



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 07:04 PM UTC

PDB ID : 4U7U / pdb_00004u7u
Title : Crystal structure of RNA-guided immune Cascade complex from E.coli
Authors : Zhao, H.; Sheng, G.; Wang, J.; Wang, M.; Bunkoczi, G.; Gong, W.; Wei, Z.; Wang, Y.
Deposited on : 2014-07-31
Resolution : 3.00 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

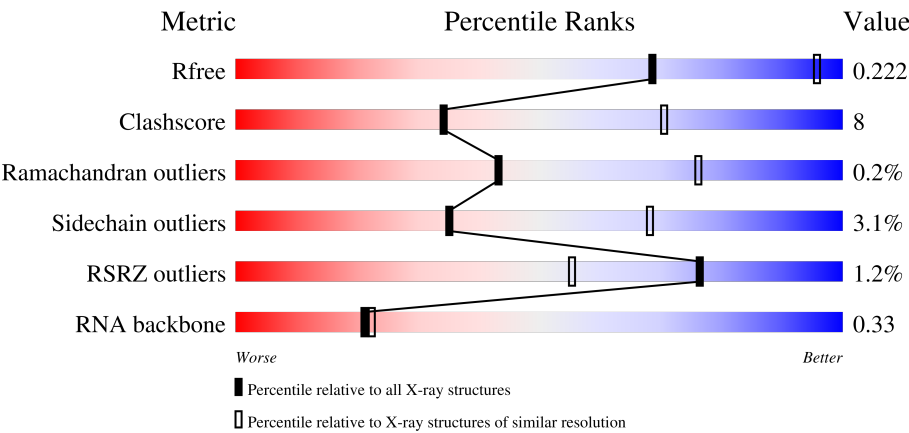
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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.



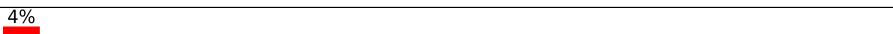
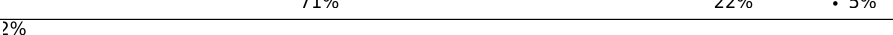
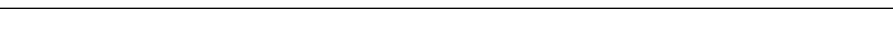
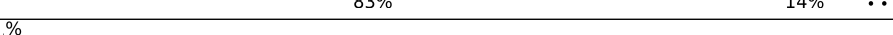
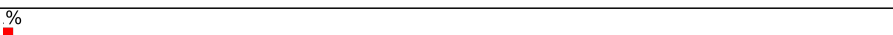
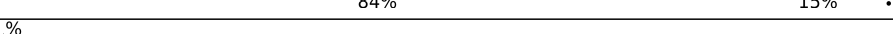
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)
RNA backbone	3983	1109 (3.20-2.80)

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

Mol	Chain	Length	Quality of chain
1	A	502	% 74% 21% • •
1	M	502	80% 15% • •
2	B	160	% 81% 17% •
2	C	160	% 84% 11% • • •

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Mol	Chain	Length	Quality of chain
2	N	160	
2	O	160	
3	D	201	
3	P	201	
4	E	363	
4	F	363	
4	G	363	
4	H	363	
4	I	363	
4	J	363	
4	Q	363	
4	R	363	
4	S	363	
4	T	363	
4	U	363	
4	V	363	
5	K	224	
5	W	224	
6	L	61	
6	X	61	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 54555 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 CRISPR system Cascade subunit CasA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	480	Total	C	N	O	S	0	0	0
			3739	2386	659	674	20			
1	M	489	Total	C	N	O	S	0	0	0
			3812	2428	673	691	20			

- Molecule 2 is a protein called CRISPR system Cascade subunit CasB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	157	Total	C	N	O	S	0	0	0
			1291	808	249	227	7			
2	C	157	Total	C	N	O	S	0	0	0
			1292	809	249	227	7			
2	N	152	Total	C	N	O	S	0	0	0
			1246	784	240	215	7			
2	O	156	Total	C	N	O	S	0	0	0
			1247	785	234	221	7			

- Molecule 3 is a protein called CRISPR system Cascade subunit CasE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	191	Total	C	N	O	S	0	0	0
			1451	931	255	258	7			
3	P	191	Total	C	N	O	S	0	0	0
			1459	936	258	258	7			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-1	ALA	-	expression tag	UNP Q46897
D	0	TRP	-	expression tag	UNP Q46897
P	-1	ALA	-	expression tag	UNP Q46897
P	0	TRP	-	expression tag	UNP Q46897

- Molecule 4 is a protein called CRISPR system Cascade subunit CasC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	357	Total	C	N	O	S	0	0	0
			2752	1721	490	525	16			
4	F	359	Total	C	N	O	S	0	0	0
			2760	1727	489	528	16			
4	G	356	Total	C	N	O	S	0	0	0
			2753	1720	490	527	16			
4	H	363	Total	C	N	O	S	0	0	0
			2774	1736	493	529	16			
4	I	355	Total	C	N	O	S	0	0	0
			2731	1711	485	519	16			
4	J	351	Total	C	N	O	S	0	0	0
			2680	1678	473	513	16			
4	Q	362	Total	C	N	O	S	0	0	0
			2790	1744	495	535	16			
4	R	359	Total	C	N	O	S	0	0	0
			2736	1712	484	524	16			
4	S	361	Total	C	N	O	S	0	0	0
			2773	1734	494	529	16			
4	T	360	Total	C	N	O	S	0	0	0
			2777	1738	494	529	16			
4	U	354	Total	C	N	O	S	0	0	0
			2723	1704	482	521	16			
4	V	355	Total	C	N	O	S	0	0	0
			2725	1704	482	523	16			

- Molecule 5 is a protein called CRISPR system Cascade subunit CasD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	K	218	Total	C	N	O	S	0	0	0
			1722	1090	305	318	9			
5	W	218	Total	C	N	O	S	0	0	0
			1726	1093	306	318	9			

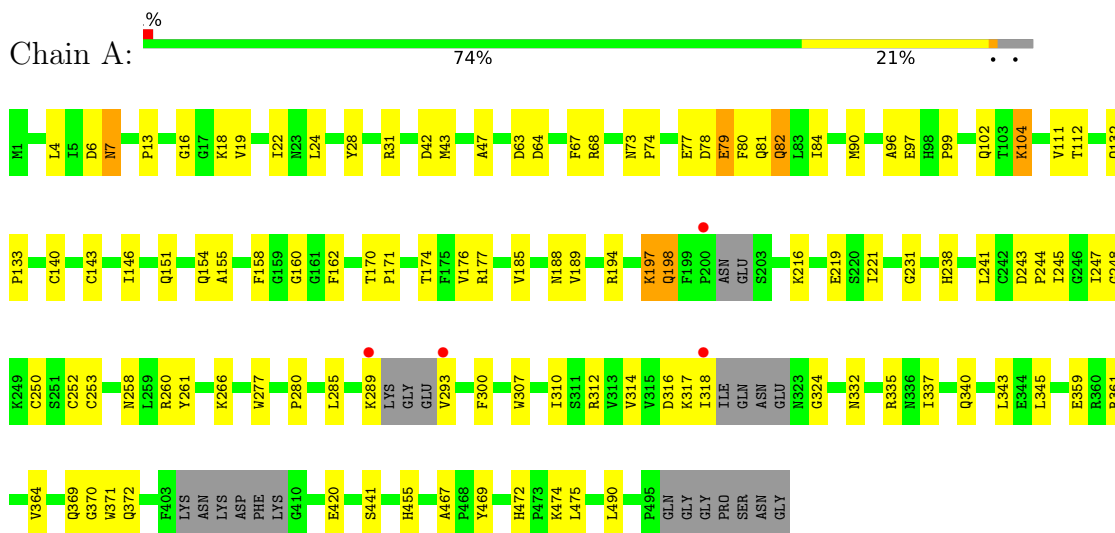
- Molecule 6 is a RNA chain called crRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	L	61	Total	C	N	O	P	0	0	0
			1298	580	230	428	60			
6	X	61	Total	C	N	O	P	0	0	0
			1298	580	230	428	60			

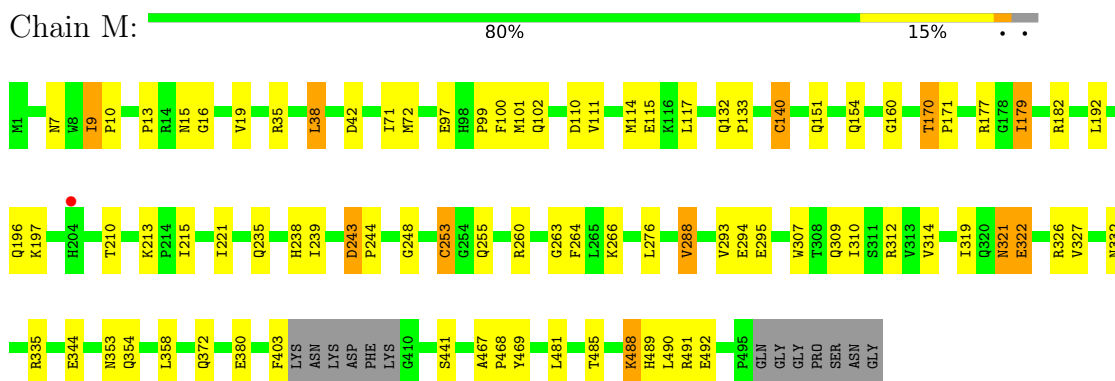
3 Residue-property plots

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.

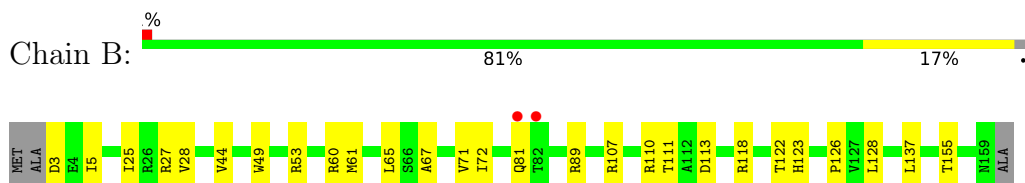
• Molecule 1: CRISPR system Cascade subunit CasA



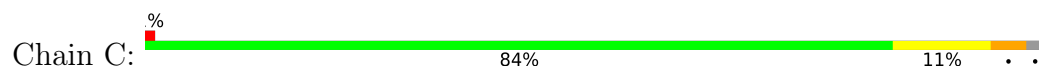
• Molecule 1: CRISPR system Cascade subunit CasA



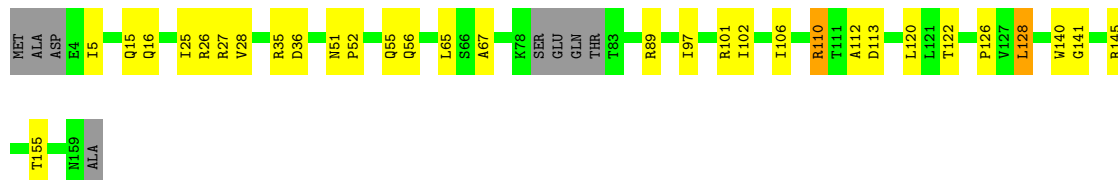
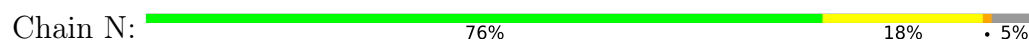
• Molecule 2: CRISPR system Cascade subunit CasB



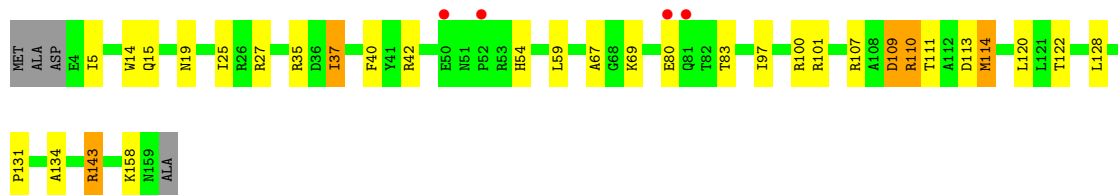
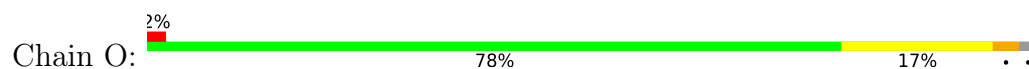
- Molecule 2: CRISPR system Cascade subunit CasB



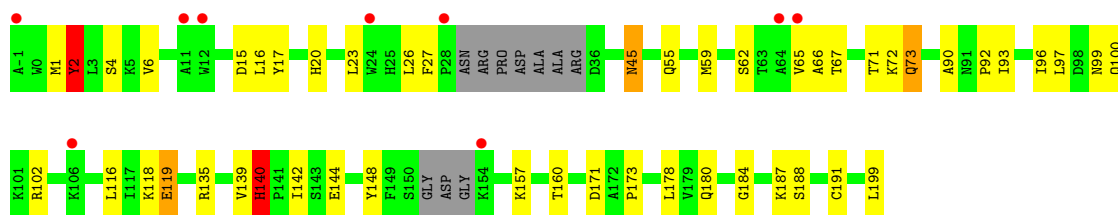
- Molecule 2: CRISPR system Cascade subunit CasB



