:K:263:ILE:HG23	3:K:310:MET:HE1	1.64	0.77
3:O:86:THR:OG1	3:O:87:ILE:N	2.15	0.77
3:O:203:THR:HG23	3:O:215:PRO:HG3	1.67	0.77
3:C:263:ILE:HG23	3:C:310:MET:HE1	1.65	0.77
1:E:107:LEU:C	1:E:109:PRO:HD3	2.09	0.77
3:O:81:ARG:NH1	3:O:94:THR:O	2.16	0.77
3:C:84:GLN:NE2	3:C:86:THR:O	2.19	0.76
3:G:170:LEU:HB2	3:G:315:ALA:HB3	1.66	0.76
3:S:170:LEU:HB2	3:S:315:ALA:HB3	1.67	0.76
1:I:110:ASN:H	1:I:110:ASN:HD22	1.32	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:GLY:HA3	2:B:68:ARG:HH12	1.50	0.75
3:O:84:GLN:OE1	3:O:86:THR:N	2.19	0.75
1:M:107:LEU:C	1:M:109:PRO:HD3	2.12	0.75
3:K:130:ASN:HA	3:K:309:PRO:HG2	1.67	0.75
1:I:110:ASN:H	1:I:110:ASN:ND2	1.84	0.75
1:A:107:LEU:C	1:A:109:PRO:HD3	2.12	0.75
3:S:81:ARG:NH1	3:S:94:THR:O	2.20	0.74
3:S:84:GLN:OE1	3:S:86:THR:N	2.18	0.74
1:I:294:GLY:HA3	2:J:68:ARG:HH12	1.54	0.73
3:G:203:THR:HG23	3:G:215:PRO:HG3	1.70	0.73
3:C:170:LEU:HB2	3:C:315:ALA:HB3	1.71	0.73
2:R:109:THR:HB	2:R:228:LEU:HB3	1.70	0.73
2:J:85:VAL:HG11	2:J:194:VAL:H	1.52	0.73
1:M:223:GLU:HG3	1:M:225:ASP:O	1.88	0.73
3:O:95:GLN:HB2	3:O:99:ASN:HA	1.71	0.73
2:B:85:VAL:HG21	2:B:194:VAL:O	1.88	0.72
2:R:137:PRO:HG3	3:K:317:LEU:HB3	1.72	0.72
3:C:295:GLN:HA	3:C:295:GLN:NE2	2.00	0.72
2:R:74:SER:OG	2:R:76:GLN:OE1	2.07	0.72
2:B:76:GLN:HG3	2:B:77:ALA:N	2.05	0.71
3:G:130:ASN:HA	3:G:309:PRO:HG2	1.72	0.71
3:C:169:TYR:H	3:C:316:GLY:HA3	1.55	0.71
3:G:86:THR:OG1	3:G:87:ILE:N	2.16	0.71
2:J:109:THR:HB	2:J:228:LEU:HB3	1.73	0.71
2:F:109:THR:HB	2:F:228:LEU:HB3	1.72	0.70
1:Q:294:GLY:HA3	2:R:68:ARG:HH12	1.53	0.70
1:I:97:LEU:O	1:I:104:ARG:NH1	2.23	0.70
3:S:203:THR:HG23	3:S:215:PRO:HG3	1.73	0.70
3:G:263:ILE:HG23	3:G:310:MET:HE1	1.73	0.69
3:O:170:LEU:HB2	3:O:315:ALA:HB3	1.74	0.69
2:N:109:THR:HB	2:N:228:LEU:HB3	1.74	0.69
2:N:177:TYR:OH	2:N:190:THR:O	2.09	0.69
1:M:109:PRO:HB2	1:M:112:TYR:H	1.55	0.69
2:R:177:TYR:OH	2:R:190:THR:O	2.10	0.69
3:K:108:PRO:HG2	3:K:310:MET:HE3	1.75	0.69
3:O:121:LYS:HB3	3:O:122:PRO:CD	2.23	0.69
3:G:108:PRO:HG2	3:G:310:MET:HE3	1.76	0.68
3:O:108:PRO:HG2	3:O:310:MET:HE3	1.76	0.68
1:I:223:GLU:HG2	3:K:217:TYR:CE1	2.29	0.68
1:M:109:PRO:HB3	1:M:112:TYR:O	1.94	0.68
1:A:300:ILE:HA	2:B:84:ALA:H	1.59	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:170:LEU:HB2	3:K:315:ALA:HB3	1.74	0.68
3:K:166:GLN:HA	3:K:276:LEU:HD11	1.76	0.68
1:I:275:GLN:NE2	1:I:290:ILE:O	2.25	0.67
2:B:109:THR:HB	2:B:228:LEU:HB3	1.75	0.67
3:S:86:THR:OG1	3:S:87:ILE:N	2.14	0.67
3:C:86:THR:HG23	3:C:88:GLY:H	1.59	0.67
1:Q:99:GLY:O	1:Q:104:ARG:NH2	2.26	0.67
2:F:177:TYR:OH	2:F:190:THR:O	2.12	0.67
1:M:101:GLU:O	1:M:102:ARG:NE	2.28	0.66
1:Q:293:THR:O	2:R:68:ARG:NH2	2.27	0.66
1:Q:106:ARG:HG2	1:Q:107:LEU:HD22	1.77	0.66
3:C:108:PRO:HG2	3:C:310:MET:HE3	1.76	0.66
1:E:105:ALA:C	1:E:109:PRO:HD2	2.20	0.66
2:F:234:ASP:OD1	2:F:235:ILE:N	2.29	0.66
3:S:130:ASN:HA	3:S:309:PRO:HG2	1.77	0.66
1:M:105:ALA:CA	1:M:108:THR:HA	2.24	0.66
1:Q:275:GLN:NE2	1:Q:290:ILE:O	2.26	0.66
3:G:166:GLN:HA	3:G:276:LEU:HD11	1.76	0.66
1:M:105:ALA:C	1:M:109:PRO:HD2	2.20	0.66
3:S:169:TYR:H	3:S:316:GLY:HA3	1.61	0.66
1:Q:107:LEU:C	1:Q:109:PRO:HD3	2.21	0.66
3:S:318:ARG:O	3:S:319:GLN:HG2	1.95	0.66
2:J:59:PRO:HD2	2:J:68:ARG:HD2	1.78	0.66
3:G:95:GLN:CG	3:G:99:ASN:HA	2.25	0.66
1:A:105:ALA:C	1:A:109:PRO:HD2	2.21	0.66
1:I:107:LEU:C	1:I:109:PRO:HD3	2.21	0.65
3:O:169:TYR:H	3:O:316:GLY:HA3	1.61	0.65
3:G:86:THR:HG23	3:G:88:GLY:H	1.59	0.65
2:N:6:LEU:H	2:B:10:THR:HB	1.61	0.65
3:S:166:GLN:HA	3:S:276:LEU:HD11	1.78	0.65
3:K:169:TYR:H	3:K:316:GLY:HA3	1.61	0.65
3:K:318:ARG:O	3:K:319:GLN:HG2	1.96	0.65
2:J:85:VAL:HG21	2:J:194:VAL:O	1.95	0.65
2:B:37:PRO:HG2	3:C:267:ILE:HG12	1.79	0.65
3:S:108:PRO:HG2	3:S:310:MET:HE3	1.79	0.65
3:S:188:GLN:HE21	3:S:292:ASP:HB3	1.61	0.65
3:C:86:THR:HG21	3:C:131:ARG:HB2	1.79	0.65
1:M:275:GLN:NE2	1:M:290:ILE:O	2.30	0.65
3:O:86:THR:HG21	3:O:131:ARG:HB2	1.76	0.64
3:O:84:GLN:OE1	3:O:85:LEU:N	2.31	0.64
3:C:203:THR:HG23	3:C:215:PRO:HG3	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:293:THR:O	2:F:68:ARG:NH2	2.27	0.64
1:E:294:GLY:HA3	2:F:68:ARG:HH12	1.62	0.64
1:Q:103:LYS:HB3	1:Q:105:ALA:HB3	1.78	0.64
2:R:59:PRO:HD2	2:R:68:ARG:HD2	1.78	0.64
1:M:97:LEU:O	1:M:104:ARG:NH1	2.31	0.64
2:J:73:VAL:HG23	2:J:74:SER:H	1.63	0.64
2:N:73:VAL:HG23	2:N:74:SER:H	1.62	0.64
1:A:105:ALA:HA	1:A:109:PRO:HD2	1.80	0.64
3:O:166:GLN:HA	3:O:276:LEU:HD11	1.79	0.64
3:K:203:THR:HG23	3:K:215:PRO:HG3	1.79	0.63
3:O:130:ASN:HA	3:O:309:PRO:HG2	1.80	0.63
1:A:109:PRO:HB3	1:A:112:TYR:O	1.99	0.63
2:N:234:ASP:OD1	2:N:235:ILE:N	2.31	0.63
3:C:166:GLN:HA	3:C:276:LEU:HD11	1.80	0.63
1:I:294:GLY:HA2	2:J:57:ASN:HB2	1.80	0.63
3:S:86:THR:HG23	3:S:88:GLY:H	1.62	0.63
1:A:100:THR:O	1:A:100:THR:OG1	2.05	0.63
2:N:135:TYR:O	3:C:318:ARG:NH2	2.31	0.63
2:B:234:ASP:OD1	2:B:235:ILE:N	2.31	0.63
3:C:118:ALA:HB3	3:C:121:LYS:HG2	1.80	0.63
2:R:37:PRO:HG2	3:S:267:ILE:HG12	1.78	0.63
2:R:85:VAL:CG2	2:R:195:SER:HA	2.23	0.63
3:K:179:VAL:HG22	3:K:305:ILE:HG12	1.79	0.63
1:Q:94:ASP:HB3	1:Q:106:ARG:HB3	1.81	0.62
2:N:136:THR:HB	2:N:193:LEU:HB2	1.81	0.62
3:K:85:LEU:HB3	3:K:86:THR:HG22	1.81	0.62
3:S:124:ARG:HG2	3:S:313:GLU:HG3	1.81	0.62
1:E:99:GLY:O	1:E:104:ARG:NH2	2.32	0.62
3:G:318:ARG:O	3:G:319:GLN:HG2	1.99	0.62
1:Q:219:GLU:HB3	1:Q:222:GLN:HB3	1.81	0.62
1:I:105:ALA:C	1:I:109:PRO:HD2	2.24	0.62
3:C:86:THR:OG1	3:C:87:ILE:N	2.19	0.62
2:F:73:VAL:HG23	2:F:74:SER:H	1.63	0.62
3:G:86:THR:HG21	3:G:131:ARG:HB2	1.82	0.62
2:R:73:VAL:HG23	2:R:74:SER:H	1.65	0.62
2:F:152:GLY:HA2	3:S:318:ARG:HD2	1.81	0.62
1:M:293:THR:O	2:N:68:ARG:NH2	2.26	0.62
2:F:37:PRO:HG2	3:G:267:ILE:HG12	1.82	0.62
1:M:109:PRO:HB3	1:M:112:TYR:C	2.25	0.61
2:J:85:VAL:HG11	2:J:194:VAL:N	2.14	0.61
2:N:137:PRO:HG3	3:C:317:LEU:HB3	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:73:VAL:HG23	2:B:74:SER:H	1.64	0.61
3:S:113:ASP:OD1	3:S:114:SER:N	2.29	0.61
1:Q:109:PRO:HB3	1:Q:112:TYR:O	2.00	0.61
3:O:121:LYS:HB3	3:O:122:PRO:HD3	1.83	0.61
1:E:287:GLY:HA3	3:G:207:GLY:HA2	1.83	0.61
1:A:109:PRO:HB3	1:A:112:TYR:C	2.26	0.61
1:A:293:THR:O	2:B:68:ARG:NH2	2.31	0.61
2:R:75:ALA:HA	2:R:202:TYR:HB3	1.83	0.61
3:S:84:GLN:OE1	3:S:85:LEU:N	2.33	0.61
3:S:121:LYS:HB2	3:S:122:PRO:HD3	1.82	0.61
3:S:295:GLN:HA	3:S:295:GLN:NE2	2.14	0.61
3:G:84:GLN:NE2	3:G:89:ASN:HB2	2.16	0.61
1:Q:297:ARG:HH22	1:Q:303:LEU:HD12	1.64	0.61
2:R:85:VAL:HG21	2:R:195:SER:CA	2.23	0.61
2:R:234:ASP:OD1	2:R:235:ILE:N	2.31	0.61
2:J:91:GLY:HA3	2:J:111:TRP:CZ2	2.36	0.60
3:C:169:TYR:HB3	3:C:316:GLY:HA2	1.83	0.60
1:I:109:PRO:HB2	1:I:112:TYR:H	1.67	0.60
2:N:136:THR:N	2:N:193:LEU:O	2.27	0.60
2:N:142:LEU:HD12	2:N:143:PRO:HD2	1.82	0.60
3:O:168:HIS:C	3:O:319:GLN:HE21	2.10	0.60
1:E:297:ARG:HH22	1:E:303:LEU:HD12	1.67	0.60
2:J:142:LEU:HD12	2:J:143:PRO:HD2	1.84	0.60
1:M:223:GLU:HB2	3:O:217:TYR:CE1	2.36	0.60
2:N:59:PRO:HD2	2:N:68:ARG:HD2	1.84	0.60
3:S:118:ALA:O	3:S:121:LYS:HB3	2.02	0.60
2:F:59:PRO:HD2	2:F:68:ARG:HD2	1.83	0.60
1:M:102:ARG:NH2	1:M:104:ARG:HH21	1.99	0.60
3:O:118:ALA:O	3:O:121:LYS:HB2	2.02	0.60
1:E:165:GLY:HA2	2:B:178:ARG:HB3	1.83	0.59
1:E:109:PRO:HB2	1:E:112:TYR:H	1.67	0.59
3:G:169:TYR:H	3:G:316:GLY:HA3	1.67	0.59
1:Q:105:ALA:HA	1:Q:108:THR:HA	1.83	0.59
1:Q:109:PRO:HB2	1:Q:112:TYR:H	1.66	0.59
1:M:214:TYR:HE2	1:M:228:TYR:HB2	1.67	0.59
2:B:142:LEU:HD12	2:B:143:PRO:HD2	1.85	0.59
2:F:10:THR:HB	2:B:6:LEU:H	1.67	0.59
2:F:130:LYS:HB2	2:F:200:THR:HG23	1.84	0.59
2:J:163:SER:C	2:J:165:VAL:H	2.11	0.59
3:O:118:ALA:H	3:O:121:LYS:HE2	1.68	0.59
2:F:91:GLY:HA3	2:F:111:TRP:CZ2	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:105:ALA:CA	1:Q:109:PRO:HD2	2.28	0.58
2:B:237:GLN:NE2	2:B:238:THR:O	2.36	0.58
3:S:169:TYR:HB3	3:S:316:GLY:HA2	1.85	0.58
1:Q:219:GLU:HB3	1:Q:222:GLN:CB	2.33	0.58
2:N:152:GLY:HA3	3:C:318:ARG:HD3	1.85	0.58
2:B:72:PRO:O	2:B:82:LEU:HD11	2.03	0.58
3:S:86:THR:HG21	3:S:131:ARG:HB2	1.84	0.58
3:C:124:ARG:HG2	3:C:313:GLU:HG3	1.85	0.58
2:F:72:PRO:O	2:F:82:LEU:HD11	2.04	0.58
2:R:73:VAL:O	2:R:74:SER:HB3	2.02	0.58
2:F:142:LEU:HD12	2:F:143:PRO:HD2	1.86	0.58
1:I:293:THR:O	2:J:68:ARG:NH2	2.32	0.58
1:M:97:LEU:HD11	1:M:252:PRO:HD3	1.86	0.58