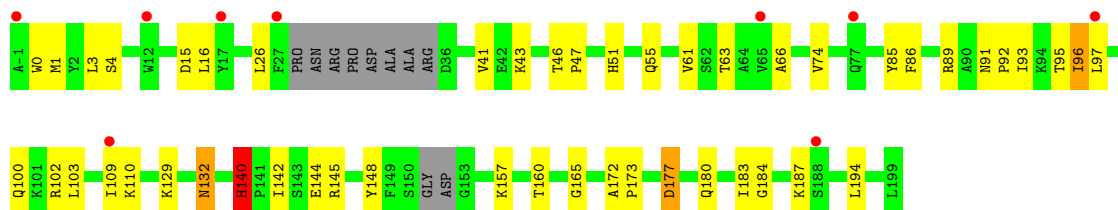
- Molecule 2: CRISPR system Cascade subunit CasB



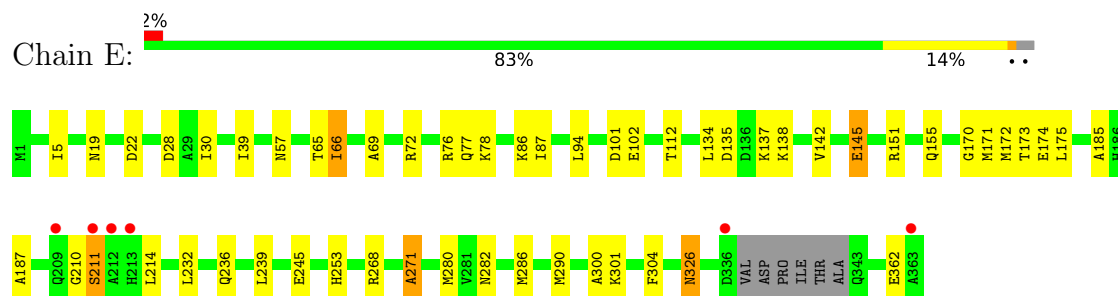
- Molecule 3: CRISPR system Cascade subunit CasE



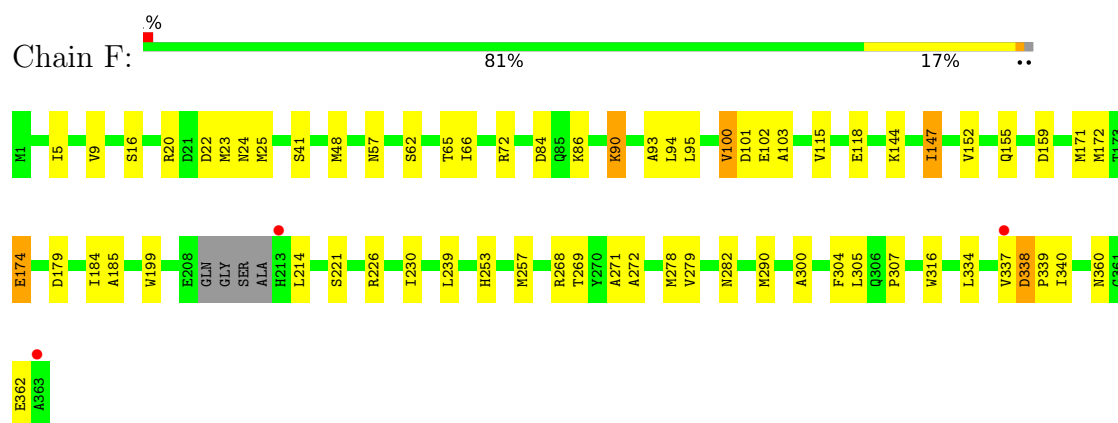
- Molecule 3: CRISPR system Cascade subunit CasE



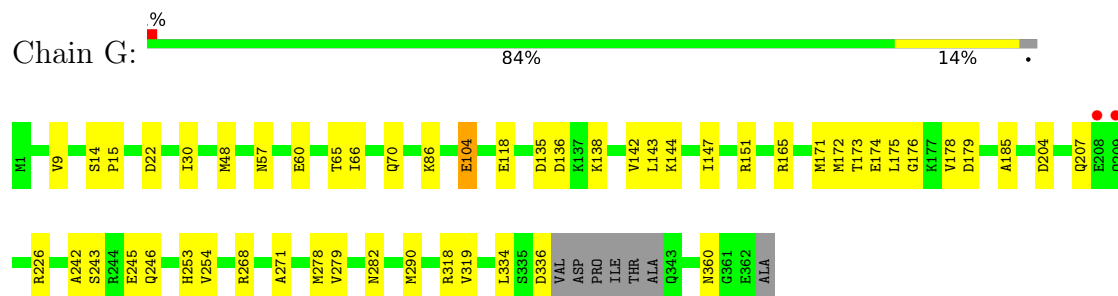
- Molecule 4: CRISPR system Cascade subunit CasC



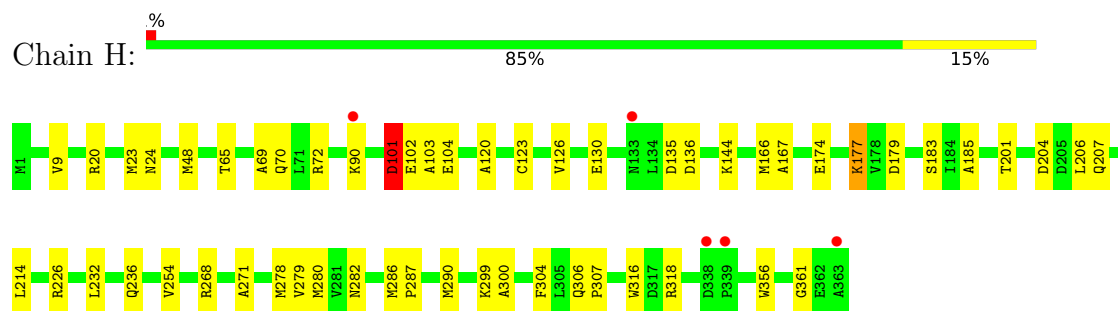
- Molecule 4: CRISPR system Cascade subunit CasC



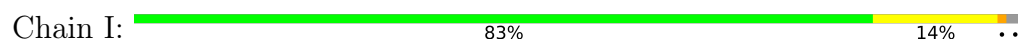
- Molecule 4: CRISPR system Cascade subunit CasC

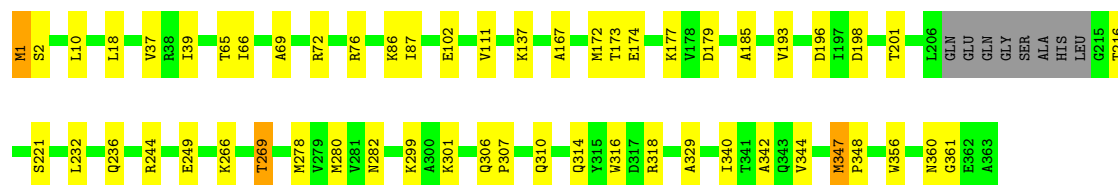


- Molecule 4: CRISPR system Cascade subunit CasC

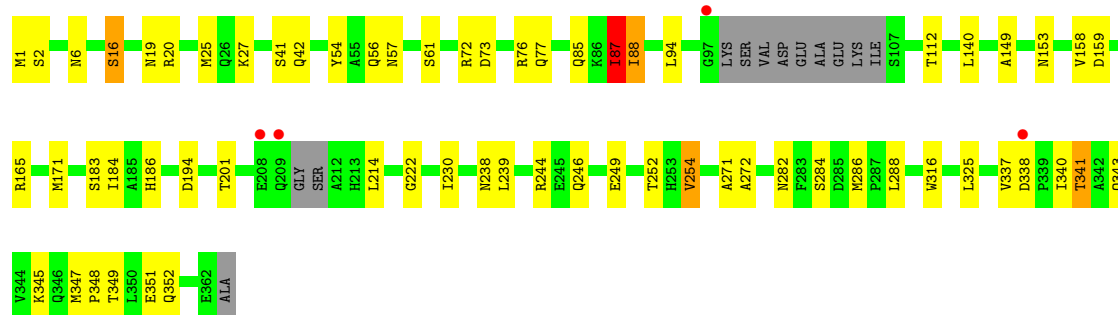
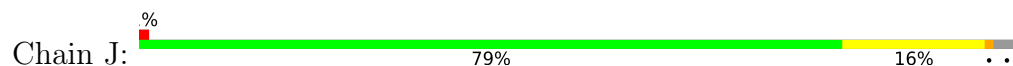


- Molecule 4: CRISPR system Cascade subunit CasC

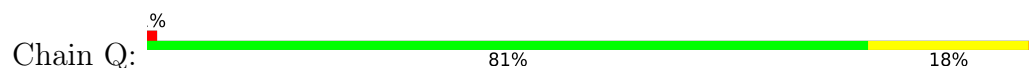




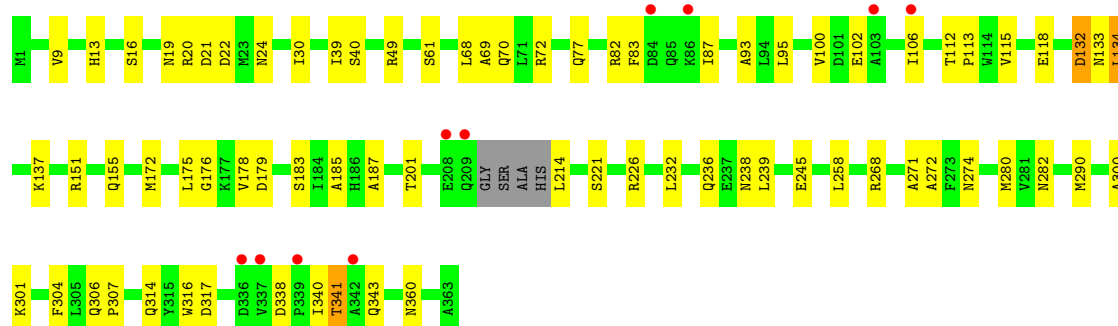
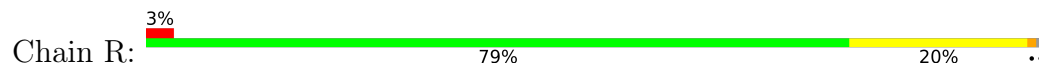
• Molecule 4: CRISPR system Cascade subunit CasC



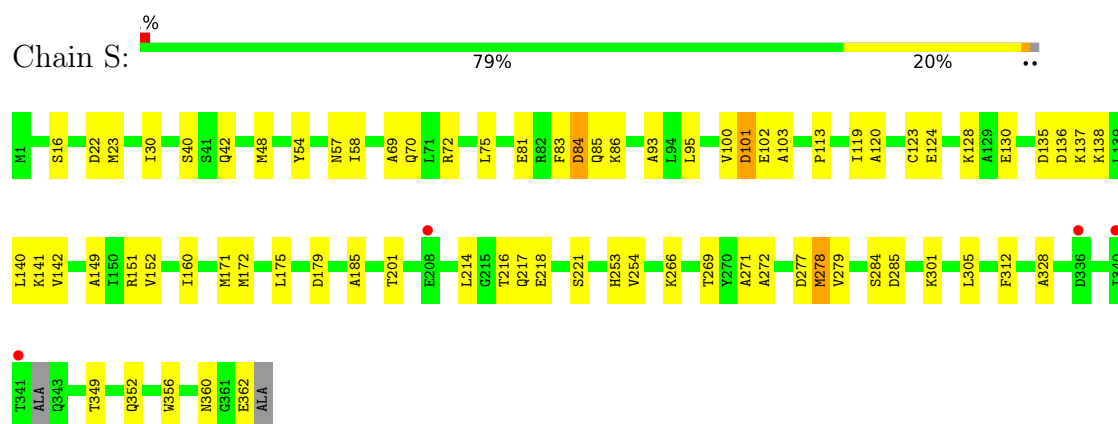
• Molecule 4: CRISPR system Cascade subunit CasC



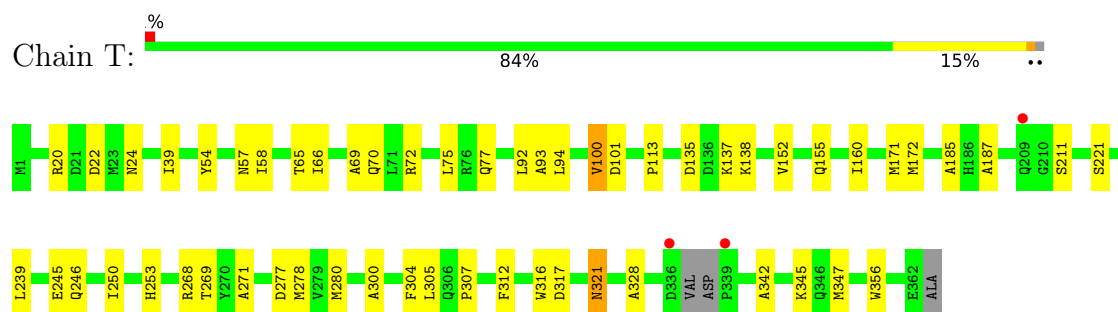
• Molecule 4: CRISPR system Cascade subunit CasC



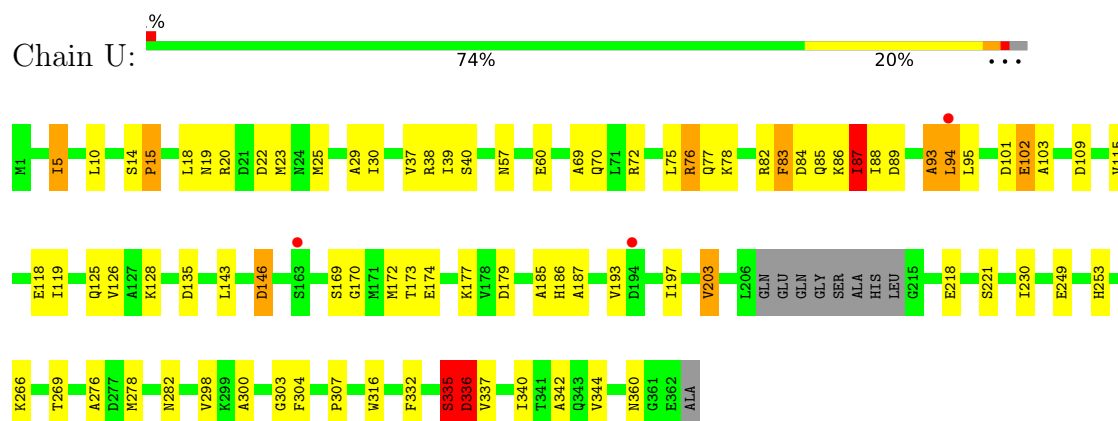
• Molecule 4: CRISPR system Cascade subunit CasC



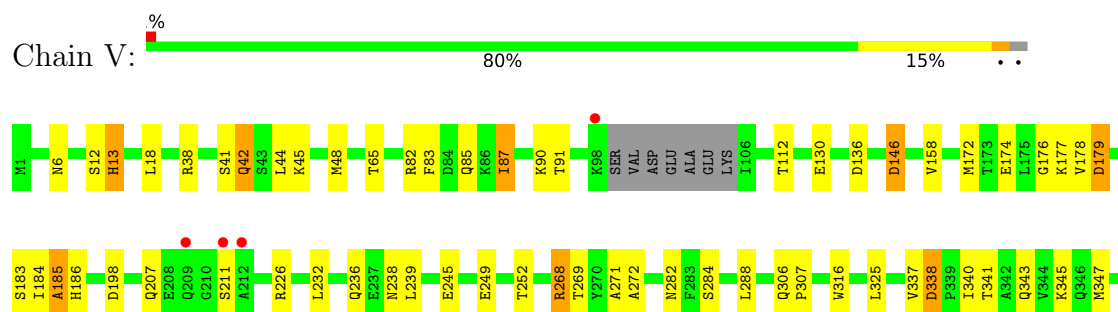
• Molecule 4: CRISPR system Cascade subunit CasC



• Molecule 4: CRISPR system Cascade subunit CasC

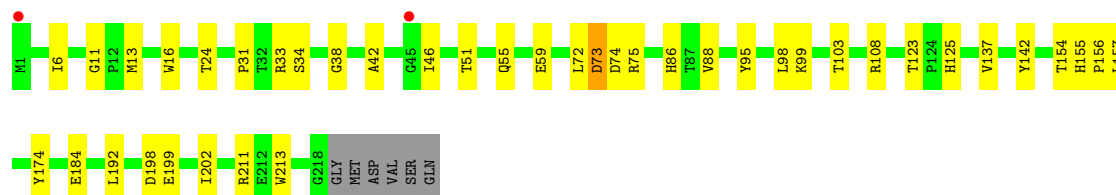
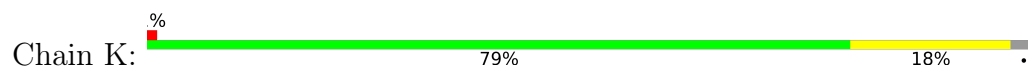


• Molecule 4: CRISPR system Cascade subunit CasC

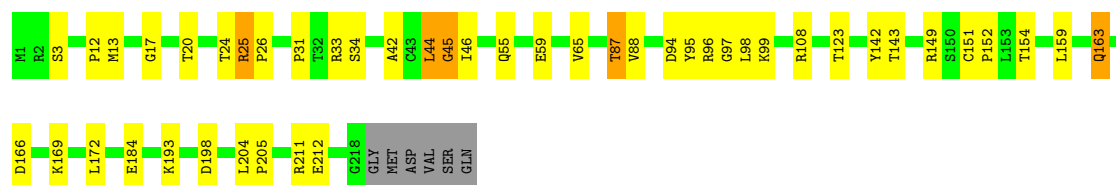
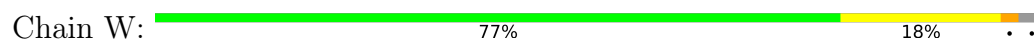




- Molecule 5: CRISPR system Cascade subunit CasD



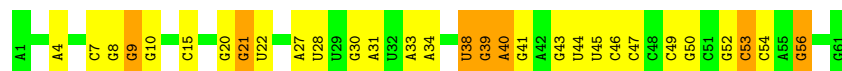
- Molecule 5: CRISPR system Cascade subunit CasD



- Molecule 6: crRNA



- Molecule 6: crRNA



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	111.41Å 118.14Å 225.87Å 92.23° 93.55° 106.06°	Depositor
Resolution (Å)	43.80 – 3.00 43.80 – 3.00	Depositor EDS
% Data completeness (in resolution range)	88.8 (43.80-3.00) 88.7 (43.80-3.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.22 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.179 , 0.218 0.186 , 0.222	Depositor DCC
R_{free} test set	9794 reflections (4.45%)	wwPDB-VP
Wilson B-factor (Å ²)	55.6	Xtriage
Anisotropy	0.128	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 39.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	54555	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.83% 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	0.58	0/3825	0.88	10/5197 (0.2%)
1	M	0.84	1/3901 (0.0%)	0.88	9/5303 (0.2%)
2	B	0.82	0/1316	0.83	1/1777 (0.1%)
2	C	0.81	1/1317 (0.1%)	1.03	6/1778 (0.3%)
2	N	0.68	0/1270	0.83	2/1714 (0.1%)
2	O	0.62	0/1272	0.96	9/1724 (0.5%)
3	D	0.64	0/1480	1.08	7/2011 (0.3%)
3	P	0.54	0/1488	0.97	3/2019 (0.1%)
4	E	0.83	1/2795 (0.0%)	0.82	1/3768 (0.0%)
4	F	0.82	0/2803	0.83	4/3785 (0.1%)
4	G	0.87	0/2796	0.81	0/3771
4	H	0.87	0/2819	0.85	0/3809
4	I	0.84	0/2774	0.84	4/3744 (0.1%)
4	J	0.72	0/2722	0.84	4/3681 (0.1%)
4	Q	0.97	0/2834	0.84	2/3823 (0.1%)
4	R	0.81	0/2779	0.88	7/3758 (0.2%)
4	S	0.81	0/2817	0.85	1/3802 (0.0%)
4	T	0.82	0/2821	0.84	2/3805 (0.1%)
4	U	0.70	0/2766	0.91	7/3737 (0.2%)
4	V	0.97	0/2768	0.93	6/3741 (0.2%)
5	K	0.63	0/1764	0.88	2/2398 (0.1%)
5	W	0.90	0/1768	0.93	5/2402 (0.2%)
6	L	0.60	0/1450	0.58	0/2259
6	X	0.62	0/1450	0.56	0/2259
All	All	0.79	3/55795 (0.0%)	0.86	92/76065 (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
4	R	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
4	U	0	2
All	All	0	4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	112	ALA	N-CA	-5.65	1.39	1.46
4	E	19	ASN	C-O	-5.24	1.17	1.24
1	M	170	THR	C-O	-5.04	1.21	1.23

All (92) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	112	ALA	N-CA-C	-17.31	92.42	111.28
3	D	140	HIS	CA-C-N	12.75	135.78	119.84
3	D	140	HIS	C-N-CA	12.75	135.78	119.84
2	C	108	ALA	N-CA-C	9.94	124.72	112.59
2	C	110	ARG	N-CA-C	-9.57	97.90	110.43
2	C	113	ASP	N-CA-C	9.12	121.22	111.28
4	I	306	GLN	CA-C-N	-8.29	110.40	119.19
4	I	306	GLN	C-N-CA	-8.29	110.40	119.19
2	O	110	ARG	N-CA-C	7.71	119.32	111.07
1	A	467	ALA	CA-C-N	-7.65	111.95	120.45
1	A	467	ALA	C-N-CA	-7.65	111.95	120.45
2	C	37	ILE	CA-C-N	7.11	126.36	118.97
2	C	37	ILE	C-N-CA	7.11	126.36	118.97
4	R	133	ASN	CB-CA-C	-6.89	99.99	111.23
4	E	271	ALA	N-CA-C	6.78	120.60	111.24
2	O	109	ASP	CA-C-N	-6.77	111.64	120.44
2	O	109	ASP	C-N-CA	-6.77	111.64	120.44
5	W	25	ARG	CA-C-N	6.45	126.63	120.31
5	W	25	ARG	C-N-CA	6.45	126.63	120.31
4	T	342	ALA	N-CA-C	6.39	118.88	108.08
4	Q	12	SER	CA-C-N	-6.37	111.72	122.92
4	Q	12	SER	C-N-CA	-6.37	111.72	122.92
2	O	114	MET	N-CA-C	6.36	118.29	111.36
2	N	140	TRP	N-CA-C	6.34	118.95	111.02
4	T	342	ALA	CB-CA-C	-6.34	109.28	116.63
4	V	12	SER	CA-C-N	-6.24	111.93	122.92
4	V	12	SER	C-N-CA	-6.24	111.93	122.92
4	U	87	ILE	N-CA-C	-6.21	103.33	111.09
4	V	186	HIS	N-CA-CB	6.19	119.70	110.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	37	ILE	CA-C-N	6.17	125.66	119.24
2	O	37	ILE	C-N-CA	6.17	125.66	119.24
4	F	338	ASP	CA-C-N	6.16	127.55	119.84
4	F	338	ASP	C-N-CA	6.16	127.55	119.84
2	B	71	VAL	N-CA-C	-6.14	105.83	111.67
1	A	472	HIS	CA-C-N	6.08	126.25	119.32
1	A	472	HIS	C-N-CA	6.08	126.25	119.32
2	O	80	GLU	N-CA-C	-6.08	104.66	111.28
1	M	467	ALA	CA-C-N	-6.07	113.56	119.87
1	M	467	ALA	C-N-CA	-6.07	113.56	119.87
5	W	17	GLY	N-CA-C	6.05	121.17	112.82
1	A	6	ASP	CA-C-N	-6.05	114.65	123.00
1	A	6	ASP	C-N-CA	-6.05	114.65	123.00
4	F	102	GLU	N-CA-C	-6.04	105.74	112.57
4	R	341	THR	N-CA-C	5.94	118.37	110.53
5	W	151	CYS	CA-C-N	5.93	125.91	120.21
5	W	151	CYS	C-N-CA	5.93	125.91	120.21
4	S	102	GLU	N-CA-C	-5.89	105.40	112.59
1	A	170	THR	CB-CA-C	-5.86	107.04	111.20
3	P	140	HIS	CA-C-N	5.86	135.30	120.53
3	P	140	HIS	C-N-CA	5.86	135.30	120.53
1	A	221	ILE	N-CA-C	5.85	113.66	108.63
4	F	100	VAL	N-CA-C	5.81	112.42	106.21
4	R	133	ASN	N-CA-CB	-5.80	103.90	112.78
4	V	185	ALA	CA-C-O	-5.79	114.89	121.72
5	K	73	ASP	N-CA-C	-5.74	103.73	111.54
1	M	243	ASP	CA-C-N	5.68	125.59	119.85
1	M	243	ASP	C-N-CA	5.68	125.59	119.85
4	U	95	LEU	N-CA-C	-5.68	105.17	111.36
3	D	2	TYR	N-CA-C	5.63	117.83	108.99
1	A	243	ASP	CA-C-N	5.62	126.86	119.84
1	A	243	ASP	C-N-CA	5.62	126.86	119.84
4	U	93	ALA	CA-C-N	-5.61	113.69	122.49
4	U	93	ALA	C-N-CA	-5.61	113.69	122.49
1	M	213	LYS	CA-C-N	5.59	125.54	119.78
1	M	213	LYS	C-N-CA	5.59	125.54	119.78
2	O	109	ASP	O-C-N	-5.59	115.77	122.65
4	V	338	ASP	CA-C-N	5.59	125.54	119.78
4	V	338	ASP	C-N-CA	5.59	125.54	119.78
4	U	146	ASP	CA-C-N	5.56	129.41	120.30
4	U	146	ASP	C-N-CA	5.56	129.41	120.30
4	J	88	ILE	N-CA-C	5.50	115.95	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	J	87	ILE	N-CA-C	-5.38	105.29	110.72
3	D	72	LYS	CA-C-N	-5.38	114.46	122.74
3	D	72	LYS	C-N-CA	-5.38	114.46	122.74
4	R	133	ASN	CA-C-N	-5.36	115.32	122.72
4	R	133	ASN	C-N-CA	-5.36	115.32	122.72
4	U	336	ASP	N-CA-C	5.36	122.21	110.80
5	K	46	ILE	N-CA-C	5.34	115.00	106.88
4	J	222	GLY	N-CA-C	5.32	118.25	110.38
1	M	221	ILE	N-CA-C	5.26	113.08	107.76
1	M	354	GLN	CB-CA-C	-5.25	110.50	116.54
3	D	139	VAL	CA-C-N	-5.17	115.64	122.56
3	D	139	VAL	C-N-CA	-5.17	115.64	122.56
2	O	128	LEU	N-CA-C	5.16	115.16	107.88
3	P	165	GLY	N-CA-C	5.16	117.55	110.58
1	M	9	ILE	CB-CA-C	-5.11	105.25	110.71
4	I	347	MET	CA-C-N	5.05	124.83	119.28
4	I	347	MET	C-N-CA	5.05	124.83	119.28
4	R	77	GLN	CA-C-N	-5.03	114.68	122.67
4	R	77	GLN	C-N-CA	-5.03	114.68	122.67
2	N	128	LEU	N-CA-C	5.01	115.14	108.38
4	J	16	SER	N-CA-C	5.00	114.84	108.24

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	R	132	ASP	Peptide
4	R	338	ASP	Peptide
4	U	335	SER	Peptide
4	U	94	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	3739	0	3705	67	0
1	M	3812	0	3775	50	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1291	0	1295	17	0
2	C	1292	0	1300	26	0
2	N	1246	0	1253	16	0
2	O	1247	0	1226	19	0
3	D	1451	0	1447	38	0
3	P	1459	0	1466	34	0
4	E	2752	0	2729	36	0
4	F	2760	0	2730	42	0
4	G	2753	0	2727	36	0
4	H	2774	0	2731	36	0
4	I	2731	0	2714	38	0
4	J	2680	0	2624	41	0
4	Q	2790	0	2764	44	0
4	R	2736	0	2672	44	0
4	S	2773	0	2734	49	0
4	T	2777	0	2761	38	0
4	U	2723	0	2690	90	0
4	V	2725	0	2682	41	0
5	K	1722	0	1700	33	0
5	W	1726	0	1711	33	0
6	L	1298	0	658	13	0
6	X	1298	0	658	15	0
All	All	54555	0	52752	813	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 8.