3:O:84:GLN:HE21	3:O:89:ASN:HB2	1.68	0.58
2:R:85:VAL:HG11	2:R:194:VAL:C	2.29	0.57
3:S:167:PHE:HA	3:S:319:GLN:HB2	1.85	0.57
3:K:94:THR:OG1	3:K:95:GLN:HG3	2.03	0.57
3:G:118:ALA:HB3	3:G:121:LYS:HG2	1.85	0.57
3:G:205:ALA:HB1	3:G:211:GLU:H	1.69	0.57
2:R:72:PRO:O	2:R:82:LEU:HD11	2.03	0.57
2:R:134:ALA:HB3	2:R:195:SER:OG	2.03	0.57
3:C:81:ARG:NH1	3:C:94:THR:O	2.37	0.57
2:J:72:PRO:O	2:J:82:LEU:HD11	2.04	0.57
2:B:162:GLN:HG2	2:B:163:SER:H	1.69	0.57
1:Q:103:LYS:HB3	1:Q:105:ALA:CB	2.34	0.57
1:M:291:LYS:HE3	2:N:65:LEU:HD21	1.86	0.57
2:R:85:VAL:HG11	2:R:194:VAL:O	2.04	0.57
3:C:295:GLN:HE21	3:C:295:GLN:CA	2.02	0.57
1:A:109:PRO:HB2	1:A:112:TYR:H	1.70	0.57
1:M:291:LYS:HE2	2:N:60:THR:HA	1.86	0.57
1:A:105:ALA:CA	1:A:109:PRO:HD2	2.35	0.57
2:R:130:LYS:HB2	2:R:200:THR:HG23	1.87	0.57
2:J:130:LYS:HB2	2:J:200:THR:HG23	1.86	0.57
2:F:153:THR:OG1	3:S:317:LEU:HD21	2.04	0.56
2:B:177:TYR:OH	2:B:190:THR:O	2.23	0.56
1:I:105:ALA:HA	1:I:109:PRO:HD2	1.87	0.56
2:J:24:ILE:HG23	2:J:25:LEU:HG	1.87	0.56
2:J:136:THR:N	2:J:193:LEU:O	2.28	0.56
3:C:293:TYR:HE1	3:C:295:GLN:HE22	1.51	0.56
1:E:267:TRP:CE3	2:F:36:ILE:HB	2.40	0.56
1:M:164:PRO:HB2	2:J:178:ARG:HH11	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:59:PRO:HD2	2:B:68:ARG:HD2	1.87	0.56
1:E:279:PHE:CZ	3:G:212:ASP:HB3	2.40	0.56
1:Q:287:GLY:HA3	3:S:207:GLY:HA2	1.86	0.56
1:I:124:GLN:HG3	2:J:233:SER:HB3	1.88	0.56
2:J:85:VAL:HG22	2:J:86:PHE:CD2	2.41	0.56
3:O:318:ARG:O	3:O:319:GLN:HG2	2.06	0.56
2:J:37:PRO:HG2	3:K:267:ILE:HG12	1.87	0.56
2:N:130:LYS:HB2	2:N:200:THR:HG23	1.87	0.56
2:B:65:LEU:O	2:B:68:ARG:HG3	2.06	0.56
1:I:109:PRO:HB3	1:I:112:TYR:O	2.06	0.56
2:J:163:SER:O	2:J:165:VAL:N	2.39	0.56
3:C:130:ASN:HA	3:C:309:PRO:HG2	1.87	0.56
1:E:99:GLY:H	1:E:104:ARG:HH22	1.53	0.56
1:I:101:GLU:C	1:I:102:ARG:HG2	2.30	0.56
1:I:291:LYS:HE2	2:J:60:THR:HG22	1.88	0.56
1:A:222:GLN:O	1:A:224:LYS:N	2.39	0.56
2:J:234:ASP:OD1	2:J:235:ILE:N	2.36	0.56
3:K:85:LEU:HD22	3:K:86:THR:HG22	1.88	0.56
3:K:118:ALA:HB3	3:K:121:LYS:HG2	1.87	0.56
1:E:105:ALA:CA	1:E:109:PRO:HD2	2.36	0.56
2:R:6:LEU:H	2:J:10:THR:HB	1.71	0.56
2:J:65:LEU:O	2:J:68:ARG:HG3	2.06	0.56
2:N:10:THR:OG1	2:N:11:ASN:N	2.38	0.56
1:E:105:ALA:HA	1:E:109:PRO:HD2	1.89	0.55
1:Q:225:ASP:O	1:Q:227:GLU:N	2.38	0.55
1:M:124:GLN:HG3	2:N:233:SER:HB3	1.88	0.55
2:F:159:PHE:HB3	3:G:255:ARG:NH2	2.21	0.55
1:A:124:GLN:HG3	2:B:233:SER:HB3	1.89	0.55
2:J:85:VAL:CG1	2:J:194:VAL:H	2.18	0.55
2:B:134:ALA:O	2:B:195:SER:N	2.39	0.55
3:C:188:GLN:HE21	3:C:292:ASP:HB3	1.70	0.55
1:A:275:GLN:NE2	1:A:290:ILE:O	2.35	0.55
2:N:91:GLY:HA3	2:N:111:TRP:CZ2	2.42	0.55
3:S:205:ALA:HB1	3:S:211:GLU:H	1.72	0.55
2:F:24:ILE:HG23	2:F:25:LEU:HG	1.89	0.55
1:Q:98:GLU:HA	1:Q:104:ARG:NH1	2.22	0.55
2:J:75:ALA:HA	2:J:202:TYR:HB3	1.89	0.55
2:N:159:PHE:HB3	3:O:255:ARG:NH2	2.22	0.55
2:F:73:VAL:O	2:F:74:SER:HB3	2.07	0.55
2:R:73:VAL:O	2:R:198:TYR:OH	2.24	0.55
1:E:109:PRO:HB3	1:E:112:TYR:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:24:ILE:HG23	2:N:25:LEU:HG	1.89	0.55
2:N:37:PRO:HG2	3:O:267:ILE:HG12	1.89	0.55
2:N:134:ALA:O	2:N:195:SER:N	2.36	0.55
2:F:178:ARG:NH1	1:Q:164:PRO:HB2	2.22	0.54
1:M:105:ALA:HA	1:M:108:THR:CA	2.29	0.54
2:R:24:ILE:HG23	2:R:25:LEU:HG	1.89	0.54
2:B:163:SER:C	2:B:165:VAL:H	2.16	0.54
3:O:205:ALA:HB1	3:O:211:GLU:H	1.73	0.54
2:F:178:ARG:HB3	1:Q:165:GLY:HA2	1.90	0.54
1:M:223:GLU:C	1:M:225:ASP:H	2.14	0.54
2:N:5:GLU:HA	2:B:10:THR:HG22	1.89	0.54
3:O:118:ALA:H	3:O:121:LYS:HG2	1.71	0.54
2:F:75:ALA:HA	2:F:202:TYR:HB3	1.88	0.54
1:I:109:PRO:HB3	1:I:112:TYR:C	2.33	0.54
1:M:226:LEU:O	3:O:214:HIS:ND1	2.37	0.54
1:E:300:ILE:C	2:F:84:ALA:HB2	2.33	0.54
1:Q:97:LEU:O	1:Q:104:ARG:NH1	2.41	0.54
1:I:220:HIS:O	1:I:222:GLN:HG2	2.08	0.54
1:A:293:THR:C	2:B:68:ARG:HH22	2.16	0.54
1:Q:291:LYS:HE2	2:R:60:THR:HG22	1.89	0.54
1:E:226:LEU:HB2	3:G:214:HIS:ND1	2.23	0.54
1:E:271:PRO:HB2	3:G:239:ILE:HG12	1.89	0.54
2:B:163:SER:O	2:B:165:VAL:N	2.41	0.54
2:B:174:ASN:HA	2:B:177:TYR:HD2	1.73	0.54
3:S:179:VAL:HG22	3:S:305:ILE:HG12	1.90	0.54
2:F:14:LEU:HB3	2:F:17:ASP:HB2	1.90	0.53
1:I:105:ALA:CA	1:I:109:PRO:HD2	2.38	0.53
1:Q:280:LYS:H	1:Q:280:LYS:HD2	1.73	0.53
2:N:75:ALA:HA	2:N:202:TYR:HB3	1.89	0.53
2:B:73:VAL:O	2:B:198:TYR:OH	2.27	0.53
1:M:274:ASN:HB2	3:O:240:PRO:HD3	1.91	0.53
1:A:277:TYR:H	2:B:235:ILE:HG21	1.73	0.53
2:N:73:VAL:O	2:N:74:SER:HB3	2.08	0.53
1:E:274:ASN:HB2	3:G:240:PRO:HD3	1.90	0.53
1:Q:105:ALA:C	1:Q:109:PRO:HD2	2.33	0.53
2:J:159:PHE:HB3	3:K:255:ARG:NH2	2.24	0.53
1:Q:274:ASN:HB2	3:S:240:PRO:HD3	1.90	0.53
2:F:6:LEU:H	2:R:10:THR:HB	1.73	0.53
2:F:163:SER:C	2:F:165:VAL:H	2.17	0.53
3:C:179:VAL:HG22	3:C:305:ILE:HG12	1.89	0.53
1:M:96:PRO:HG2	1:M:104:ARG:HG2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:165:GLY:HA2	2:J:178:ARG:HB3	1.89	0.53
1:A:220:HIS:NE2	3:C:276:LEU:O	2.42	0.53
2:B:24:ILE:HG23	2:B:25:LEU:HG	1.89	0.53
1:A:274:ASN:HB2	3:C:240:PRO:HD3	1.91	0.53
2:R:194:VAL:O	2:R:194:VAL:HG12	2.08	0.53
1:M:105:ALA:HA	1:M:109:PRO:HD2	1.91	0.53
2:J:162:GLN:HG2	2:J:163:SER:H	1.74	0.53
1:Q:294:GLY:HA2	2:R:57:ASN:HB2	1.91	0.53
1:M:267:TRP:CE3	2:N:36:ILE:HB	2.43	0.53
1:I:164:PRO:HB2	2:R:178:ARG:NH1	2.24	0.52
1:M:279:PHE:CE1	3:O:212:ASP:HB3	2.44	0.52
1:A:165:GLY:HA2	2:N:178:ARG:HB3	1.91	0.52
2:N:135:TYR:CE1	2:N:169:ILE:HG23	2.43	0.52
1:E:219:GLU:HB2	1:E:222:GLN:HG2	1.91	0.52
1:A:223:GLU:C	1:A:225:ASP:H	2.16	0.52
2:N:72:PRO:O	2:N:82:LEU:HD11	2.08	0.52
1:Q:109:PRO:HB3	1:Q:112:TYR:C	2.34	0.52
2:J:73:VAL:O	2:J:74:SER:HB3	2.09	0.52
2:B:14:LEU:HB3	2:B:17:ASP:HB2	1.92	0.52
1:Q:112:TYR:O	1:Q:112:TYR:CG	2.62	0.52
1:I:172:ARG:NH2	1:I:243:THR:OG1	2.42	0.52
2:B:194:VAL:O	2:B:194:VAL:HG12	2.09	0.52
2:J:204:VAL:HB	2:J:208:ALA:HB3	1.92	0.52
3:O:115:ASP:OD1	3:O:121:LYS:HE3	2.09	0.52
3:G:168:HIS:C	3:G:319:GLN:HE21	2.17	0.52
1:I:105:ALA:HB1	1:I:106:ARG:HB2	1.92	0.52
1:I:112:TYR:O	1:I:112:TYR:CG	2.62	0.52
1:A:226:LEU:HB3	3:C:214:HIS:HB2	1.91	0.52
2:J:194:VAL:O	2:J:194:VAL:HG12	2.09	0.52
1:M:112:TYR:O	1:M:112:TYR:CG	2.63	0.52
2:F:123:GLY:HA2	3:G:188:GLN:NE2	2.25	0.52
2:F:123:GLY:HA2	3:G:188:GLN:HE21	1.75	0.52
2:F:178:ARG:HH11	1:Q:164:PRO:HB2	1.75	0.52
1:A:287:GLY:HA3	3:C:207:GLY:HA2	1.92	0.52
2:F:152:GLY:HA2	3:S:318:ARG:CD	2.39	0.51
2:R:10:THR:OG1	2:R:11:ASN:N	2.42	0.51
1:M:105:ALA:CA	1:M:109:PRO:HD2	2.40	0.51
2:B:130:LYS:HB2	2:B:200:THR:HG23	1.93	0.51
3:O:169:TYR:HB3	3:O:316:GLY:HA2	1.92	0.51
1:M:291:LYS:H	1:M:291:LYS:CD	2.11	0.51
2:B:73:VAL:O	2:B:74:SER:HB3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:168:HIS:O	3:O:319:GLN:NE2	2.43	0.51
1:A:220:HIS:NE2	3:C:276:LEU:C	2.69	0.51
2:F:204:VAL:HB	2:F:208:ALA:HB3	1.93	0.51
1:A:98:GLU:HA	1:A:104:ARG:NH1	2.26	0.51
2:J:73:VAL:O	2:J:198:TYR:OH	2.28	0.51
2:B:61:ASN:O	2:B:65:LEU:HG	2.11	0.51
1:E:84:PHE:HB3	1:E:261:MET:HE3	1.93	0.51
2:N:163:SER:C	2:N:165:VAL:H	2.18	0.51
2:R:5:GLU:HA	2:J:10:THR:HG22	1.93	0.51
3:K:114:SER:HB3	3:K:115:ASP:HB2	1.92	0.51
1:A:112:TYR:O	1:A:112:TYR:CG	2.64	0.50
1:E:280:LYS:H	1:E:280:LYS:HD2	1.76	0.50
1:Q:267:TRP:CE3	2:R:36:ILE:HB	2.46	0.50
1:Q:293:THR:C	2:R:68:ARG:HH22	2.18	0.50
1:I:293:THR:C	2:J:68:ARG:HH22	2.17	0.50
1:A:133:THR:HB	1:A:268:ILE:HB	1.93	0.50
2:N:65:LEU:O	2:N:68:ARG:HG3	2.12	0.50
1:E:109:PRO:HB3	1:E:112:TYR:C	2.36	0.50
3:S:316:GLY:O	3:S:317:LEU:HB2	2.10	0.50
1:A:267:TRP:CE3	2:B:36:ILE:HB	2.46	0.50
2:R:91:GLY:HA3	2:R:111:TRP:CZ2	2.47	0.50
3:G:121:LYS:HB3	3:G:122:PRO:HD3	1.92	0.50
1:Q:271:PRO:HB2	3:S:239:ILE:HG12	1.93	0.50
1:I:267:TRP:CE3	2:J:36:ILE:HB	2.46	0.50
3:C:148:TYR:HB3	3:C:284:LEU:HD23	1.94	0.50
1:Q:105:ALA:HB1	1:Q:106:ARG:HG3	1.93	0.50
1:A:277:TYR:H	2:B:235:ILE:CG2	2.25	0.50
1:I:136:ARG:NH2	2:J:31:THR:O	2.36	0.50
2:R:14:LEU:HB3	2:R:17:ASP:HB2	1.93	0.50
2:R:65:LEU:O	2:R:68:ARG:HG3	2.12	0.50
2:N:153:THR:OG1	3:C:317:LEU:HD21	2.10	0.50
1:E:293:THR:C	2:F:68:ARG:HH22	2.19	0.50
1:I:133:THR:HB	1:I:268:ILE:HB	1.94	0.50
3:C:121:LYS:HB3	3:C:122:PRO:HD3	1.94	0.50
1:Q:105:ALA:HB1	1:Q:106:ARG:HA	1.94	0.49
3:S:121:LYS:HB2	3:S:122:PRO:CD	2.41	0.49
3:K:122:PRO:HB3	3:K:313:GLU:HG2	1.94	0.49
1:M:287:GLY:HA3	3:O:207:GLY:HA2	1.93	0.49
3:S:317:LEU:HG	3:S:318:ARG:HG2	1.93	0.49
3:K:169:TYR:HB3	3:K:316:GLY:HA2	1.94	0.49
2:R:159:PHE:HB3	3:S:255:ARG:NH2	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:167:LEU:CD2	2:J:194:VAL:HG13	2.42	0.49
2:F:65:LEU:O	2:F:68:ARG:HG3	2.12	0.49
1:M:223:GLU:HB2	3:O:217:TYR:HE1	1.74	0.49
1:Q:124:GLN:HG3	2:R:233:SER:HB3	1.94	0.49
1:Q:300:ILE:O	2:R:84:ALA:HB2	2.12	0.49
1:M:279:PHE:CZ	3:O:212:ASP:HB3	2.48	0.49
2:R:163:SER:C	2:R:165:VAL:H	2.20	0.49
2:B:91:GLY:HA3	2:B:111:TRP:CZ2	2.48	0.49
2:R:87:ARG:O	2:R:89:ASP:N	2.45	0.49
2:N:162:GLN:HG2	2:N:163:SER:H	1.77	0.49
3:O:124:ARG:HG2	3:O:313:GLU:HG3	1.94	0.49
3:C:316:GLY:O	3:C:317:LEU:HB2	2.13	0.49
2:F:10:THR:OG1	2:F:11:ASN:N	2.46	0.49
1:I:220:HIS:O	1:I:222:GLN:N	2.45	0.49
3:S:114:SER:HB3	3:S:115:ASP:HB2	1.95	0.49
3:O:118:ALA:N	3:O:121:LYS:HG2	2.27	0.49
3:G:263:ILE:HD12	3:G:310:MET:HE1	1.95	0.49
1:E:275:GLN:NE2	1:E:290:ILE:O	2.36	0.49
1:Q:104:ARG:N	1:Q:105:ALA:HB3	2.28	0.49
1:Q:220:HIS:O	1:Q:222:GLN:N	2.46	0.49
2:R:142:LEU:HD12	2:R:143:PRO:HD2	1.94	0.49
3:S:148:TYR:HB3	3:S:284:LEU:HD23	1.94	0.49
3:C:122:PRO:HB3	3:C:313:GLU:HG2	1.95	0.49
1:E:291:LYS:HE2	2:F:60:THR:HG22	1.95	0.48
2:F:163:SER:O	2:F:165:VAL:N	2.46	0.48
2:R:167:LEU:CD2	2:R:194:VAL:HG13	2.43	0.48
3:S:317:LEU:HG	3:S:318:ARG:NE	2.27	0.48
3:K:86:THR:HG21	3:K:132:PHE:H	1.77	0.48
1:E:112:TYR:O	1:E:112:TYR:CG	2.66	0.48
1:Q:293:THR:HG21	2:R:97:GLN:OE1	2.13	0.48
1:E:164:PRO:HB2	2:B:178:ARG:NH1	2.28	0.48
1:M:99:GLY:O	1:M:104:ARG:NH2	2.46	0.48
1:M:219:GLU:H	1:M:222:GLN:NE2	2.12	0.48
1:M:267:TRP:HA	2:N:39:GLU:HA	1.95	0.48
1:M:164:PRO:HB2	2:J:178:ARG:NH1	2.29	0.48
1:M:273:ARG:HA	3:O:239:ILE:HD12	1.95	0.48
1:A:164:PRO:HB2	2:N:178:ARG:NH1	2.28	0.48
1:E:102:ARG:HG2	1:E:103:LYS:HG3	1.95	0.48
3:G:115:ASP:OD1	3:G:115:ASP:C	2.56	0.48
1:I:164:PRO:HB2	2:R:178:ARG:HH11	1.79	0.48
2:B:125:PHE:CD1	3:C:185:LYS:HD3	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:210:THR:O	3:K:210:THR:OG1	2.30	0.48
2:B:87:ARG:O	2:B:89:ASP:N	2.47	0.48
1:M:220:HIS:O	1:M:222:GLN:N	2.46	0.48
2:R:162:GLN:HG2	2:R:163:SER:H	1.79	0.48
3:S:122:PRO:CB	3:S:313:GLU:HG2	2.44	0.48
3:K:92:ILE:HD12	3:K:178:HIS:NE2	2.28	0.48
3:G:116:ALA:N	3:G:117:THR:HA	2.29	0.48
3:G:122:PRO:HB3	3:G:313:GLU:HG2	1.96	0.48
1:M:291:LYS:HE2	2:N:60:THR:CA	2.43	0.48
2:R:134:ALA:O	2:R:195:SER:N	2.46	0.48
1:I:225:ASP:O	1:I:227:GLU:N	2.46	0.48
1:M:219:GLU:HG2	1:M:222:GLN:NE2	2.29	0.48
2:B:100:LEU:HD22	3:C:246:VAL:HG21	1.95	0.48
2:B:167:LEU:CD2	2:B:194:VAL:HG13	2.44	0.48
3:S:170:LEU:HB3	3:S:272:PHE:HB3	1.96	0.48
1:M:158:GLN:HG3	1:M:186:PHE:CE1	2.48	0.47
1:A:105:ALA:HB1	1:A:106:ARG:HB2	1.96	0.47
3:S:122:PRO:HB3	3:S:313:GLU:HG2	1.96	0.47
3:K:86:THR:HG21	3:K:131:ARG:HB2	1.95	0.47
2:F:10:THR:HG22	2:B:5:GLU:HA	1.96	0.47
2:B:10:THR:OG1	2:B:11:ASN:N	2.47	0.47
3:O:102:VAL:HA	3:O:263:ILE:HB	1.96	0.47
3:G:124:ARG:HG2	3:G:313:GLU:HG3	1.94	0.47
2:N:163:SER:O	2:N:165:VAL:N	2.46	0.47
2:R:153:THR:OG1	3:K:317:LEU:HD21	2.14	0.47
1:E:172:ARG:NH2	1:E:243:THR:OG1	2.47	0.47
2:J:177:TYR:OH	2:J:190:THR:HG23	2.15	0.47
3:K:121:LYS:HB3	3:K:122:PRO:HD3	1.96	0.47
3:O:114:SER:HA	3:O:115:ASP:HA	1.72	0.47
3:O:123:THR:O	3:O:125:PRO:HD3	2.14	0.47
1:E:267:TRP:HA	2:F:39:GLU:HA	1.97	0.47
2:F:228:LEU:HD21	1:Q:163:PRO:HB3	1.96	0.47
1:A:214:TYR:CE1	3:C:217:TYR:CZ	3.03	0.47
1:A:300:ILE:O	2:B:84:ALA:HB2	2.15	0.47
3:K:89:ASN:OD1	3:K:90:SER:N	2.48	0.47
1:Q:221:LYS:HA	1:Q:221:LYS:HD3	1.75	0.47
1:I:123:ALA:HA	2:J:236:LEU:HD23	1.97	0.47
1:M:99:GLY:H	1:M:104:ARG:HH22	1.63	0.47
1:M:294:GLY:HA3	2:N:68:ARG:HH12	1.80	0.47
1:A:200:PHE:CZ	1:A:202:SER:HB3	2.50	0.47
3:K:318:ARG:HG3	3:K:319:GLN:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:167:PHE:HA	3:O:319:GLN:HB2	1.96	0.47
3:G:293:TYR:CZ	3:G:299:PRO:HA	2.50	0.47
1:I:110:ASN:ND2	1:I:110:ASN:N	2.57	0.47
3:O:115:ASP:OD1	3:O:115:ASP:N	2.46	0.47
3:G:274:SER:OG	3:G:277:ASN:HB2	2.15	0.47
1:I:268:ILE:HG21	3:K:197:PRO:HG2	1.96	0.47
1:A:293:THR:HG21	2:B:97:GLN:OE1	2.15	0.47
2:B:85:VAL:HG11	2:B:194:VAL:C	2.40	0.47
3:K:124:ARG:HG2	3:K:313:GLU:HG3	1.95	0.47
2:F:136:THR:HB	2:F:193:LEU:HB2	1.97	0.47
2:F:162:GLN:HG2	2:F:163:SER:H	1.80	0.47
3:O:118:ALA:HB3	3:O:121:LYS:HD3	1.97	0.47
1:Q:126:ARG:HD3	2:R:236:LEU:HD13	1.96	0.46
2:B:2:PHE:HA	2:B:3:PRO:HD3	1.80	0.46
3:G:148:TYR:HB3	3:G:284:LEU:HD23	1.97	0.46
1:Q:224:LYS:HG3	1:Q:224:LYS:O	2.14	0.46
1:I:274:ASN:HB2	3:K:240:PRO:HD3	1.96	0.46
1:E:279:PHE:CE2	3:G:212:ASP:HB3	2.50	0.46
1:M:102:ARG:CG	1:M:103:LYS:HA	2.46	0.46
2:B:157:TRP:CD2	2:B:165:VAL:HG21	2.51	0.46
1:Q:101:GLU:C	1:Q:102:ARG:HD3	2.41	0.46
1:Q:133:THR:HB	1:Q:268:ILE:HB	1.96	0.46
1:I:84:PHE:HB3	1:I:261:MET:HE3	1.98	0.46
1:A:291:LYS:HE2	2:B:60:THR:HG22	1.96	0.46
2:N:100:LEU:HD22	3:O:246:VAL:HG21	1.98	0.46
2:N:157:TRP:CD2	2:N:165:VAL:HG21	2.51	0.46
1:Q:105:ALA:CA	1:Q:108:THR:HA	2.45	0.46
1:M:232:PRO:HG2	2:J:176:HIS:NE2	2.31	0.46
2:J:100:LEU:HD22	3:K:246:VAL:HG21	1.97	0.46
2:B:124:SER:N	3:C:188:GLN:HG2	2.30	0.46
3:C:205:ALA:HB1	3:C:211:GLU:H	1.81	0.46
1:M:99:GLY:N	1:M:104:ARG:HH22	2.13	0.46
3:K:94:THR:HA	3:K:95:GLN:HA	1.70	0.46
3:C:215:PRO:HA	3:C:216:PRO:HD3	1.80	0.46
1:E:274:ASN:ND2	1:E:292:PRO:HG3	2.31	0.46
2:N:85:VAL:HG23	2:N:85:VAL:O	2.15	0.46
2:B:162:GLN:CD	2:B:162:GLN:H	2.24	0.46
1:Q:220:HIS:N	1:Q:222:GLN:OE1	2.49	0.46
1:M:133:THR:HB	1:M:268:ILE:HB	1.97	0.46
1:M:268:ILE:HG21	3:O:197:PRO:HG2	1.98	0.46
1:Q:268:ILE:HG21	3:S:197:PRO:HG2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:267:TRP:HA	2:J:39:GLU:HA	1.97	0.46
1:I:294:GLY:CA	2:J:68:ARG:HH12	2.25	0.46
2:J:212:ALA:HA	3:K:188:GLN:NE2	2.31	0.46
2:N:135:TYR:O	3:C:318:ARG:NH1	2.47	0.46
1:Q:104:ARG:CA	1:Q:105:ALA:HB3	2.46	0.45
1:Q:300:ILE:HA	2:R:84:ALA:N	2.23	0.45
3:S:204:VAL:HG12	3:S:206:GLY:H	1.81	0.45
3:O:172:ARG:O	3:O:313:GLU:N	2.47	0.45
2:F:120:MET:HA	2:F:163:SER:HB3	1.98	0.45
1:Q:105:ALA:HB1	1:Q:106:ARG:CA	2.46	0.45
1:Q:105:ALA:H	1:Q:108:THR:HA	1.81	0.45
1:A:297:ARG:HH22	1:A:303:LEU:HD13	1.81	0.45
2:N:111:TRP:HB3	2:N:226:MET:HG2	1.99	0.45
2:F:159:PHE:HB3	3:G:255:ARG:HH22	1.81	0.45
3:G:94:THR:HA	3:G:95:GLN:HA	1.59	0.45
1:I:224:LYS:HA	1:I:224:LYS:HD2	1.23	0.45
1:A:294:GLY:CA	2:B:68:ARG:HH12	2.23	0.45
3:O:318:ARG:HG3	3:O:319:GLN:N	2.31	0.45
3:C:149:TRP:HB3	3:C:154:VAL:HG11	1.98	0.45
1:M:300:ILE:C	2:N:84:ALA:HB2	2.40	0.45
2:R:161:LEU:HD21	2:R:164:SER:C	2.41	0.45
2:N:73:VAL:O	2:N:198:TYR:OH	2.35	0.45
3:O:86:THR:HG23	3:O:88:GLY:H	1.82	0.45
2:F:73:VAL:O	2:F:198:TYR:OH	2.34	0.45
2:B:85:VAL:HG21	2:B:194:VAL:C	2.41	0.45
1:M:294:GLY:CA	2:N:68:ARG:HH12	2.30	0.45
2:J:6:LEU:H	2:N:10:THR:HB	1.80	0.45
2:F:35:HIS:NE2	3:G:106:GLU:OE2	2.50	0.45
2:F:85:VAL:HG12	2:F:195:SER:HA	1.97	0.45
1:I:231:CYS:HA	1:I:232:PRO:HD3	1.81	0.45
3:S:149:TRP:HB3	3:S:154:VAL:HG11	1.98	0.45
1:A:172:ARG:NH2	1:A:243:THR:OG1	2.49	0.45
1:A:278:LEU:O	2:B:237:GLN:HG3	2.17	0.45
2:R:134:ALA:N	2:R:195:SER:O	2.37	0.45
3:O:126:ASP:HB2	3:O:127:VAL:HA	1.99	0.45
3:C:92:ILE:HD11	3:C:178:HIS:NE2	2.32	0.45
1:A:101:GLU:HG3	1:A:104:ARG:NE	2.32	0.45
2:J:87:ARG:O	2:J:89:ASP:N	2.49	0.45
2:J:120:MET:HA	2:J:163:SER:HB3	1.98	0.45
3:O:92:ILE:HD12	3:O:93:THR:H	1.82	0.45
1:A:104:ARG:HA	1:A:105:ALA:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S:149:TRP:HB3	3:S:154:VAL:CG1	2.47	0.45
3:S:263:ILE:HD12	3:S:310:MET:HE1	1.98	0.45
1:E:236:MET:HE3	1:E:236:MET:HB2	1.86	0.44
1:Q:84:PHE:HB3	1:Q:261:MET:HE3	1.98	0.44
1:M:84:PHE:HB3	1:M:261:MET:HE3	1.99	0.44
3:O:179:VAL:HG22	3:O:305:ILE:HG12	1.99	0.44
3:K:204:VAL:HG12	3:K:206:GLY:N	2.33	0.44
1:E:164:PRO:HB2	2:B:178:ARG:HH11	1.83	0.44
3:G:216:PRO:HB2	3:G:218:LYS:HG3	1.99	0.44
1:E:133:THR:HB	1:E:268:ILE:HB	1.99	0.44
2:F:52:ILE:HG21	2:F:69:LEU:HB3	2.00	0.44
2:F:100:LEU:HD22	3:G:246:VAL:HG21	1.99	0.44
1:I:82:SER:O	1:I:86:ARG:NH2	2.50	0.44
2:R:93:SER:HA	2:R:97:GLN:OE1	2.17	0.44
2:B:204:VAL:HB	2:B:208:ALA:HB3	1.99	0.44
1:Q:226:LEU:O	3:S:214:HIS:CE1	2.71	0.44
1:I:104:ARG:HA	1:I:105:ALA:HB3	2.00	0.44
1:M:104:ARG:HA	1:M:105:ALA:O	2.18	0.44
1:M:271:PRO:HB2	3:O:239:ILE:HG13	2.00	0.44
2:R:157:TRP:CD2	2:R:165:VAL:HG21	2.51	0.44