All (813) 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)
4:U:82:ARG:CG	4:U:83:PHE:CE2	1.79	1.60
4:U:82:ARG:CG	4:U:83:PHE:HE2	1.03	1.58
4:U:82:ARG:C	4:U:83:PHE:CD2	1.88	1.51
4:U:82:ARG:CB	4:U:83:PHE:CE2	1.92	1.50
4:U:82:ARG:C	4:U:83:PHE:HD2	1.23	1.44
4:U:82:ARG:HB3	4:U:83:PHE:CE2	1.50	1.40
4:U:82:ARG:CB	4:U:83:PHE:HE2	1.24	1.38
4:U:101:ASP:OD1	4:U:103:ALA:N	1.57	1.37
4:U:82:ARG:HG2	4:U:83:PHE:CE2	1.51	1.33
4:Q:62:SER:OG	4:Q:159:ASP:OD2	1.53	1.26
4:U:84:ASP:O	4:U:87:ILE:HD13	1.33	1.26

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:108:ALA:O	2:C:112:ALA:HB3	1.39	1.20
4:U:82:ARG:CD	4:U:83:PHE:CE2	2.24	1.20
4:U:82:ARG:HB3	4:U:83:PHE:CD2	1.81	1.14
4:U:82:ARG:CB	4:U:83:PHE:CD2	2.33	1.12
4:U:82:ARG:CD	4:U:83:PHE:HE2	1.62	1.09
4:U:82:ARG:O	4:U:83:PHE:CD2	2.10	1.05
4:I:196:ASP:OD2	4:I:299:LYS:NZ	1.91	1.04
4:U:82:ARG:HD3	4:U:83:PHE:CE2	1.94	1.00
4:U:82:ARG:CD	4:U:83:PHE:CZ	2.45	0.98
4:U:83:PHE:HD2	4:U:83:PHE:N	1.57	0.98
4:U:82:ARG:HD3	4:U:83:PHE:CZ	1.99	0.98
4:E:271:ALA:HB3	4:F:185:ALA:HB2	1.46	0.95
2:C:108:ALA:O	2:C:109:ASP:HB2	1.69	0.93
4:U:82:ARG:CA	4:U:83:PHE:CD2	2.52	0.92
4:U:82:ARG:CA	4:U:83:PHE:HD2	1.81	0.91
3:P:132:ASN:N	3:P:132:ASN:HD22	1.64	0.91
4:S:86:LYS:N	4:S:86:LYS:HD3	1.89	0.87
1:A:7:ASN:N	1:A:7:ASN:HD22	1.70	0.86
4:T:93:ALA:HB2	4:T:100:VAL:HG23	1.56	0.86
3:D:2:TYR:HB3	3:D:73:GLN:HA	1.57	0.85
1:M:295:GLU:OE2	1:M:326:ARG:NH2	2.10	0.85
4:U:76:ARG:HH11	4:U:85:GLN:HG3	1.43	0.83
2:C:120:LEU:HD23	4:H:23:MET:HE1	1.61	0.83
4:S:138:LYS:HG3	4:S:141:LYS:HE3	1.60	0.82
3:P:132:ASN:HD22	3:P:132:ASN:H	1.23	0.81
5:W:166:ASP:HB2	5:W:169:LYS:HG2	1.63	0.80
4:R:93:ALA:HB2	4:R:100:VAL:HG12	1.62	0.80
4:U:84:ASP:O	4:U:87:ILE:CD1	2.24	0.80
3:D:140:HIS:HE2	3:D:142:ILE:HG12	1.46	0.79
4:Q:271:ALA:HB3	4:R:185:ALA:HB2	1.62	0.79
3:P:140:HIS:CE1	3:P:142:ILE:HG12	2.18	0.79
4:U:76:ARG:HD3	4:U:85:GLN:HG3	1.64	0.78
4:E:101:ASP:OD1	4:E:102:GLU:N	2.17	0.78
4:T:345:LYS:HG2	4:T:347:MET:HE2	1.66	0.78
1:A:96:ALA:O	1:A:104:LYS:NZ	2.15	0.77
5:K:33:ARG:HB3	5:K:198:ASP:HB3	1.66	0.77
2:C:108:ALA:O	2:C:109:ASP:CB	2.33	0.77
4:J:20:ARG:NH1	6:L:11:C:OP2	2.18	0.76
3:P:96:ILE:HG22	3:P:97:LEU:H	1.51	0.76
5:W:87:THR:HG21	6:X:8:G:H21	1.51	0.75
4:I:221:SER:HB2	4:I:269:THR:HG21	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:U:82:ARG:CG	4:U:83:PHE:CZ	2.65	0.75
4:V:341:THR:OG1	4:V:343:GLN:OE1	2.03	0.75
1:A:140:CYS:HB2	1:A:143:CYS:H	1.51	0.75
4:I:86:LYS:H	4:I:86:LYS:HD2	1.51	0.75
3:P:140:HIS:HE1	3:P:142:ILE:HG12	1.51	0.75
4:R:151:ARG:NH2	4:R:175:LEU:O	2.20	0.74
5:K:33:ARG:NH1	5:K:184:GLU:OE2	2.21	0.74
4:U:170:GLY:O	4:U:173:THR:HG22	1.88	0.73
5:K:199:GLU:HG2	5:K:211:ARG:HD2	1.70	0.73
4:I:173:THR:HG23	4:I:174:GLU:HG3	1.71	0.73
4:Q:13:HIS:CD2	4:Q:18:LEU:HD11	2.24	0.73
4:V:345:LYS:NZ	4:V:347:MET:SD	2.61	0.73
5:K:198:ASP:HB2	5:K:211:ARG:HD3	1.71	0.72
3:D:184:GLY:O	3:D:187:LYS:NZ	2.22	0.72
4:Q:173:THR:HG23	4:Q:174:GLU:HG2	1.72	0.72
3:D:2:TYR:HE1	3:D:59:MET:HA	1.54	0.71
3:P:0:TRP:O	3:P:180:GLN:NE2	2.24	0.71
3:D:20:HIS:CD2	3:D:188:SER:HB2	2.25	0.71
4:I:167:ALA:O	4:I:177:LYS:NZ	2.19	0.71
4:Q:62:SER:OG	4:Q:159:ASP:CG	2.33	0.71
1:A:7:ASN:HB3	1:A:22:ILE:C	2.17	0.70
4:I:37:VAL:HG23	4:I:193:VAL:HG21	1.73	0.70
6:L:49:C:H2'	6:L:50:G:H8	1.56	0.70
4:T:155:GLN:HG2	4:T:239:LEU:HD22	1.73	0.70
3:D:140:HIS:NE2	3:D:142:ILE:HG12	2.07	0.70
3:P:140:HIS:CD2	4:U:15:PRO:HG2	2.28	0.69
4:S:86:LYS:HD3	4:S:86:LYS:H	1.57	0.69
4:U:82:ARG:HG2	4:U:83:PHE:CZ	2.22	0.69
4:V:174:GLU:OE2	4:V:177:LYS:NZ	2.25	0.69
4:J:345:LYS:HD3	4:J:347:MET:HE2	1.73	0.69
2:N:89:ARG:NE	2:N:155:THR:OG1	2.25	0.69
4:T:135:ASP:HB3	4:T:138:LYS:HG3	1.74	0.69
1:A:247:ILE:HG13	1:A:258:ASN:HA	1.74	0.69
4:R:268:ARG:NH1	4:S:179:ASP:OD1	2.26	0.69
5:W:198:ASP:HB2	5:W:211:ARG:HD3	1.75	0.68
2:C:108:ALA:O	2:C:112:ALA:CB	2.30	0.68
3:D:102:ARG:NH2	6:L:46:C:OP2	2.27	0.68
4:U:173:THR:HG23	4:U:174:GLU:OE1	1.92	0.68
5:W:44:LEU:O	5:W:46:ILE:HG13	1.93	0.68
4:Q:210:GLY:O	6:X:21:G:N2	2.21	0.67
3:P:15:ASP:OD1	3:P:16:LEU:N	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:V:85:GLN:N	4:V:85:GLN:OE1	2.27	0.67
1:A:63:ASP:OD1	1:A:64:ASP:N	2.26	0.67
3:D:119:GLU:OE1	4:I:266:LYS:NZ	2.22	0.67
4:E:185:ALA:HB2	4:J:271:ALA:HB3	1.76	0.67
4:I:316:TRP:CD1	4:I:340:ILE:HD11	2.30	0.67
4:S:271:ALA:HB3	4:T:185:ALA:HB2	1.76	0.67
4:R:271:ALA:HB3	4:S:185:ALA:HB2	1.76	0.66
4:R:21:ASP:C	4:R:21:ASP:OD1	2.35	0.66
4:J:112:THR:HG23	4:J:238:ASN:HA	1.76	0.66
5:K:108:ARG:NH2	6:L:7:C:O2	2.29	0.66
2:C:110:ARG:O	2:C:112:ALA:N	2.27	0.66
2:C:111:THR:HG22	2:C:112:ALA:N	2.09	0.66
2:C:111:THR:O	2:C:112:ALA:C	2.30	0.66
4:Q:185:ALA:HB2	4:V:271:ALA:HB3	1.77	0.66
5:W:55:GLN:O	5:W:59:GLU:HG3	1.96	0.66
2:O:113:ASP:OD1	2:O:114:MET:N	2.28	0.66
4:T:271:ALA:HB3	4:U:185:ALA:HB2	1.77	0.66
3:P:145:ARG:HD2	4:U:23:MET:HE3	1.77	0.65
4:E:268:ARG:NH1	4:F:179:ASP:OD1	2.29	0.65
4:T:317:ASP:O	4:T:321:ASN:HB2	1.96	0.65
4:V:38:ARG:HD3	5:W:13:MET:HE1	1.78	0.65
1:M:321:ASN:OD1	1:M:322:GLU:HB2	1.97	0.65
4:U:102:GLU:CA	4:U:102:GLU:OE1	2.45	0.64
4:G:151:ARG:NH2	4:G:175:LEU:O	2.28	0.64
4:J:94:LEU:HD22	4:J:140:LEU:HD11	1.79	0.64
1:A:99:PRO:HB2	1:A:102:GLN:HB2	1.80	0.64
4:Q:11:ILE:HG12	4:Q:13:HIS:CE1	2.33	0.64
4:Q:345:LYS:HG2	4:Q:347:MET:HE2	1.80	0.64
3:D:199:LEU:HD21	4:I:216:THR:HG22	1.79	0.64
4:H:167:ALA:H	4:H:177:LYS:HE3	1.62	0.64
4:E:142:VAL:O	4:E:145:GLU:HB2	1.97	0.64
1:M:101:MET:HE2	1:M:235:GLN:HB2	1.80	0.64
4:U:76:ARG:HH11	4:U:85:GLN:CG	2.10	0.63
4:U:101:ASP:OD1	4:U:102:GLU:N	2.30	0.63
5:W:94:ASP:OD1	5:W:95:TYR:N	2.30	0.63
5:W:87:THR:HG21	6:X:8:G:N2	2.13	0.63
4:S:84:ASP:OD1	4:S:84:ASP:N	2.29	0.63
2:C:109:ASP:C	2:C:110:ARG:O	2.37	0.63
3:P:132:ASN:N	3:P:132:ASN:ND2	2.39	0.63
1:A:250:CYS:SG	1:A:253:CYS:N	2.71	0.63
4:S:217:GLN:OE1	4:S:266:LYS:HE3	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:ASN:OD1	1:A:335:ARG:NH1	2.30	0.62
2:B:107:ARG:NH2	4:E:28:ASP:OD2	2.32	0.62
3:D:4:SER:HB3	3:D:71:THR:HG23	1.82	0.62
3:D:20:HIS:HD2	3:D:188:SER:HB2	1.63	0.62
1:A:31:ARG:HG3	1:A:74:PRO:HG2	1.82	0.62
4:G:334:LEU:O	4:H:318:ARG:NH1	2.32	0.62
4:H:271:ALA:HB3	4:I:185:ALA:HB2	1.82	0.62
4:U:316:TRP:CD1	4:U:340:ILE:HD11	2.35	0.62
5:W:44:LEU:O	5:W:46:ILE:N	2.32	0.61
4:F:271:ALA:HB3	4:G:185:ALA:HB2	1.82	0.61
4:F:300:ALA:HB2	4:F:304:PHE:CE1	2.35	0.61
4:R:201:THR:HG22	4:R:214:LEU:HG	1.80	0.61
4:U:82:ARG:NE	4:U:83:PHE:HZ	1.98	0.61
1:M:10:PRO:HG2	1:M:38:LEU:HD11	1.81	0.61
4:E:65:THR:OG1	4:E:66:ILE:N	2.33	0.61
4:G:143:LEU:HD12	4:G:171:MET:HE1	1.82	0.61
1:A:151:GLN:HA	1:A:155:ALA:HB3	1.83	0.60
5:W:34:SER:HB3	5:W:198:ASP:O	2.01	0.60
4:S:140:LEU:HB2	4:S:171:MET:HE2	1.82	0.60
4:U:87:ILE:HG12	4:U:88:ILE:N	2.11	0.60
4:U:82:ARG:CD	4:U:83:PHE:HZ	2.08	0.60
1:A:7:ASN:N	1:A:7:ASN:ND2	2.42	0.60
4:G:271:ALA:HB3	4:H:185:ALA:HB2	1.82	0.60
4:Q:48:MET:HE1	4:Q:254:VAL:HG13	1.84	0.60