3:O:121:LYS:HA	3:O:121:LYS:HD2	1.75	0.44
1:E:126:ARG:HD3	2:F:236:LEU:HD13	1.99	0.44
1:Q:101:GLU:O	1:Q:102:ARG:HD3	2.17	0.44
1:M:106:ARG:HA	1:M:108:THR:N	2.32	0.44
1:A:107:LEU:HD11	1:A:115:TRP:HD1	1.82	0.44
1:A:161:PHE:HB3	1:A:183:PRO:HG2	1.98	0.44
2:J:10:THR:OG1	2:J:11:ASN:N	2.50	0.44
1:I:203:PRO:HB3	2:R:110:GLN:OE1	2.18	0.44
1:A:84:PHE:HB3	1:A:261:MET:HE3	1.99	0.44
1:A:214:TYR:CZ	3:C:217:TYR:CE1	3.06	0.44
2:R:163:SER:O	2:R:165:VAL:N	2.50	0.44
2:N:161:LEU:HD21	2:N:164:SER:C	2.42	0.44
2:B:85:VAL:HG21	2:B:194:VAL:HB	1.99	0.44
3:C:114:SER:HA	3:C:115:ASP:HA	1.67	0.44
2:F:85:VAL:HG23	2:F:85:VAL:O	2.17	0.44
3:G:86:THR:HG21	3:G:132:PHE:H	1.82	0.44
1:Q:231:CYS:HA	1:Q:232:PRO:HD3	1.79	0.44
1:M:109:PRO:CB	1:M:112:TYR:H	2.29	0.44
2:J:6:LEU:HB3	2:J:10:THR:HG21	2.00	0.44
1:Q:155:GLN:HG2	1:Q:253:LEU:HD11	2.00	0.43
1:A:99:GLY:O	1:A:101:GLU:HG2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:93:SER:HA	2:N:97:GLN:OE1	2.18	0.43
3:S:195:VAL:O	3:S:247:CYS:HB3	2.18	0.43
2:F:236:LEU:HD12	2:F:237:GLN:H	1.83	0.43
3:S:167:PHE:CE1	3:S:321:VAL:HG13	2.54	0.43
2:N:162:GLN:CD	2:N:162:GLN:H	2.26	0.43
3:K:195:VAL:HG13	3:K:281:PHE:CD1	2.53	0.43
2:R:72:PRO:HB3	2:R:213:TYR:CD1	2.53	0.43
2:B:85:VAL:HG23	2:B:86:PHE:CD2	2.53	0.43
3:K:96:GLU:OE2	3:K:259:CYS:N	2.51	0.43
3:O:316:GLY:O	3:O:317:LEU:HB2	2.18	0.43
3:C:126:ASP:HA	3:C:127:VAL:HA	1.76	0.43
1:I:300:ILE:HA	2:J:84:ALA:N	2.22	0.43
1:M:214:TYR:CE2	1:M:228:TYR:HB2	2.50	0.43
3:O:122:PRO:CB	3:O:313:GLU:HG2	2.49	0.43
3:C:96:GLU:HG3	3:C:97:ALA:H	1.83	0.43
3:C:319:GLN:HE21	3:C:319:GLN:HB2	1.60	0.43
1:E:300:ILE:HA	2:F:84:ALA:H	1.82	0.43
2:F:2:PHE:HA	2:F:3:PRO:HD3	1.83	0.43
1:A:109:PRO:CB	1:A:112:TYR:H	2.31	0.43
1:A:294:GLY:HA2	2:B:57:ASN:HB2	2.00	0.43
3:O:141:GLU:HG3	3:O:300:VAL:HG12	2.00	0.43
3:C:195:VAL:O	3:C:247:CYS:HB3	2.18	0.43
1:E:98:GLU:HA	1:E:104:ARG:NH1	2.34	0.43
2:F:157:TRP:CD2	2:F:165:VAL:HG21	2.54	0.43
1:I:215:PRO:HD2	1:I:227:GLU:CD	2.44	0.43
2:J:74:SER:OG	2:J:76:GLN:HB2	2.17	0.43
3:S:126:ASP:HA	3:S:127:VAL:HA	1.79	0.43
2:F:134:ALA:HB3	2:F:195:SER:OG	2.19	0.43
1:E:220:HIS:HB3	1:E:221:LYS:H	1.13	0.43
1:E:294:GLY:CA	2:F:68:ARG:HH12	2.31	0.43
1:M:105:ALA:HB1	1:M:106:ARG:HB2	1.99	0.43
2:N:87:ARG:O	2:N:89:ASP:N	2.51	0.43
1:A:268:ILE:HG21	3:C:197:PRO:HG2	2.00	0.43
2:J:153:THR:OG1	3:O:317:LEU:HD21	2.18	0.43
2:F:236:LEU:HD12	2:F:237:GLN:N	2.35	0.42
1:A:226:LEU:HD23	3:C:214:HIS:O	2.18	0.42
2:J:36:ILE:HA	2:J:37:PRO:HD3	1.86	0.42
3:S:204:VAL:HG12	3:S:206:GLY:N	2.33	0.42
2:F:161:LEU:HD21	2:F:164:SER:C	2.44	0.42
1:M:223:GLU:C	1:M:225:ASP:N	2.77	0.42
1:M:291:LYS:HG3	2:N:65:LEU:CD2	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:PHE:O	1:A:163:PRO:HD3	2.19	0.42
1:E:268:ILE:HG21	3:G:197:PRO:HG2	2.02	0.42
3:G:92:ILE:HD12	3:G:93:THR:H	1.83	0.42
2:R:195:SER:HB2	2:R:197:TRP:NE1	2.34	0.42
3:S:268:ASN:HB3	3:S:270:LEU:O	2.20	0.42
3:K:80:ASP:HB2	3:K:81:ARG:HD3	2.00	0.42
1:I:279:PHE:CZ	3:K:212:ASP:HB3	2.55	0.42
2:J:161:LEU:HD21	2:J:164:SER:C	2.45	0.42
3:O:96:GLU:HG3	3:O:97:ALA:H	1.85	0.42
3:G:243:GLN:O	3:G:246:VAL:HG23	2.20	0.42
1:M:161:PHE:O	1:M:163:PRO:HD3	2.20	0.42
1:A:274:ASN:ND2	1:A:292:PRO:HG3	2.34	0.42
2:R:124:SER:N	3:S:188:GLN:HG2	2.35	0.42
1:E:104:ARG:HA	1:E:105:ALA:O	2.20	0.42
1:Q:227:GLU:C	1:Q:227:GLU:CD	2.88	0.42
1:A:75:THR:HG22	2:B:225:THR:HG22	2.01	0.42
3:C:263:ILE:HD12	3:C:310:MET:HE1	2.01	0.42
2:F:36:ILE:HA	2:F:37:PRO:HD3	1.82	0.42
2:R:100:LEU:HD22	3:S:246:VAL:HG21	2.00	0.42
3:S:81:ARG:CZ	3:S:94:THR:H	2.33	0.42
3:O:169:TYR:CD2	3:O:170:LEU:HG	2.54	0.42
2:F:152:GLY:CA	3:S:318:ARG:HD2	2.47	0.42
3:G:92:ILE:HD11	3:G:178:HIS:NE2	2.35	0.42
1:I:119:ILE:HG22	1:I:259:MET:HE1	2.02	0.42
1:A:106:ARG:N	1:A:109:PRO:HD2	2.35	0.42
2:J:163:SER:C	2:J:165:VAL:N	2.78	0.42
3:S:169:TYR:CD2	3:S:170:LEU:HG	2.55	0.42
3:O:263:ILE:HD12	3:O:310:MET:HE1	2.01	0.42
1:E:293:THR:HG21	2:F:97:GLN:OE1	2.20	0.42
2:F:7:LYS:O	2:F:10:THR:HG23	2.20	0.42
1:Q:215:PRO:HD2	1:Q:227:GLU:CD	2.45	0.42
1:I:236:MET:HE3	1:I:236:MET:HB2	1.90	0.42
1:M:172:ARG:NH2	1:M:243:THR:OG1	2.53	0.42
1:A:224:LYS:O	1:A:224:LYS:HG3	2.19	0.42
3:S:243:GLN:O	3:S:246:VAL:HG23	2.19	0.42
1:A:300:ILE:C	2:B:84:ALA:HB2	2.45	0.42
2:N:85:VAL:HB	2:N:194:VAL:N	2.35	0.42
3:G:170:LEU:HB3	3:G:272:PHE:HB3	2.02	0.41
2:R:52:ILE:HG21	2:R:69:LEU:HB3	2.00	0.41
2:B:93:SER:HA	2:B:97:GLN:OE1	2.20	0.41
1:E:105:ALA:HB1	1:E:106:ARG:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:85:VAL:HG12	2:F:195:SER:CA	2.50	0.41
3:G:149:TRP:HB3	3:G:154:VAL:HG11	2.02	0.41
1:A:297:ARG:NH2	1:A:303:LEU:HD13	2.35	0.41
1:Q:294:GLY:CA	2:R:68:ARG:HH12	2.26	0.41
1:A:236:MET:HB2	1:A:236:MET:HE3	1.85	0.41
2:B:75:ALA:HA	2:B:202:TYR:HB3	2.02	0.41
3:S:96:GLU:HG3	3:S:97:ALA:H	1.85	0.41
3:K:316:GLY:O	3:K:317:LEU:HB2	2.19	0.41
3:C:167:PHE:HE1	3:C:321:VAL:H	1.69	0.41
1:Q:103:LYS:O	1:Q:104:ARG:HG3	2.20	0.41
1:I:274:ASN:ND2	3:K:240:PRO:HB3	2.36	0.41
1:I:279:PHE:CE1	3:K:212:ASP:HB3	2.56	0.41
2:N:65:LEU:HD23	2:N:65:LEU:HA	1.85	0.41
2:B:71:PHE:HA	2:B:72:PRO:HD3	1.95	0.41
3:S:116:ALA:HB3	3:S:118:ALA:N	2.36	0.41
1:I:200:PHE:CZ	1:I:202:SER:HB3	2.56	0.41
2:B:36:ILE:HA	2:B:37:PRO:HD3	1.85	0.41
1:Q:236:MET:HE3	1:Q:236:MET:HB2	1.88	0.41
1:M:293:THR:HG21	2:N:97:GLN:OE1	2.20	0.41
3:O:243:GLN:O	3:O:246:VAL:HG23	2.21	0.41
3:C:102:VAL:HA	3:C:263:ILE:HB	2.03	0.41
1:A:226:LEU:HA	1:A:226:LEU:HD12	1.72	0.41
2:R:85:VAL:HG11	2:R:194:VAL:HB	2.03	0.41
2:N:36:ILE:HA	2:N:37:PRO:HD3	1.85	0.41
3:S:216:PRO:HB2	3:S:218:LYS:HG3	2.02	0.41
1:I:208:GLN:O	1:I:234:ASN:ND2	2.44	0.41
3:O:195:VAL:O	3:O:247:CYS:HB3	2.21	0.41
1:E:277:TYR:H	2:F:235:ILE:CG2	2.33	0.41
2:F:56:ASN:HB2	2:F:71:PHE:HB3	2.03	0.41
3:G:212:ASP:OD1	3:G:212:ASP:O	2.38	0.41
1:Q:172:ARG:NH2	1:Q:243:THR:OG1	2.54	0.41
1:Q:226:LEU:O	3:S:214:HIS:ND1	2.54	0.41
1:Q:299:ALA:O	2:R:84:ALA:N	2.54	0.41
1:A:126:ARG:HD3	2:B:236:LEU:HD13	2.03	0.41
2:J:10:THR:C	2:J:12:GLN:H	2.29	0.41
2:B:7:LYS:O	2:B:10:THR:HG23	2.21	0.41
3:S:215:PRO:HA	3:S:216:PRO:HD3	1.83	0.41
3:S:318:ARG:C	3:S:319:GLN:HG2	2.45	0.41
3:K:204:VAL:HG12	3:K:206:GLY:H	1.85	0.41
3:K:205:ALA:HB1	3:K:211:GLU:H	1.85	0.41
3:G:172:ARG:O	3:G:313:GLU:N	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:TRP:CZ3	1:A:117:ILE:HA	2.56	0.41
2:N:142:LEU:HA	2:N:143:PRO:HD2	1.93	0.41
3:S:85:LEU:HB3	3:S:86:THR:HG22	2.03	0.41
3:K:308:ALA:HA	3:K:309:PRO:HD2	1.95	0.41
3:K:318:ARG:C	3:K:319:GLN:HG2	2.44	0.41
2:F:5:GLU:HA	2:R:10:THR:HG22	2.04	0.40
3:G:195:VAL:O	3:G:247:CYS:HB3	2.22	0.40
2:J:7:LYS:O	2:J:10:THR:HG23	2.21	0.40
2:J:177:TYR:OH	2:J:190:THR:O	2.32	0.40
2:F:6:LEU:HB3	2:F:10:THR:HG21	2.03	0.40
1:Q:119:ILE:HG22	1:Q:259:MET:HE1	2.03	0.40
2:J:136:THR:HB	2:J:193:LEU:HB2	2.03	0.40
3:O:121:LYS:CB	3:O:122:PRO:HD3	2.51	0.40
3:C:204:VAL:HG12	3:C:206:GLY:H	1.85	0.40
1:E:274:ASN:HB2	3:G:240:PRO:CD	2.52	0.40
2:F:174:ASN:HA	2:F:177:TYR:HD2	1.87	0.40
1:I:90:VAL:HG12	1:I:115:TRP:HZ2	1.87	0.40
1:M:164:PRO:HB2	2:J:178:ARG:HD3	2.03	0.40
1:M:220:HIS:HB3	1:M:221:LYS:H	1.61	0.40
2:F:10:THR:C	2:F:12:GLN:H	2.29	0.40
3:G:169:TYR:HB3	3:G:316:GLY:HA2	2.03	0.40
2:N:137:PRO:HG3	3:C:318:ARG:H	1.86	0.40
2:B:10:THR:C	2:B:12:GLN:H	2.29	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	230/303 (76%)	207 (90%)	19 (8%)	4 (2%)	7	30
1	E	230/303 (76%)	207 (90%)	18 (8%)	5 (2%)	5	24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	230/303 (76%)	208 (90%)	17 (7%)	5 (2%)	5	24
1	M	230/303 (76%)	208 (90%)	19 (8%)	3 (1%)	9	35
1	Q	230/303 (76%)	208 (90%)	18 (8%)	4 (2%)	7	30
2	B	226/242 (93%)	206 (91%)	18 (8%)	2 (1%)	14	44
2	F	226/242 (93%)	204 (90%)	20 (9%)	2 (1%)	14	44
2	J	226/242 (93%)	204 (90%)	20 (9%)	2 (1%)	14	44
2	N	226/242 (93%)	204 (90%)	20 (9%)	2 (1%)	14	44
2	R	226/242 (93%)	204 (90%)	20 (9%)	2 (1%)	14	44
3	C	240/323 (74%)	218 (91%)	19 (8%)	3 (1%)	9	35
3	G	240/323 (74%)	221 (92%)	16 (7%)	3 (1%)	9	35
3	K	240/323 (74%)	221 (92%)	16 (7%)	3 (1%)	9	35
3	O	240/323 (74%)	225 (94%)	11 (5%)	4 (2%)	7	30
3	S	240/323 (74%)	223 (93%)	15 (6%)	2 (1%)	16	47
All	All	3480/4340 (80%)	3168 (91%)	266 (8%)	46 (1%)	9	35