1:A:245:ILE:HG22	1:A:260:ARG:HB2	1.82	0.60
3:D:100:GLN:OE1	3:D:102:ARG:NH1	2.35	0.60
3:D:140:HIS:C	3:D:140:HIS:CD2	2.80	0.60
5:K:33:ARG:NE	5:K:199:GLU:OE1	2.32	0.60
3:P:129:LYS:HD2	3:P:183:ILE:HG23	1.84	0.60
4:T:113:PRO:HB2	4:T:160:ILE:HD11	1.83	0.60
4:U:83:PHE:CB	4:U:87:ILE:HD11	2.32	0.60
1:A:469:TYR:HB3	1:A:475:LEU:HD13	1.84	0.59
4:E:76:ARG:NH2	4:E:102:GLU:OE1	2.32	0.59
4:H:278:MET:HG2	4:H:279:VAL:N	2.17	0.59
2:O:15:GLN:NE2	2:O:69:LYS:O	2.32	0.59
4:R:221:SER:OG	4:S:30:ILE:O	2.20	0.59
3:P:140:HIS:HD2	4:U:15:PRO:HG2	1.67	0.59
4:S:86:LYS:H	4:S:86:LYS:CD	2.12	0.59
4:S:217:GLN:HG3	4:S:218:GLU:N	2.16	0.59
4:G:204:ASP:HB3	4:G:207:GLN:HB3	1.83	0.59
4:I:2:SER:O	4:I:244:ARG:NH2	2.34	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:155:GLN:HG2	4:F:239:LEU:HD22	1.85	0.59
4:I:10:LEU:HB2	4:I:278:MET:HB3	1.85	0.59
2:C:110:ARG:HG3	2:C:111:THR:HB	1.85	0.59
4:R:132:ASP:O	4:R:134:LEU:N	2.36	0.59
4:G:135:ASP:OD1	4:G:136:ASP:N	2.36	0.59
4:R:83:PHE:HB3	4:R:87:ILE:HD11	1.84	0.58
4:U:102:GLU:OE1	4:U:102:GLU:HA	2.03	0.58
1:A:300:PHE:CZ	1:A:361:ARG:HD2	2.38	0.58
4:G:290:MET:HE1	4:G:319:VAL:HG21	1.85	0.58
4:H:268:ARG:NH1	4:I:179:ASP:OD1	2.36	0.58
3:P:89:ARG:NH1	3:P:144:GLU:OE2	2.36	0.58
4:U:82:ARG:NE	4:U:83:PHE:CZ	2.70	0.58
4:J:165:ARG:O	6:L:6:C:O2'	2.16	0.58
1:M:117:LEU:HD23	1:M:151:GLN:HG3	1.86	0.58
4:Q:316:TRP:CD1	4:Q:340:ILE:HD11	2.39	0.58
4:S:95:LEU:HD22	4:S:172:MET:HE3	1.85	0.58
4:T:268:ARG:NH1	4:U:179:ASP:OD1	2.37	0.57
1:A:194:ARG:HA	1:A:197:LYS:HG3	1.84	0.57
1:A:335:ARG:HG3	1:A:372:GLN:HB3	1.86	0.57
4:I:198:ASP:OD2	4:I:201:THR:HG23	2.04	0.57
4:R:316:TRP:CD1	4:R:340:ILE:HD11	2.39	0.57
4:I:1:MET:HE2	4:I:244:ARG:HD3	1.86	0.57
1:A:285:LEU:HD21	1:A:312:ARG:HD3	1.87	0.57
4:H:204:ASP:HB3	4:H:207:GLN:HG2	1.86	0.57
4:V:45:LYS:HA	4:V:48:MET:HE3	1.87	0.57
5:W:31:PRO:HD2	5:W:65:VAL:HG11	1.87	0.57
4:U:221:SER:HB2	4:U:269:THR:HG21	1.87	0.57
3:D:45:ASN:OD1	3:D:45:ASN:N	2.38	0.57
4:J:341:THR:HG22	4:J:343:GLN:H	1.70	0.57
4:R:245:GLU:N	4:R:245:GLU:OE1	2.38	0.57
3:P:132:ASN:H	3:P:132:ASN:ND2	2.00	0.56
4:S:278:MET:HE1	4:S:312:PHE:CE2	2.41	0.56
2:C:111:THR:C	2:C:113:ASP:N	2.52	0.56
4:Q:288:LEU:HD21	4:Q:325:LEU:HD11	1.86	0.56
4:U:335:SER:O	4:U:337:VAL:N	2.38	0.56
1:A:307:TRP:HA	1:A:310:ILE:HG13	1.87	0.56
3:D:140:HIS:HD2	3:D:140:HIS:O	1.88	0.56
1:M:133:PRO:HG3	5:W:95:TYR:CE1	2.40	0.56
1:M:307:TRP:HA	1:M:310:ILE:HG13	1.86	0.56
1:A:79:GLU:HA	1:A:82:GLN:HB2	1.87	0.56
4:F:199:TRP:HB3	4:F:214:LEU:HD23	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:72:ARG:NH1	4:J:73:ASP:OD1	2.39	0.56
5:W:193:LYS:HE2	5:W:212:GLU:HB3	1.87	0.56
2:B:67:ALA:HB1	2:B:122:THR:HG22	1.85	0.56
4:J:186:HIS:HB2	5:K:13:MET:HE1	1.88	0.56
4:S:135:ASP:OD1	4:S:136:ASP:N	2.39	0.56
2:C:52:PRO:HA	2:C:55:GLN:HG3	1.88	0.56
4:H:101:ASP:HB2	4:H:103:ALA:H	1.70	0.55
4:H:135:ASP:OD1	4:H:136:ASP:N	2.40	0.55
4:U:109:ASP:OD1	4:U:109:ASP:N	2.27	0.55
5:W:88:VAL:HG22	6:X:7:C:H1'	1.88	0.55
4:I:86:LYS:H	4:I:86:LYS:CD	2.19	0.55
4:I:360:ASN:O	4:I:360:ASN:ND2	2.39	0.55
1:M:332:ASN:OD1	1:M:335:ARG:NH1	2.40	0.55
4:S:172:MET:HE2	4:S:172:MET:HA	1.89	0.55
4:U:83:PHE:CD2	4:U:83:PHE:N	2.29	0.55
4:G:243:SER:H	4:G:246:GLN:NE2	2.05	0.55
4:J:349:THR:HG22	4:J:351:GLU:H	1.71	0.55
4:S:151:ARG:NH2	4:S:175:LEU:O	2.38	0.55
4:E:94:LEU:HD22	4:E:171:MET:HE3	1.89	0.55
4:U:10:LEU:HB2	4:U:278:MET:HB3	1.89	0.55
1:M:492:GLU:N	1:M:492:GLU:OE1	2.40	0.55
4:F:62:SER:OG	4:F:159:ASP:OD2	2.25	0.55
4:G:278:MET:HG2	4:G:279:VAL:N	2.19	0.55
4:F:9:VAL:HB	4:F:226:ARG:HB2	1.89	0.55
5:W:3:SER:HB3	5:W:163:GLN:HE21	1.70	0.54
4:T:77:GLN:O	4:T:77:GLN:NE2	2.40	0.54
1:A:174:THR:HB	1:A:345:LEU:HD11	1.88	0.54
4:F:316:TRP:HD1	4:F:340:ILE:HG21	1.72	0.54
4:J:337:VAL:HG12	4:J:338:ASP:H	1.72	0.54
2:B:27:ARG:NH2	4:G:22:ASP:OD1	2.41	0.54
1:M:100:PHE:O	1:M:102:GLN:HG3	2.07	0.54
1:A:340:GLN:HA	1:A:369:GLN:HE21	1.72	0.54
3:P:1:MET:HE3	3:P:3:LEU:HB2	1.89	0.54
4:T:278:MET:HE1	4:T:312:PHE:CE1	2.43	0.54
4:S:124:GLU:O	4:S:128:LYS:HG3	2.07	0.54
4:V:179:ASP:N	4:V:179:ASP:OD1	2.41	0.54
4:J:19:ASN:OD1	4:J:27:LYS:HD2	2.08	0.54
1:A:316:ASP:OD2	1:A:332:ASN:ND2	2.31	0.54
4:I:76:ARG:NH2	4:I:102:GLU:OE2	2.39	0.54
4:R:214:LEU:HD22	4:S:22:ASP:HB3	1.90	0.54
2:C:109:ASP:O	2:C:110:ARG:C	2.49	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:T:172:MET:HA	4:T:172:MET:HE2	1.90	0.53
4:F:48:MET:HG2	4:F:257:MET:HB3	1.90	0.53
4:I:86:LYS:HD2	4:I:86:LYS:N	2.22	0.53
4:Q:179:ASP:OD1	4:V:268:ARG:NH1	2.41	0.53
5:K:74:ASP:OD1	5:K:74:ASP:C	2.49	0.53
1:A:97:GLU:HA	1:A:104:LYS:NZ	2.24	0.53
2:N:67:ALA:HB1	2:N:122:THR:HG22	1.90	0.53
4:R:179:ASP:O	4:R:238:ASN:ND2	2.38	0.53
1:A:248:GLY:HA3	1:A:260:ARG:CZ	2.38	0.53
6:L:49:C:H2'	6:L:50:G:C8	2.41	0.53
3:P:140:HIS:CE1	3:P:142:ILE:CG1	2.91	0.53
4:U:83:PHE:HB2	4:U:87:ILE:HD11	1.89	0.53
4:T:101:ASP:OD1	4:T:101:ASP:C	2.46	0.53
4:V:245:GLU:N	4:V:245:GLU:OE2	2.40	0.53
5:W:3:SER:HA	5:W:163:GLN:HG3	1.91	0.53
4:E:173:THR:HG23	4:E:174:GLU:HG2	1.91	0.52
4:E:214:LEU:HD13	4:F:22:ASP:HB3	1.90	0.52
2:B:89:ARG:NE	2:B:155:THR:OG1	2.43	0.52
2:N:35:ARG:NH2	2:N:55:GLN:OE1	2.43	0.52
4:V:13:HIS:CD2	4:V:18:LEU:HD11	2.43	0.52
5:W:204:LEU:HD12	5:W:205:PRO:HD2	1.91	0.52
5:K:72:LEU:O	5:K:73:ASP:C	2.51	0.52
4:V:90:LYS:NZ	4:V:130:GLU:OE1	2.39	0.52
4:V:136:ASP:OD1	4:V:136:ASP:N	2.41	0.52
4:I:69:ALA:O	4:I:72:ARG:HB3	2.10	0.52
4:J:87:ILE:C	4:J:87:ILE:HD12	2.34	0.52
4:S:113:PRO:HB2	4:S:160:ILE:HD11	1.91	0.52
1:A:154:GLN:HA	1:A:171:PRO:HD2	1.92	0.52
2:C:110:ARG:CG	2:C:111:THR:HB	2.38	0.52
4:Q:170:GLY:O	4:Q:173:THR:HG22	2.10	0.52
1:A:359:GLU:OE2	1:A:361:ARG:NH2	2.42	0.52
2:B:60:ARG:NH1	2:B:137:LEU:O	2.41	0.52
4:F:93:ALA:HB2	4:F:100:VAL:HG23	1.91	0.52
4:S:360:ASN:O	4:S:360:ASN:ND2	2.43	0.52
4:T:39:ILE:HB	4:T:187:ALA:HB3	1.91	0.52
2:B:3:ASP:OD1	2:B:53:ARG:NH2	2.43	0.51
4:J:42:GLN:HG2	5:K:86:HIS:CE1	2.45	0.51
2:C:111:THR:N	2:C:113:ASP:OD1	2.44	0.51
3:D:2:TYR:HE1	3:D:59:MET:CA	2.23	0.51
4:G:172:MET:HE2	4:G:172:MET:HA	1.91	0.51
5:K:88:VAL:HG22	6:L:7:C:H1'	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:27:ARG:HD2	4:S:23:MET:SD	2.51	0.51
4:Q:232:LEU:O	4:Q:236:GLN:HG3	2.11	0.51
2:B:126:PRO:HB2	2:B:128:LEU:HD23	1.92	0.51
4:R:72:ARG:NH1	4:R:102:GLU:HA	2.26	0.51
4:S:75:LEU:HD11	4:S:119:ILE:HD13	1.92	0.51
4:H:300:ALA:HB2	4:H:304:PHE:CE1	2.46	0.51
5:K:74:ASP:OD1	5:K:74:ASP:O	2.29	0.51
1:M:110:ASP:OD1	1:M:111:VAL:N	2.43	0.51
3:P:43:LYS:HB2	3:P:51:HIS:HB2	1.92	0.51
1:A:112:THR:HG21	1:A:266:LYS:HE3	1.93	0.51
4:I:280:MET:HE3	4:I:329:ALA:HB1	1.92	0.51
5:K:55:GLN:O	5:K:59:GLU:HG3	2.10	0.51
5:K:73:ASP:O	5:K:74:ASP:OD1	2.29	0.51
4:E:172:MET:HE2	4:E:172:MET:HA	1.92	0.51
2:N:36:ASP:OD2	2:O:107:ARG:NH2	2.44	0.51
4:J:27:LYS:NZ	6:L:9:G:OP1	2.44	0.50
2:O:110:ARG:O	2:O:113:ASP:OD1	2.29	0.50
5:K:38:GLY:HA3	6:L:2:U:O4'	2.12	0.50
3:P:85:TYR:CD2	4:U:197:ILE:HD11	2.47	0.50