All (46) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	G	121	LYS
3	G	317	LEU
1	Q	226	LEU
1	I	226	LEU
1	M	221	LYS
1	A	100	THR
3	S	121	LYS
3	S	317	LEU
3	K	121	LYS
3	K	317	LEU
3	O	121	LYS
3	O	126	ASP
3	O	317	LEU
3	C	121	LYS
3	C	317	LEU
1	E	221	LYS
1	Q	221	LYS
1	E	111	GLY
1	Q	293	THR

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Mol	Chain	Res	Type
1	I	108	THR
1	I	220	HIS
1	A	293	THR
1	Q	111	GLY
1	I	111	GLY
1	I	293	THR
1	A	111	GLY
1	E	220	HIS
1	E	293	THR
2	F	74	SER
1	M	111	GLY
1	M	293	THR
2	R	74	SER
3	K	126	ASP
3	C	315	ALA
3	G	315	ALA
2	J	74	SER
2	N	74	SER
3	O	315	ALA
1	E	109	PRO
1	A	109	PRO
2	R	58	VAL
2	N	58	VAL
2	B	58	VAL
2	B	239	GLY
2	F	58	VAL
2	J	58	VAL

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	199/256 (78%)	190 (96%)	9 (4%)	24	56
1	E	199/256 (78%)	190 (96%)	9 (4%)	24	56
1	I	199/256 (78%)	189 (95%)	10 (5%)	22	53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	M	199/256 (78%)	193 (97%)	6 (3%)	36	65
1	Q	199/256 (78%)	193 (97%)	6 (3%)	36	65
2	B	193/202 (96%)	186 (96%)	7 (4%)	31	62
2	F	193/202 (96%)	187 (97%)	6 (3%)	35	64
2	J	193/202 (96%)	185 (96%)	8 (4%)	27	59
2	N	193/202 (96%)	186 (96%)	7 (4%)	31	62
2	R	193/202 (96%)	185 (96%)	8 (4%)	27	59
3	C	205/272 (75%)	194 (95%)	11 (5%)	20	50
3	G	205/272 (75%)	197 (96%)	8 (4%)	28	60
3	K	205/272 (75%)	196 (96%)	9 (4%)	25	56
3	O	205/272 (75%)	195 (95%)	10 (5%)	22	53
3	S	205/272 (75%)	195 (95%)	10 (5%)	22	53
All	All	2985/3650 (82%)	2861 (96%)	124 (4%)	26	58