3:P:100:GLN:OE1	3:P:102:ARG:NH1	2.44	0.50
4:U:75:LEU:HD11	4:U:119:ILE:HD13	1.92	0.50
6:X:49:C:H2'	6:X:50:G:H8	1.75	0.50
4:G:57:ASN:HB3	4:G:253:HIS:CE1	2.46	0.50
3:P:144:GLU:OE1	3:P:160:THR:OG1	2.28	0.50
4:V:207:GLN:O	4:V:207:GLN:OE1	2.29	0.50
4:F:95:LEU:HD22	4:F:172:MET:HE3	1.94	0.50
6:L:41:G:H2'	6:L:42:A:O4'	2.11	0.50
4:Q:120:ALA:O	4:Q:123:CYS:HB2	2.11	0.50
2:C:109:ASP:O	2:C:110:ARG:O	2.30	0.50
4:J:316:TRP:HB3	4:J:340:ILE:HD11	1.94	0.50
1:A:285:LEU:HD11	1:A:312:ARG:HD3	1.93	0.50
1:A:133:PRO:HG3	5:K:95:TYR:CD1	2.46	0.50
2:B:65:LEU:HD23	2:B:72:ILE:HD12	1.93	0.50
4:H:144:LYS:NZ	4:H:174:GLU:OE2	2.43	0.50
4:F:144:LYS:HD2	4:F:174:GLU:HG2	1.93	0.49
4:Q:290:MET:HA	4:Q:290:MET:HE2	1.94	0.49
4:V:112:THR:HG23	4:V:238:ASN:HA	1.94	0.49
3:D:23:LEU:O	3:D:26:LEU:HG	2.12	0.49
4:H:20:ARG:HD2	4:H:24:ASN:HA	1.94	0.49
4:H:280:MET:HE1	4:H:316:TRP:CE2	2.47	0.49
4:Q:172:MET:HE2	4:Q:172:MET:HA	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:176:GLY:O	4:G:178:VAL:HG23	2.12	0.49
1:M:13:PRO:HB2	1:M:16:GLY:H	1.77	0.49
4:U:83:PHE:HB3	4:U:87:ILE:HD11	1.94	0.49
4:V:249:GLU:O	4:V:252:THR:OG1	2.30	0.49
4:V:288:LEU:HD12	4:V:325:LEU:HD21	1.94	0.49
2:C:108:ALA:O	2:C:109:ASP:O	2.30	0.49
3:D:2:TYR:HB3	3:D:73:GLN:CA	2.36	0.49
4:J:76:ARG:HD2	4:J:85:GLN:HG2	1.93	0.49
1:M:15:ASN:OD1	1:M:15:ASN:N	2.41	0.49
1:M:71:ILE:O	1:M:182:ARG:NH2	2.46	0.49
4:G:173:THR:HG23	4:G:174:GLU:HG2	1.95	0.49
4:T:69:ALA:O	4:T:72:ARG:HB3	2.12	0.49
4:V:13:HIS:HB3	4:V:272:ALA:HB1	1.93	0.49
4:E:290:MET:HE2	4:E:290:MET:HA	1.94	0.49
4:G:268:ARG:NH1	4:H:179:ASP:OD1	2.45	0.49
2:O:27:ARG:NH2	4:U:22:ASP:OD1	2.36	0.49
4:T:137:LYS:HD3	4:T:137:LYS:N	2.27	0.49
4:E:301:LYS:O	4:E:301:LYS:HG3	2.12	0.49
4:G:9:VAL:HB	4:G:226:ARG:HB2	1.94	0.49
4:J:345:LYS:HD3	4:J:347:MET:CE	2.41	0.49
4:Q:280:MET:HE1	4:Q:316:TRP:CE2	2.48	0.49
4:T:93:ALA:CB	4:T:100:VAL:HG23	2.36	0.49
4:H:306:GLN:HB2	4:H:307:PRO:HD3	1.94	0.49
4:T:300:ALA:HB2	4:T:304:PHE:CE1	2.47	0.49
4:T:304:PHE:C	4:T:307:PRO:HD2	2.37	0.49
4:U:72:ARG:HG3	4:U:76:ARG:NH2	2.27	0.49
2:C:15:GLN:NE2	2:C:69:LYS:O	2.42	0.49
4:H:72:ARG:NH1	4:H:102:GLU:HA	2.27	0.49
4:Q:155:GLN:HG2	4:Q:239:LEU:HD22	1.95	0.49
4:S:48:MET:HE1	4:S:254:VAL:HG13	1.95	0.49
4:F:90:LYS:HE2	4:F:94:LEU:HD11	1.95	0.49
4:U:82:ARG:C	4:U:83:PHE:CG	2.76	0.49
4:U:304:PHE:O	4:U:307:PRO:HD2	2.12	0.49
4:H:9:VAL:HB	4:H:226:ARG:HB2	1.93	0.48
4:H:201:THR:HG23	4:H:214:LEU:HG	1.95	0.48
4:F:290:MET:HE2	4:F:290:MET:HA	1.95	0.48
4:J:61:SER:HB3	4:J:158:VAL:HG21	1.94	0.48
4:S:201:THR:HG22	4:S:214:LEU:HG	1.95	0.48
4:J:153:ASN:ND2	4:J:171:MET:HE2	2.29	0.48
4:J:2:SER:O	4:J:244:ARG:NH2	2.34	0.48
4:E:280:MET:HE2	4:E:282:ASN:HB2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:90:LYS:HE2	4:H:126:VAL:HB	1.96	0.48
4:I:65:THR:OG1	4:I:66:ILE:N	2.45	0.48
1:M:253:CYS:HB2	1:M:255:GLN:H	1.78	0.48
4:G:204:ASP:OD1	4:H:65:THR:OG1	2.32	0.48
1:M:114:MET:HE2	1:M:263:GLY:N	2.29	0.48
4:U:360:ASN:O	4:U:360:ASN:ND2	2.46	0.48
6:X:38:U:H2'	6:X:39:G:H4'	1.96	0.48
4:E:326:ASN:OD1	4:E:326:ASN:N	2.37	0.48
4:I:342:ALA:O	4:I:344:VAL:N	2.47	0.48
4:T:57:ASN:HB3	4:T:253:HIS:CE1	2.49	0.48
4:I:137:LYS:N	4:I:137:LYS:CD	2.78	0.47
4:Q:81:GLU:HG3	4:Q:82:ARG:HG3	1.95	0.47
5:W:33:ARG:HB3	5:W:198:ASP:HB3	1.95	0.47
4:J:149:ALA:HB2	5:K:98:LEU:HD11	1.95	0.47
4:R:20:ARG:HD2	4:R:24:ASN:HA	1.96	0.47
4:V:207:GLN:O	4:V:207:GLN:CG	2.61	0.47
4:E:155:GLN:HG2	4:E:239:LEU:HD22	1.95	0.47
3:P:46:THR:HB	3:P:47:PRO:HD2	1.96	0.47
4:R:360:ASN:O	4:R:360:ASN:ND2	2.47	0.47
4:E:22:ASP:OD1	4:E:22:ASP:N	2.48	0.47
4:F:65:THR:OG1	4:F:66:ILE:N	2.48	0.47
5:K:155:HIS:ND1	5:K:156:PRO:O	2.45	0.47
4:T:246:GLN:O	4:T:250:ILE:HG13	2.15	0.47
4:V:176:GLY:O	4:V:178:VAL:HG23	2.14	0.47
1:A:216:LYS:N	1:A:219:GLU:OE1	2.48	0.47
4:U:69:ALA:HA	4:U:72:ARG:NH1	2.29	0.47
4:V:87:ILE:O	4:V:91:THR:OG1	2.28	0.47
2:B:65:LEU:C	2:B:67:ALA:H	2.21	0.47
4:E:232:LEU:O	4:E:236:GLN:HG3	2.15	0.47
5:K:6:ILE:HG13	5:K:174:TYR:CE1	2.49	0.47
5:K:34:SER:OG	6:L:3:A:OP1	2.29	0.47
2:N:141:GLY:O	2:N:145:ARG:HG3	2.15	0.47
4:Q:57:ASN:HB3	4:Q:253:HIS:CE1	2.50	0.47
4:R:232:LEU:O	4:R:236:GLN:HG3	2.15	0.47
4:S:120:ALA:O	4:S:123:CYS:HB2	2.14	0.47
4:T:278:MET:HE1	4:T:312:PHE:CD1	2.50	0.47
4:U:336:ASP:OD1	4:U:336:ASP:N	2.44	0.47
4:G:138:LYS:O	4:G:142:VAL:HG23	2.14	0.47
3:D:15:ASP:OD1	3:D:16:LEU:N	2.48	0.47
4:H:206:LEU:HD12	4:I:65:THR:HG21	1.96	0.47
1:M:133:PRO:HG3	5:W:95:TYR:CD1	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:48:MET:HE3	4:F:257:MET:HE3	1.96	0.47
4:F:316:TRP:CD1	4:F:340:ILE:HG21	2.49	0.47
4:H:70:GLN:OE1	4:H:70:GLN:N	2.40	0.47
4:I:356:TRP:CE2	4:I:361:GLY:HA2	2.50	0.47
4:T:277:ASP:CG	4:T:305:LEU:HD21	2.40	0.47
4:U:14:SER:HB3	4:U:266:LYS:HD3	1.97	0.47
1:A:24:LEU:HB3	1:A:80:PHE:HZ	1.80	0.46
1:A:132:GLN:HA	1:A:133:PRO:HD3	1.82	0.46
2:O:101:ARG:NH2	4:T:22:ASP:OD1	2.37	0.46
2:B:25:ILE:O	2:B:28:VAL:HG22	2.15	0.46
1:M:488:LYS:O	1:M:491:ARG:N	2.47	0.46
4:S:54:TYR:CD2	4:S:58:ILE:HD12	2.51	0.46
6:X:52:G:O3'	6:X:53:C:H6	1.97	0.46
1:A:31:ARG:NH2	1:A:73:ASN:OD1	2.48	0.46
2:C:60:ARG:NH1	2:C:137:LEU:O	2.48	0.46
3:D:90:ALA:HA	3:D:191:CYS:HB3	1.97	0.46
2:N:25:ILE:O	2:N:28:VAL:HG22	2.15	0.46
2:N:110:ARG:O	2:N:112:ALA:N	2.44	0.46
2:O:67:ALA:HB1	2:O:122:THR:HG22	1.98	0.46
4:U:115:VAL:HB	4:U:118:GLU:HB2	1.97	0.46
3:D:2:TYR:HB3	3:D:73:GLN:HB2	1.97	0.46
4:J:249:GLU:O	4:J:252:THR:HB	2.15	0.46
2:N:97:ILE:HD12	2:N:120:LEU:HD22	1.96	0.46
4:G:65:THR:OG1	4:G:66:ILE:N	2.49	0.46
4:J:341:THR:CG2	4:J:343:GLN:H	2.28	0.46
5:K:11:GLY:HA2	5:K:154:THR:HG23	1.97	0.46
1:M:42:ASP:N	1:M:42:ASP:OD1	2.49	0.46
2:O:35:ARG:NH1	2:O:59:LEU:HD11	2.30	0.46
4:S:85:GLN:HE21	4:S:85:GLN:HB3	1.46	0.46
4:U:276:ALA:HB3	4:U:332:PHE:HE2	1.80	0.46
3:D:96:ILE:HG22	3:D:97:LEU:N	2.30	0.46
5:K:34:SER:HB3	5:K:198:ASP:O	2.15	0.46
4:S:137:LYS:HB3	4:S:137:LYS:HE2	1.63	0.46
2:B:118:ARG:O	2:B:122:THR:HG23	2.16	0.46
2:C:37:ILE:HA	2:C:38:PRO:HD3	1.77	0.46
4:J:76:ARG:HG2	4:J:88:ILE:HG21	1.98	0.46
3:P:110:LYS:HD3	6:X:47:C:OP2	2.15	0.46
4:R:82:ARG:HB3	4:R:83:PHE:CD2	2.51	0.46
4:S:93:ALA:HB2	4:S:100:VAL:HG23	1.97	0.46
1:A:68:ARG:NH1	1:A:337:ILE:O	2.42	0.46
4:I:172:MET:HE2	4:I:172:MET:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:K:16:TRP:CG	5:K:31:PRO:HA	2.50	0.46
1:M:100:PHE:CE2	1:M:101:MET:HG3	2.51	0.46
1:M:154:GLN:HA	1:M:171:PRO:HD2	1.98	0.46
1:M:321:ASN:OD1	1:M:322:GLU:N	2.49	0.46
3:P:91:ASN:HA	3:P:92:PRO:HD2	1.79	0.46
4:S:328:ALA:HB1	4:S:356:TRP:CZ2	2.50	0.46
2:B:110:ARG:O	2:B:111:THR:HB	2.15	0.46
4:J:54:TYR:OH	4:J:159:ASP:OD1	2.28	0.46
4:J:288:LEU:HD12	4:J:325:LEU:HD21	1.97	0.46
1:A:13:PRO:HB2	1:A:16:GLY:H	1.81	0.45
3:D:199:LEU:HD23	3:D:199:LEU:O	2.16	0.45
4:E:69:ALA:O	4:E:72:ARG:HB3	2.16	0.45
4:E:78:LYS:HD2	4:E:78:LYS:O	2.16	0.45
4:H:304:PHE:C	4:H:307:PRO:HD2	2.42	0.45
2:O:113:ASP:OD1	2:O:113:ASP:C	2.58	0.45
4:R:13:HIS:HA	4:R:274:ASN:OD1	2.16	0.45
4:F:334:LEU:O	4:G:318:ARG:HD3	2.17	0.45
5:K:73:ASP:O	5:K:74:ASP:CG	2.58	0.45
4:S:138:LYS:O	4:S:142:VAL:HG23	2.17	0.45
4:U:135:ASP:OD1	4:U:135:ASP:N	2.49	0.45
1:A:102:GLN:OE1	1:A:241:LEU:N	2.31	0.45
1:A:455:HIS:CE1	1:A:490:LEU:HD13	2.52	0.45
2:C:59:LEU:HD23	2:C:59:LEU:HA	1.81	0.45
4:H:120:ALA:O	4:H:123:CYS:HB2	2.16	0.45
4:R:16:SER:HB3	4:R:272:ALA:HB2	1.98	0.45
4:S:349:THR:OG1	4:S:352:GLN:HG3	2.16	0.45
4:V:42:GLN:H	4:V:42:GLN:HG3	1.05	0.45
3:D:2:TYR:HB3	3:D:73:GLN:CB	2.47	0.45
4:H:166:MET:O	4:H:166:MET:HG3	2.16	0.45
4:J:230:ILE:HD11	4:J:254:VAL:HG11	1.99	0.45
4:Q:243:SER:OG	4:Q:246:GLN:HG3	2.15	0.45
4:S:278:MET:HE1	4:S:312:PHE:CD2	2.52	0.45
4:U:37:VAL:HG23	4:U:193:VAL:HG21	1.97	0.45
4:V:146:ASP:OD1	4:V:146:ASP:N	2.46	0.45
3:D:178:LEU:HD23	3:D:178:LEU:HA	1.84	0.45
4:E:39:ILE:HB	4:E:187:ALA:HB3	1.99	0.45
4:F:338:ASP:HA	4:F:339:PRO:HD3	1.56	0.45
5:K:74:ASP:C	5:K:75:ARG:HG2	2.42	0.45
4:T:70:GLN:OE1	4:T:70:GLN:N	2.48	0.45
4:U:40:SER:HA	4:U:186:HIS:ND1	2.32	0.45
4:V:6:ASN:HD21	4:V:284:SER:HB3	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:W:87:THR:HB	6:X:9:G:H5"	1.98	0.45
2:C:113:ASP:N	2:C:113:ASP:OD1	2.47	0.45
3:D:140:HIS:CD2	3:D:140:HIS:O	2.68	0.45
4:H:90:LYS:HE3	4:H:130:GLU:OE2	2.16	0.45
4:Q:26:GLN:N	4:Q:218:GLU:OE1	2.47	0.45
4:R:69:ALA:O	4:R:72:ARG:HB3	2.17	0.45
4:U:39:ILE:HB	4:U:187:ALA:HB3	1.98	0.45
2:O:14:TRP:HZ3	2:O:25:ILE:HD12	1.81	0.45
4:R:115:VAL:HG12	4:R:118:GLU:H	1.81	0.45
4:R:280:MET:HE1	4:R:316:TRP:CE2	2.52	0.45
4:U:115:VAL:HG12	4:U:118:GLU:H	1.81	0.45
4:V:337:VAL:HG12	4:V:338:ASP:H	1.82	0.45
1:A:317:LYS:C	1:A:318:ILE:HD13	2.41	0.45
1:M:288:VAL:HB	1:M:293:VAL:HG12	1.99	0.45
4:Q:27:LYS:NZ	4:V:198:ASP:OD1	2.44	0.45
4:U:14:SER:O	4:U:18:LEU:HD11	2.17	0.45
1:A:24:LEU:HB3	1:A:80:PHE:CZ	2.53	0.44
4:G:243:SER:OG	4:G:246:GLN:HG3	2.17	0.44
4:J:42:GLN:HG2	5:K:86:HIS:NE2	2.32	0.44
1:M:314:VAL:O	1:M:335:ARG:NH2	2.49	0.44
4:U:29:ALA:HB2	4:U:38:ARG:HD3	1.99	0.44
4:U:173:THR:HA	4:U:177:LYS:NZ	2.33	0.44
4:V:239:LEU:HD23	4:V:239:LEU:HA	1.78	0.44
2:B:123:HIS:CD2	4:F:23:MET:HE2	2.52	0.44
4:E:300:ALA:HB2	4:E:304:PHE:CE1	2.52	0.44
4:H:356:TRP:CE2	4:H:361:GLY:HA2	2.53	0.44
1:M:71:ILE:HG22	1:M:72:MET:HE2	1.99	0.44
4:T:245:GLU:OE1	4:T:245:GLU:N	2.49	0.44
1:A:198:GLN:HG3	1:A:198:GLN:O	2.17	0.44
3:D:144:GLU:OE1	3:D:160:THR:OG1	2.33	0.44
4:F:268:ARG:NH1	4:G:179:ASP:OD1	2.51	0.44
4:F:360:ASN:O	4:F:360:ASN:ND2	2.50	0.44
1:M:238:HIS:O	1:M:266:LYS:HA	2.17	0.44
1:M:248:GLY:HA3	1:M:260:ARG:CZ	2.47	0.44
4:Q:70:GLN:OE1	4:Q:70:GLN:N	2.45	0.44
4:R:300:ALA:HB2	4:R:304:PHE:CE1	2.52	0.44
4:S:70:GLN:OE1	4:S:70:GLN:N	2.46	0.44
4:U:82:ARG:O	4:U:83:PHE:CE2	2.68	0.44
4:U:218:GLU:CG	4:U:303:GLY:HA2	2.47	0.44
3:D:96:ILE:HG22	3:D:97:LEU:H	1.83	0.44
4:H:48:MET:HE1	4:H:254:VAL:HG13	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:7:ASN:OD1	1:M:7:ASN:N	2.51	0.44
4:U:143:LEU:HD23	4:U:143:LEU:HA	1.85	0.44
1:A:244:PRO:HG3	1:A:261:TYR:CE2	2.53	0.44
4:F:290:MET:SD	4:F:316:TRP:HE3	2.41	0.44
4:R:95:LEU:HD13	4:R:172:MET:HE2	1.98	0.44
2:C:87:LEU:HD21	2:C:117:LEU:HD11	2.00	0.44
4:J:246:GLN:O	4:J:249:GLU:HB3	2.18	0.44
2:O:5:ILE:HD11	2:O:54:HIS:HB3	2.00	0.44
3:P:86:PHE:HB2	3:P:194:LEU:HD11	1.99	0.44
4:S:284:SER:OG	4:S:285:ASP:N	2.50	0.44
4:V:48:MET:HE1	4:V:184:ILE:HG12	1.99	0.44
5:W:42:ALA:O	5:W:142:TYR:HB2	2.18	0.44
1:A:332:ASN:OD1	1:A:335:ARG:HD2	2.17	0.44
3:D:17:TYR:O	3:D:20:HIS:HB3	2.17	0.44
4:G:70:GLN:OE1	4:G:70:GLN:N	2.47	0.44
1:M:353:ASN:HB2	1:M:358:LEU:HD11	1.99	0.44
2:N:113:ASP:OD1	2:N:113:ASP:N	2.51	0.44
4:S:57:ASN:HB3	4:S:253:HIS:CE1	2.53	0.44
4:T:75:LEU:HD12	4:T:92:LEU:HD22	1.99	0.44
1:A:4:LEU:HD23	1:A:84:ILE:HB	1.99	0.44
1:A:24:LEU:HD22	1:A:28:TYR:HD2	1.83	0.44
3:D:171:ASP:OD1	3:D:173:PRO:HD2	2.17	0.44
1:A:176:VAL:N	1:A:188:ASN:OD1	2.49	0.43
4:F:278:MET:HG2	4:F:279:VAL:N	2.30	0.43
3:P:26:LEU:HD21	3:P:66:ALA:HB3	1.99	0.43
4:R:317:ASP:OD1	4:R:341:THR:HG22	2.17	0.43
1:M:177:ARG:NH1	1:M:344:GLU:OE2	2.51	0.43
4:Q:301:LYS:O	4:Q:301:LYS:HG3	2.18	0.43
4:T:280:MET:HE1	4:T:316:TRP:CE2	2.53	0.43
1:A:250:CYS:C	1:A:252:CYS:H	2.25	0.43
1:A:250:CYS:HB3	1:A:253:CYS:HB2	1.75	0.43
3:D:62:SER:OG	3:D:67:THR:HA	2.18	0.43
4:J:201:THR:HG22	4:J:214:LEU:HG	1.99	0.43
1:M:9:ILE:HA	1:M:10:PRO:HD3	1.86	0.43
4:U:57:ASN:HB3	4:U:253:HIS:CE1	2.53	0.43
4:V:82:ARG:HB2	4:V:83:PHE:CD2	2.52	0.43
4:E:134:LEU:HD12	4:E:135:ASP:H	1.84	0.43
4:I:66:ILE:HB	4:I:111:VAL:HG22	2.00	0.43
4:R:70:GLN:OE1	4:R:70:GLN:N	2.43	0.43
4:U:89:ASP:O	4:U:93:ALA:HB2	2.19	0.43
4:G:48:MET:HE1	4:G:254:VAL:HG13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:360:ASN:O	4:G:360:ASN:ND2	2.51	0.43
4:J:25:MET:HE2	4:J:25:MET:HB3	1.90	0.43
4:F:5:ILE:CG2	4:F:230:ILE:HB	2.49	0.43
4:F:23:MET:O	4:F:25:MET:HG2	2.17	0.43
2:N:65:LEU:C	2:N:67:ALA:H	2.27	0.43
4:R:290:MET:HE2	4:R:290:MET:HA	2.00	0.43
4:V:306:GLN:HB2	4:V:307:PRO:HD3	2.01	0.43
1:A:238:HIS:O	1:A:266:LYS:HA	2.19	0.43
4:G:336:ASP:CG	4:H:318:ARG:HH22	2.25	0.43
4:I:310:GLN:O	4:I:314:GLN:HG3	2.19	0.43
1:M:13:PRO:HB2	1:M:16:GLY:HA3	2.00	0.43
4:Q:256:HIS:HB2	4:Q:354:LYS:HD3	2.00	0.43
4:H:232:LEU:O	4:H:236:GLN:HG3	2.19	0.43
1:M:309:GLN:OE1	1:M:312:ARG:HD2	2.18	0.43
2:N:101:ARG:HG3	4:Q:199:TRP:CH2	2.54	0.43
4:V:13:HIS:ND1	4:V:13:HIS:N	2.67	0.43
4:V:44:LEU:HD21	4:V:226:ARG:HD3	2.01	0.43
5:W:97:GLY:O	5:W:98:LEU:HD23	2.19	0.43
3:D:148:TYR:CE2	3:D:157:LYS:HD2	2.54	0.43
5:K:137:VAL:HG13	5:K:157:LEU:HB3	2.01	0.43
4:Q:13:HIS:CD2	4:Q:18:LEU:CD1	3.00	0.43
4:V:316:TRP:CG	4:V:340:ILE:HD11	2.54	0.43
3:D:1:MET:SD	3:D:55:GLN:NE2	2.88	0.43
3:D:92:PRO:HB2	3:D:116:LEU:HD12	2.00	0.43
4:F:221:SER:OG	4:G:30:ILE:O	2.36	0.43
5:K:211:ARG:HH12	5:K:213:TRP:NE1	2.16	0.43
1:M:132:GLN:HA	1:M:133:PRO:HD3	1.83	0.43
1:M:488:LYS:O	1:M:489:HIS:C	2.62	0.43
2:N:102:ILE:O	2:N:106:ILE:HG23	2.18	0.43
4:Q:221:SER:OG	4:R:30:ILE:O	2.37	0.43
4:U:83:PHE:HB3	4:U:87:ILE:CD1	2.49	0.43
5:W:172:LEU:HD23	5:W:172:LEU:O	2.19	0.43
1:A:158:PHE:HB2	1:A:162:PHE:CD1	2.53	0.42
4:F:94:LEU:HD22	4:F:171:MET:HE3	2.01	0.42
1:M:35:ARG:NH2	1:M:179:ILE:O	2.52	0.42
3:P:103:LEU:HA	3:P:109:ILE:HA	2.01	0.42
4:Q:310:GLN:O	4:Q:314:GLN:HG3	2.19	0.42
3:P:177:ASP:OD1	3:P:177:ASP:C	2.63	0.42
4:R:22:ASP:HA	6:X:21:G:N7	2.35	0.42
4:S:101:ASP:HB2	4:S:103:ALA:H	1.83	0.42
4:U:298:VAL:CG1	4:U:307:PRO:HB2	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:V:347:MET:HG3	4:V:353:LEU:HA	2.02	0.42
3:D:99:ASN:N	6:L:44:U:O4	2.29	0.42
4:F:101:ASP:HB2	4:F:103:ALA:H	1.83	0.42
4:F:304:PHE:C	4:F:307:PRO:HD2	2.44	0.42
4:I:301:LYS:HE2	4:I:307:PRO:HG3	2.00	0.42
4:S:69:ALA:O	4:S:72:ARG:HB3	2.19	0.42
4:S:83:PHE:HE1	4:S:124:GLU:HB3	1.83	0.42
4:T:94:LEU:HD22	4:T:171:MET:HE3	2.02	0.42
4:T:152:VAL:O	4:T:155:GLN:HG3	2.18	0.42
4:U:146:ASP:OD1	4:U:146:ASP:O	2.38	0.42
1:A:47:ALA:HB2	1:A:146:ILE:HD13	2.02	0.42