All (124) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	103	LYS
1	E	107	LEU
1	E	152	VAL
1	E	219	GLU
1	E	220	HIS
1	E	224	LYS
1	E	226	LEU
1	E	291	LYS
1	E	300	ILE
2	F	33	CYS
2	F	70	ARG
2	F	162	GLN
2	F	165	VAL
2	F	172	ILE
2	F	235	ILE
3	G	86	THR
3	G	115	ASP
3	G	141	GLU
3	G	156	THR
3	G	211	GLU
3	G	239	ILE

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Mol	Chain	Res	Type
3	G	259	CYS
3	G	307	LEU
1	Q	98	GLU
1	Q	102	ARG
1	Q	107	LEU
1	Q	152	VAL
1	Q	291	LYS
1	Q	300	ILE
1	I	102	ARG
1	I	110	ASN
1	I	152	VAL
1	I	219	GLU
1	I	223	GLU
1	I	224	LYS
1	I	226	LEU
1	I	290	ILE
1	I	291	LYS
1	I	300	ILE
1	M	73	HIS
1	M	102	ARG
1	M	152	VAL
1	M	222	GLN
1	M	291	LYS
1	M	300	ILE
1	A	73	HIS
1	A	98	GLU
1	A	107	LEU
1	A	152	VAL
1	A	220	HIS
1	A	221	LYS
1	A	226	LEU
1	A	291	LYS
1	A	300	ILE
2	R	33	CYS
2	R	70	ARG
2	R	85	VAL
2	R	162	GLN
2	R	164	SER
2	R	165	VAL
2	R	172	ILE
2	R	235	ILE
2	J	33	CYS

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Mol	Chain	Res	Type
2	J	70	ARG
2	J	85	VAL
2	J	162	GLN
2	J	164	SER
2	J	165	VAL
2	J	172	ILE
2	J	235	ILE
2	N	33	CYS
2	N	70	ARG
2	N	162	GLN
2	N	164	SER
2	N	165	VAL
2	N	172	ILE
2	N	235	ILE
2	B	33	CYS
2	B	70	ARG
2	B	76	GLN
2	B	164	SER
2	B	165	VAL
2	B	172	ILE
2	B	235	ILE
3	S	86	THR
3	S	87	ILE
3	S	92	ILE
3	S	141	GLU
3	S	156	THR
3	S	239	ILE
3	S	259	CYS
3	S	295	GLN
3	S	307	LEU
3	S	318	ARG
3	K	81	ARG
3	K	82	VAL
3	K	86	THR
3	K	141	GLU
3	K	154	VAL
3	K	156	THR
3	K	239	ILE
3	K	259	CYS
3	K	307	LEU
3	O	85	LEU
3	O	86	THR

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Mol	Chain	Res	Type
3	O	119	VAL
3	O	154	VAL
3	O	156	THR
3	O	157	GLU
3	O	239	ILE
3	O	259	CYS
3	O	295	GLN
3	O	307	LEU
3	C	86	THR
3	C	94	THR
3	C	114	SER
3	C	141	GLU
3	C	156	THR
3	C	218	LYS
3	C	239	ILE
3	C	259	CYS
3	C	295	GLN
3	C	307	LEU
3	C	319	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
2	F	61	ASN
3	G	95	GLN
3	G	319	GLN
1	I	110	ASN
1	M	222	GLN
1	A	233	ASN
2	R	61	ASN
2	J	61	ASN
2	J	110	GLN
2	N	48	GLN
2	B	61	ASN
2	B	76	GLN
3	S	163	GLN
3	S	188	GLN
3	S	280	ASN
3	S	295	GLN
3	K	280	ASN
3	O	188	GLN
3	O	280	ASN

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Mol	Chain	Res	Type
3	C	230	GLN
3	C	280	ASN
3	C	295	GLN
3	C	319	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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	232/303 (76%)	0.52	40 (17%) 4 2	25, 40, 140, 156	0
1	E	232/303 (76%)	0.45	36 (15%) 5 2	27, 41, 140, 154	0
1	I	232/303 (76%)	0.60	37 (15%) 5 2	30, 41, 142, 157	0
1	M	232/303 (76%)	0.55	37 (15%) 5 2	28, 41, 142, 156	0
1	Q	232/303 (76%)	0.46	33 (14%) 6 3	29, 42, 140, 156	0
2	B	230/242 (95%)	0.50	26 (11%) 10 5	27, 41, 73, 147	0
2	F	230/242 (95%)	0.33	20 (8%) 16 9	32, 44, 80, 142	0
2	J	230/242 (95%)	0.43	26 (11%) 10 5	31, 44, 79, 145	0
2	N	230/242 (95%)	0.40	24 (10%) 11 6	28, 44, 76, 149	0
2	R	230/242 (95%)	0.39	26 (11%) 10 5	30, 45, 81, 145	0
3	C	242/323 (74%)	0.72	46 (19%) 3 1	25, 47, 130, 150	0
3	G	242/323 (74%)	0.55	40 (16%) 4 2	31, 50, 131, 149	0
3	K	242/323 (74%)	0.64	46 (19%) 3 1	29, 50, 130, 148	0
3	O	242/323 (74%)	0.57	44 (18%) 3 1	31, 52, 131, 148	0
3	S	242/323 (74%)	0.67	46 (19%) 3 1	31, 52, 133, 148	0
All	All	3520/4340 (81%)	0.52	527 (14%) 5 3	25, 44, 129, 157	0

All (527) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	107	LEU	8.8
1	E	107	LEU	8.5
1	I	107	LEU	8.5
1	A	107	LEU	8.0
1	Q	107	LEU	7.8
2	B	84	ALA	7.2
3	O	321	VAL	6.9

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Mol	Chain	Res	Type	RSRZ
3	K	119	VAL	6.9
3	S	119	VAL	6.8
1	I	109	PRO	6.8
3	G	118	ALA	6.7
3	C	321	VAL	6.7
3	S	321	VAL	6.5
3	G	321	VAL	6.5
3	C	119	VAL	6.4
1	I	216	THR	6.3
2	B	83	CYS	6.3
2	R	164	SER	6.2
1	I	303	LEU	6.2
2	R	239	GLY	6.1
3	G	119	VAL	6.0
1	E	108	THR	6.0
3	K	118	ALA	6.0
3	C	320	ALA	6.0
3	C	118	ALA	5.9
3	C	117	THR	5.9
2	B	86	PHE	5.9
3	K	320	ALA	5.9
1	E	226	LEU	5.8
3	O	320	ALA	5.7
3	C	208	THR	5.7
1	A	226	LEU	5.7
3	S	318	ARG	5.7
1	I	108	THR	5.6
2	J	164	SER	5.6
3	K	321	VAL	5.6
2	J	84	ALA	5.5
2	N	189	TYR	5.5
3	K	208	THR	5.5
3	K	97	ALA	5.4
2	N	164	SER	5.4
2	N	85	VAL	5.4
3	S	93	THR	5.4
1	M	109	PRO	5.4
2	J	240	THR	5.3
2	J	85	VAL	5.3
1	M	303	LEU	5.3
2	B	240	THR	5.3
1	I	103	LYS	5.3

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Mol	Chain	Res	Type	RSRZ
2	B	239	GLY	5.2
1	I	217	PHE	5.2
1	E	303	LEU	5.2
3	O	93	THR	5.2
1	A	227	GLU	5.2
1	E	216	THR	5.2
2	F	240	THR	5.2
3	O	208	THR	5.2
2	R	86	PHE	5.1
2	N	83	CYS	5.1
3	S	208	THR	5.1
3	C	98	ALA	5.1
3	O	119	VAL	5.1
2	R	189	TYR	5.1
2	F	85	VAL	5.0
1	A	217	PHE	5.0
2	R	238	THR	5.0
1	I	72	SER	5.0
2	J	83	CYS	5.0
1	I	106	ARG	5.0
1	M	216	THR	5.0
3	S	118	ALA	4.9
1	Q	108	THR	4.9
3	K	207	GLY	4.9
1	A	216	THR	4.9
2	B	175	THR	4.9
3	K	206	GLY	4.9
1	M	105	ALA	4.9
1	E	223	GLU	4.9
3	C	97	ALA	4.9
3	O	85	LEU	4.8
2	R	83	CYS	4.8
1	A	106	ARG	4.8
3	S	80	ASP	4.8
3	S	117	THR	4.8
2	R	85	VAL	4.8
2	F	164	SER	4.8
3	K	98	ALA	4.7
1	Q	103	LYS	4.7
1	A	303	LEU	4.7
1	Q	221	LYS	4.7
3	S	97	ALA	4.7

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Mol	Chain	Res	Type	RSRZ
2	R	84	ALA	4.7
3	O	117	THR	4.7
1	Q	220	HIS	4.7
1	I	220	HIS	4.7
3	K	120	ASP	4.7
3	O	97	ALA	4.7
3	C	121	LYS	4.6
3	K	121	LYS	4.6
3	G	317	LEU	4.6
1	E	109	PRO	4.6
3	C	129	VAL	4.6
1	M	226	LEU	4.5
1	E	105	ALA	4.5
1	Q	226	LEU	4.5
3	G	120	ASP	4.5
1	I	221	LYS	4.5
2	J	86	PHE	4.5
3	G	207	GLY	4.5
1	I	287	GLY	4.4
1	A	72	SER	4.4
3	G	121	LYS	4.4
1	A	287	GLY	4.4
1	I	226	LEU	4.4
1	M	220	HIS	4.4
2	J	177	TYR	4.4
2	N	84	ALA	4.4
3	O	120	ASP	4.4
2	J	238	THR	4.3
3	G	80	ASP	4.3
3	O	86	THR	4.3
1	E	217	PHE	4.3
2	B	164	SER	4.3
1	M	223	GLU	4.3
1	Q	217	PHE	4.3
2	N	86	PHE	4.3
2	F	177	TYR	4.3
3	G	97	ALA	4.3
3	G	114	SER	4.3
1	Q	223	GLU	4.3
2	B	85	VAL	4.3
2	F	238	THR	4.3
3	C	317	LEU	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	288	ASN	4.2
3	G	98	ALA	4.2
2	J	175	THR	4.2
1	M	106	ARG	4.2
1	A	109	PRO	4.2
3	S	98	ALA	4.2
1	A	294	GLY	4.2
2	R	240	THR	4.2
1	I	227	GLU	4.2
2	R	175	THR	4.2
2	R	177	TYR	4.2
1	A	295	ALA	4.2
3	O	98	ALA	4.2
3	G	319	GLN	4.1
1	M	108	THR	4.1
1	A	108	THR	4.1
3	K	117	THR	4.1
2	J	1	GLY	4.1
3	O	82	VAL	4.1
2	B	177	TYR	4.1
3	C	318	ARG	4.1
3	C	207	GLY	4.1
1	Q	303	LEU	4.0
1	Q	216	THR	4.0
2	F	83	CYS	4.0
1	I	105	ALA	4.0
3	S	320	ALA	4.0
3	C	84	GLN	4.0
2	R	178	ARG	4.0
3	S	127	VAL	4.0
1	I	298	THR	4.0
3	C	315	ALA	4.0
1	M	103	LYS	4.0
1	Q	292	PRO	4.0
3	G	320	ALA	4.0
2	B	195	SER	4.0
3	S	210	THR	4.0
3	C	86	THR	4.0
2	J	239	GLY	3.9
3	S	120	ASP	3.9
3	K	82	VAL	3.9
1	I	96	PRO	3.9

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Mol	Chain	Res	Type	RSRZ
3	C	83	ALA	3.9
1	A	302	THR	3.9
3	C	94	THR	3.9
1	A	221	LYS	3.9
2	F	189	TYR	3.9
1	Q	100	THR	3.9
3	C	115	ASP	3.9
3	C	319	GLN	3.9
1	Q	106	ARG	3.9
1	I	100	THR	3.8
3	S	96	GLU	3.8
2	B	238	THR	3.8
3	C	316	GLY	3.8
1	M	96	PRO	3.8
1	E	288	ASN	3.8
2	F	178	ARG	3.8
1	A	105	ALA	3.8
1	M	227	GLU	3.8
2	N	238	THR	3.8
2	F	84	ALA	3.8
3	G	208	THR	3.8
3	C	203	THR	3.8
1	Q	105	ALA	3.7
1	E	103	LYS	3.7
1	I	302	THR	3.7
1	A	218	GLY	3.7
3	O	207	GLY	3.7
1	E	96	PRO	3.7
2	F	175	THR	3.7
1	M	72	SER	3.7
2	F	239	GLY	3.7
3	S	207	GLY	3.7
1	M	221	LYS	3.7
2	B	189	TYR	3.7
3	C	82	VAL	3.7
3	C	93	THR	3.7
2	B	178	ARG	3.7
2	N	235	ILE	3.7
1	I	218	GLY	3.6
1	E	106	ARG	3.6
3	C	80	ASP	3.6
3	G	93	THR	3.6

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Mol	Chain	Res	Type	RSRZ
1	Q	73	HIS	3.6
2	F	86	PHE	3.6
2	N	178	ARG	3.6
2	F	235	ILE	3.6
2	N	177	TYR	3.6
1	E	287	GLY	3.5
3	O	118	ALA	3.5
1	A	292	PRO	3.5
2	B	176	HIS	3.5
3	G	115	ASP	3.5
3	O	115	ASP	3.5
2	B	235	ILE	3.5
2	N	175	THR	3.5
3	G	89	ASN	3.5
2	J	176	HIS	3.5
1	E	227	GLU	3.4
1	Q	72	SER	3.4
1	Q	109	PRO	3.4
1	A	96	PRO	3.4
1	A	103	LYS	3.4
1	E	73	HIS	3.4
2	J	178	ARG	3.4
3	C	127	VAL	3.4
3	G	116	ALA	3.4
3	O	91	THR	3.4
1	M	100	THR	3.4
3	S	203	THR	3.4
3	S	130	ASN	3.3
2	F	236	LEU	3.3
3	G	117	THR	3.3
3	S	86	THR	3.3
2	J	189	TYR	3.3
2	N	237	GLN	3.3
1	M	217	PHE	3.3
1	A	223	GLU	3.3
2	N	239	GLY	3.3
3	S	82	VAL	3.3
3	K	116	ALA	3.3
3	K	209	GLY	3.3
3	S	128	SER	3.3
1	A	293	THR	3.3
3	O	96	GLU	3.3

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Mol	Chain	Res	Type	RSRZ
1	Q	96	PRO	3.2
2	R	176	HIS	3.2
3	K	127	VAL	3.2
1	I	293	THR	3.2
2	J	194	VAL	3.2
3	S	317	LEU	3.2
3	O	127	VAL	3.2
1	Q	287	GLY	3.1
3	G	127	VAL	3.1
3	S	204	VAL	3.1
1	E	220	HIS	3.1
2	F	162	GLN	3.1
1	Q	295	ALA	3.1
3	K	83	ALA	3.1
2	N	190	THR	3.1
3	S	129	VAL	3.1
1	I	73	HIS	3.1
1	Q	294	GLY	3.1
3	K	93	THR	3.1
2	N	176	HIS	3.1
3	K	210	THR	3.1
2	R	235	ILE	3.1
3	G	315	ALA	3.0
3	C	96	GLU	3.0
1	Q	225	ASP	3.0
1	E	225	ASP	3.0
1	E	302	THR	3.0
1	Q	298	THR	3.0
3	O	317	LEU	3.0
2	F	89	ASP	3.0
1	A	111	GLY	3.0
3	O	129	VAL	3.0
3	C	130	ASN	3.0
3	O	94	THR	3.0
3	C	210	THR	3.0
2	J	235	ILE	3.0
3	S	92	ILE	3.0
3	C	116	ALA	3.0
3	G	82	VAL	2.9
3	S	319	GLN	2.9
3	K	84	GLN	2.9
2	N	240	THR	2.9

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Mol	Chain	Res	Type	RSRZ
3	C	217	TYR	2.9
1	M	294	GLY	2.9
1	E	224	LYS	2.9
1	A	215	PRO	2.9
1	E	295	ALA	2.9
1	I	223	GLU	2.9
1	I	292	PRO	2.9
1	M	295	ALA	2.9
2	F	176	HIS	2.9
2	N	236	LEU	2.9
3	K	203	THR	2.9
3	K	89	ASN	2.9
3	G	126	ASP	2.8
3	S	83	ALA	2.8
3	K	80	ASP	2.8
3	K	205	ALA	2.8
1	Q	293	THR	2.8
1	M	292	PRO	2.8
1	M	302	THR	2.8
3	G	130	ASN	2.8
3	G	206	GLY	2.8
3	S	209	GLY	2.8
3	K	315	ALA	2.8
1	A	100	THR	2.8
1	Q	227	GLU	2.8
3	K	113	ASP	2.8
3	K	211	GLU	2.8
2	B	194	VAL	2.8
1	I	99	GLY	2.8
3	K	318	ARG	2.8
2	J	81	GLU	2.8
3	G	203	THR	2.8
1	M	111	GLY	2.7
1	M	165	GLY	2.7
2	R	1	GLY	2.7
2	R	73	VAL	2.7
3	K	317	LEU	2.7
3	C	128	SER	2.7
1	E	298	THR	2.7
3	O	203	THR	2.7
2	B	1	GLY	2.7
1	A	225	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	Q	299	ALA	2.7
1	I	299	ALA	2.7
3	O	315	ALA	2.7
2	R	236	LEU	2.7
3	C	85	LEU	2.7
1	Q	219	GLU	2.7
3	G	86	THR	2.7
2	J	89	ASP	2.7
3	G	83	ALA	2.7
3	K	319	GLN	2.7
1	I	295	ALA	2.7
3	O	83	ALA	2.7
3	C	204	VAL	2.7
3	C	120	ASP	2.7
1	M	288	ASN	2.7
1	I	294	GLY	2.6
1	A	97	LEU	2.6
3	C	114	SER	2.6
1	A	224	LYS	2.6
2	B	227	GLN	2.6
3	S	89	ASN	2.6
1	A	298	THR	2.6
3	G	128	SER	2.6
3	K	169	TYR	2.6
1	E	292	PRO	2.6
3	K	115	ASP	2.6
1	I	97	LEU	2.6
3	S	116	ALA	2.6
3	K	125	PRO	2.6
2	R	89	ASP	2.6
3	O	319	GLN	2.6
2	B	61	ASN	2.6
1	E	101	GLU	2.6
1	M	298	THR	2.6
1	A	73	HIS	2.6
1	E	232	PRO	2.6
3	O	128	SER	2.6
1	Q	288	ASN	2.6
3	G	212	ASP	2.6
2	B	236	LEU	2.6
1	I	111	GLY	2.5
1	M	287	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
3	C	209	GLY	2.5
3	S	211	GLU	2.5
3	C	211	GLU	2.5
1	M	112	TYR	2.5
2	J	236	LEU	2.5
3	G	213	SER	2.5
1	I	224	LYS	2.5
3	S	113	ASP	2.5
3	O	126	ASP	2.5
3	K	92	ILE	2.5
1	M	293	THR	2.5
3	O	80	ASP	2.5
3	C	212	ASP	2.5
1	E	100	THR	2.5
1	I	267	TRP	2.5
3	S	94	THR	2.5
1	M	73	HIS	2.5
3	O	169	TYR	2.5
3	O	114	SER	2.5
2	N	89	ASP	2.5
2	N	10	THR	2.5
3	S	91	THR	2.5
3	O	92	ILE	2.4
1	E	72	SER	2.4
2	B	190	THR	2.4
1	A	112	TYR	2.4
1	A	291	LYS	2.4
1	E	98	GLU	2.4
3	G	81	ARG	2.4
3	K	96	GLU	2.4
3	K	94	THR	2.4
1	E	99	GLY	2.4
1	A	220	HIS	2.4
2	J	80	GLY	2.4
3	O	209	GLY	2.4
3	C	206	GLY	2.4
3	K	81	ARG	2.4
1	M	219	GLU	2.4
2	N	233	SER	2.4
3	S	112	SER	2.4
1	E	218	GLY	2.3
2	B	237	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
3	G	84	GLN	2.3
1	I	219	GLU	2.3
1	E	221	LYS	2.3
1	E	294	GLY	2.3
3	O	99	ASN	2.3
3	K	212	ASP	2.3
1	A	297	ARG	2.3
2	R	38	GLY	2.3
2	R	190	THR	2.3
2	J	195	SER	2.3
2	B	163	SER	2.3
3	O	205	ALA	2.3
3	S	111	CYS	2.3
3	S	115	ASP	2.3
2	B	76	GLN	2.3
1	Q	215	PRO	2.3
2	N	1	GLY	2.3
1	I	286	ALA	2.3
1	M	286	ALA	2.3
1	M	224	LYS	2.3
1	I	297	ARG	2.3
1	M	215	PRO	2.3
3	O	125	PRO	2.3
1	Q	99	GLY	2.3
2	J	190	THR	2.3
2	R	195	SER	2.3
2	J	163	SER	2.3
3	K	99	ASN	2.3
2	J	237	GLN	2.3
2	B	110	GLN	2.3
3	C	126	ASP	2.3
3	O	215	PRO	2.2
1	E	299	ALA	2.2
1	A	299	ALA	2.2
2	R	80	GLY	2.2
3	O	210	THR	2.2
3	G	217	TYR	2.2
3	S	121	LYS	2.2
3	O	318	ARG	2.2
3	S	212	ASP	2.2
3	O	212	ASP	2.2
2	J	82	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
3	K	316	GLY	2.2
3	G	95	GLN	2.2
3	O	84	GLN	2.2
3	K	122	PRO	2.2
2	F	73	VAL	2.2
3	G	112	SER	2.2
1	I	101	GLU	2.2
3	S	99	ASN	2.2
1	Q	111	GLY	2.2
1	E	280	LYS	2.2
3	S	81	ARG	2.2
3	G	214	HIS	2.2
3	K	86	THR	2.2
2	R	194	VAL	2.2
3	C	87	ILE	2.2
3	C	295	GLN	2.2
3	G	209	GLY	2.2
3	C	88	GLY	2.2
3	S	87	ILE	2.1
2	N	162	GLN	2.1
3	S	85	LEU	2.1
3	O	90	SER	2.1
2	N	38	GLY	2.1
1	Q	224	LYS	2.1
1	A	222	GLN	2.1
3	S	205	ALA	2.1
2	N	81	GLU	2.1
3	S	206	GLY	2.1
3	K	126	ASP	2.1
3	C	100	ILE	2.1
1	I	112	TYR	2.1
3	G	318	ARG	2.1
3	O	116	ALA	2.1
2	F	81	GLU	2.1
2	R	233	SER	2.1
3	S	114	SER	2.1
1	A	267	TRP	2.1
1	E	97	LEU	2.1
1	E	112	TYR	2.1
3	G	94	THR	2.1
3	K	91	THR	2.1
1	M	299	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
2	R	237	GLN	2.1
1	M	99	GLY	2.1
3	O	211	GLU	2.1
3	C	81	ARG	2.1
1	A	286	ALA	2.1
1	M	98	GLU	2.1
2	R	82	LEU	2.0
3	K	130	ASN	2.0
2	F	152	GLY	2.0
2	B	162	GLN	2.0
1	Q	280	LYS	2.0
3	K	204	VAL	2.0
1	M	97	LEU	2.0
1	A	110	ASN	2.0
3	O	130	ASN	2.0
2	J	193	LEU	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.