1:A:177:ARG:HH11	1:A:364:VAL:HG11	1.84	0.42
1:A:317:LYS:O	1:A:324:GLY:HA3	2.20	0.42
4:G:14:SER:O	4:G:15:PRO:C	2.61	0.42
4:J:348:PRO:HD2	4:J:352:GLN:OE1	2.20	0.42
2:O:101:ARG:HH21	4:T:22:ASP:CG	2.25	0.42
4:R:9:VAL:HB	4:R:226:ARG:HB2	2.02	0.42
4:E:170:GLY:O	4:E:173:THR:HG22	2.19	0.42
4:Q:9:VAL:HG22	4:Q:279:VAL:HG22	2.01	0.42
4:U:300:ALA:HB2	4:U:304:PHE:CE1	2.53	0.42
4:U:342:ALA:O	4:U:344:VAL:N	2.53	0.42
4:E:86:LYS:HE2	4:E:86:LYS:HB2	1.87	0.42
4:E:138:LYS:O	4:E:142:VAL:HG23	2.18	0.42
4:F:147:ILE:HD13	4:F:147:ILE:HA	1.78	0.42
4:I:314:GLN:O	4:I:318:ARG:HG3	2.20	0.42
4:Q:360:ASN:ND2	4:Q:360:ASN:O	2.53	0.42
4:U:20:ARG:HG3	4:U:20:ARG:HH11	1.85	0.42
4:U:38:ARG:HA	4:U:187:ALA:O	2.19	0.42
4:U:77:GLN:HG3	4:U:78:LYS:HD2	2.01	0.42
4:V:185:ALA:HB2	5:W:152:PRO:HG3	2.00	0.42
5:W:97:GLY:C	5:W:98:LEU:HD23	2.45	0.42
3:D:26:LEU:HD23	3:D:66:ALA:HB1	2.02	0.42
5:K:42:ALA:O	5:K:142:TYR:HB2	2.19	0.42
6:L:58:G:C2	6:L:59:G:C8	3.07	0.42
1:M:210:THR:HG23	1:M:215:ILE:HG13	2.01	0.42
1:M:468:PRO:HG2	1:M:469:TYR:CE2	2.55	0.42
4:R:341:THR:O	4:R:343:GLN:N	2.52	0.42
4:S:301:LYS:O	4:S:301:LYS:HG3	2.19	0.42
1:A:24:LEU:HA	1:A:24:LEU:HD23	1.84	0.42
1:A:216:LYS:O	1:A:219:GLU:HB2	2.20	0.42
2:B:65:LEU:O	2:B:67:ALA:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:30:ILE:HD12	4:J:194:ASP:CB	2.50	0.42
4:I:10:LEU:HD23	4:I:10:LEU:HA	1.91	0.42
4:J:41:SER:OG	4:J:184:ILE:O	2.26	0.42
5:K:202:ILE:HD12	5:K:202:ILE:H	1.85	0.42
1:M:99:PRO:HB2	1:M:102:GLN:HB2	2.02	0.42
4:R:306:GLN:HB2	4:R:307:PRO:HD3	2.02	0.42
4:S:40:SER:HB2	4:S:42:GLN:NE2	2.35	0.42
4:S:277:ASP:CG	4:S:305:LEU:HD21	2.44	0.42
4:S:278:MET:HG3	4:S:279:VAL:N	2.34	0.42
6:X:40:A:H2'	6:X:41:G:O4'	2.20	0.42
2:B:113:ASP:OD1	2:B:113:ASP:N	2.53	0.42
4:E:286:MET:HB3	4:E:286:MET:HE2	1.78	0.42
4:H:69:ALA:O	4:H:72:ARG:HB3	2.19	0.42
4:J:56:GLN:HG2	4:J:57:ASN:ND2	2.35	0.42
2:N:51:ASN:HA	2:N:52:PRO:HD3	1.93	0.42
4:Q:65:THR:OG1	4:Q:66:ILE:N	2.53	0.42
4:R:39:ILE:HB	4:R:187:ALA:HB3	2.02	0.42
4:R:68:LEU:HB2	4:R:106:ILE:HG13	2.02	0.42
4:R:155:GLN:HG2	4:R:239:LEU:HD22	2.02	0.42
5:W:12:PRO:HD3	5:W:154:THR:HG23	2.01	0.42
4:E:151:ARG:NH2	4:E:175:LEU:O	2.42	0.41
4:G:144:LYS:HB3	4:G:144:LYS:HE2	1.77	0.41
1:M:239:ILE:HG23	1:M:264:PHE:CD2	2.55	0.41
4:Q:5:ILE:HG21	4:Q:5:ILE:HD13	1.83	0.41
4:T:93:ALA:HB2	4:T:100:VAL:CG2	2.40	0.41
2:B:5:ILE:HG21	2:B:61:MET:HE1	2.01	0.41
3:D:118:LYS:HE2	3:D:118:LYS:HB3	1.84	0.41
4:U:25:MET:HB3	4:U:25:MET:HE2	1.83	0.41
5:W:44:LEU:O	5:W:45:GLY:C	2.63	0.41
4:F:20:ARG:HD2	4:F:24:ASN:HA	2.02	0.41
4:G:268:ARG:HH11	4:G:268:ARG:HG3	1.85	0.41
4:V:232:LEU:O	4:V:236:GLN:HG3	2.21	0.41
5:W:25:ARG:HA	5:W:26:PRO:HD3	1.77	0.41
6:X:30:G:C6	6:X:31:A:N6	2.88	0.41
4:F:115:VAL:HG12	4:F:118:GLU:H	1.84	0.41
4:F:214:LEU:HD22	4:G:22:ASP:HB3	2.01	0.41
4:H:167:ALA:H	4:H:177:LYS:CE	2.28	0.41
4:Q:13:HIS:ND1	4:Q:13:HIS:N	2.68	0.41
4:T:65:THR:OG1	4:T:66:ILE:N	2.52	0.41
4:U:304:PHE:C	4:U:307:PRO:HD2	2.45	0.41
1:A:64:ASP:O	1:A:67:PHE:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:214:LEU:CD1	4:F:22:ASP:HB3	2.50	0.41
4:H:290:MET:HE2	4:H:290:MET:HA	2.02	0.41
4:I:18:LEU:HD13	4:I:39:ILE:HD11	2.01	0.41
1:M:170:THR:N	1:M:171:PRO:HD3	2.36	0.41
1:A:90:MET:HB2	1:A:90:MET:HE3	1.71	0.41
1:A:231:GLY:HA3	1:A:277:TRP:CZ2	2.56	0.41
4:G:118:GLU:CD	4:G:165:ARG:HH22	2.29	0.41
4:G:245:GLU:OE1	4:G:245:GLU:N	2.52	0.41
4:I:37:VAL:CG2	4:I:193:VAL:HG21	2.47	0.41
1:M:335:ARG:HG3	1:M:372:GLN:HB3	2.01	0.41
2:O:37:ILE:O	2:O:40:PHE:HB3	2.21	0.41
2:O:109:ASP:O	2:O:110:ARG:C	2.60	0.41
4:T:54:TYR:CD2	4:T:58:ILE:HD12	2.55	0.41
5:W:184:GLU:HG2	5:W:211:ARG:NH2	2.36	0.41
1:A:24:LEU:HD22	1:A:28:TYR:CD2	2.56	0.41
1:A:343:LEU:HB2	1:A:371:TRP:NE1	2.36	0.41
2:B:44:VAL:HG23	2:B:49:TRP:HB2	2.03	0.41
4:I:301:LYS:HG3	4:I:307:PRO:HG3	2.03	0.41
2:N:35:ARG:NH1	2:O:143:ARG:HD2	2.35	0.41
2:O:131:PRO:O	2:O:134:ALA:HB3	2.21	0.41
3:P:184:GLY:O	3:P:187:LYS:NZ	2.51	0.41
2:C:111:THR:CG2	2:C:112:ALA:N	2.73	0.41
4:E:87:ILE:HD13	4:E:87:ILE:HA	1.91	0.41
4:F:86:LYS:HA	4:F:86:LYS:HD2	1.92	0.41
4:I:87:ILE:HD13	4:I:87:ILE:HA	1.96	0.41
4:J:239:LEU:HD23	4:J:239:LEU:HA	1.74	0.41
4:Q:41:SER:HB2	4:Q:184:ILE:HG23	2.02	0.41
4:R:49:ARG:NH2	6:X:20:G:OP2	2.44	0.41
4:V:6:ASN:ND2	4:V:284:SER:HB3	2.36	0.41
1:A:42:ASP:OD1	1:A:43:MET:N	2.54	0.41
1:A:343:LEU:HB2	1:A:371:TRP:CE2	2.56	0.41
4:E:5:ILE:HD13	4:E:5:ILE:HG21	1.85	0.41
4:E:57:ASN:HB3	4:E:253:HIS:CE1	2.56	0.41
4:F:41:SER:HB2	4:F:184:ILE:HG23	2.03	0.41
4:G:242:ALA:HB1	4:G:246:GLN:CD	2.45	0.41
4:H:286:MET:HG3	4:H:287:PRO:HD2	2.02	0.41
4:I:347:MET:HA	4:I:348:PRO:HD3	1.81	0.41
4:J:183:SER:C	4:J:184:ILE:HD13	2.46	0.41
4:J:286:MET:HE2	5:K:157:LEU:H	1.86	0.41
1:M:9:ILE:HD13	1:M:9:ILE:HG21	1.80	0.41
1:M:319:ILE:HG22	1:M:321:ASN:OD1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:19:ASN:ND2	4:T:211:SER:HB3	2.36	0.41
3:P:95:THR:O	6:X:56:G:H5"	2.21	0.41
4:Q:22:ASP:OD1	4:Q:22:ASP:N	2.48	0.41
4:Q:190:THR:HG22	4:Q:294:PHE:CD2	2.55	0.41
4:R:49:ARG:HG2	4:R:61:SER:HB2	2.03	0.41
4:R:112:THR:HA	4:R:113:PRO:HD3	1.85	0.41
4:S:16:SER:HB3	4:S:272:ALA:HB2	2.01	0.41
4:T:221:SER:OG	4:U:30:ILE:O	2.38	0.41
4:U:316:TRP:CD1	4:U:316:TRP:C	2.99	0.41
4:V:345:LYS:HE3	4:V:345:LYS:HB3	1.68	0.41
5:W:159:LEU:HA	5:W:159:LEU:HD12	1.83	0.41
1:A:250:CYS:C	1:A:252:CYS:N	2.79	0.41
1:A:317:LYS:O	1:A:318:ILE:HD13	2.21	0.41
2:C:101:ARG:HB3	2:C:120:LEU:HD21	2.02	0.41
4:F:72:ARG:NH1	4:F:101:ASP:O	2.52	0.41
4:H:177:LYS:HA	4:H:177:LYS:HD2	1.78	0.41
1:M:488:LYS:O	1:M:490:LEU:N	2.54	0.41
2:O:97:ILE:HD12	2:O:120:LEU:HD22	2.03	0.41
3:P:172:ALA:HB3	3:P:173:PRO:HD3	2.03	0.41
4:R:301:LYS:O	4:R:301:LYS:HG3	2.21	0.41
4:T:20:ARG:HD2	4:T:24:ASN:HA	2.02	0.41
4:U:5:ILE:HG23	4:U:230:ILE:HB	2.03	0.41
4:V:183:SER:HB3	5:W:149:ARG:HG2	2.02	0.41
1:A:185:VAL:O	1:A:189:VAL:HG23	2.21	0.40
4:E:210:GLY:O	4:E:211:SER:C	2.64	0.40
1:M:192:LEU:O	1:M:196:GLN:HG2	2.21	0.40
1:M:243:ASP:HA	1:M:244:PRO:HD3	1.76	0.40
2:N:126:PRO:HB2	2:N:128:LEU:HD23	2.03	0.40
3:P:26:LEU:HD23	3:P:63:THR:HG23	2.04	0.40
3:P:96:ILE:HG22	3:P:97:LEU:N	2.29	0.40
3:P:148:TYR:CD2	3:P:157:LYS:HB2	2.56	0.40
4:R:176:GLY:O	4:R:178:VAL:HG23	2.21	0.40
4:U:101:ASP:OD1	4:U:102:GLU:C	2.50	0.40
3:D:27:PHE:HE1	3:D:59:MET:C	2.29	0.40
4:F:16:SER:HB3	4:F:272:ALA:HB2	2.03	0.40
4:J:16:SER:HB3	4:J:272:ALA:HB2	2.04	0.40
2:O:100:ARG:HD3	4:S:216:THR:HG21	2.02	0.40
4:R:19:ASN:ND2	4:R:40:SER:H	2.19	0.40
5:W:108:ARG:NH2	6:X:7:C:O2	2.50	0.40
2:C:142:LYS:HD2	2:C:142:LYS:HA	1.67	0.40
4:G:104:GLU:H	4:G:104:GLU:CD	2.28	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:K:13:MET:HE3	5:K:13:MET:HB2	1.73	0.40
4:R:258:LEU:HD12	4:R:258:LEU:HA	1.89	0.40
4:S:149:ALA:O	4:S:152:VAL:HG12	2.22	0.40
4:S:201:THR:CG2	4:S:214:LEU:HG	2.51	0.40
1:A:77:GLU:O	1:A:81:GLN:HG2	2.22	0.40
1:A:198:GLN:NE2	1:A:280:PRO:HB3	2.36	0.40
1:M:197:LYS:HE3	1:M:197:LYS:HB2	1.89	0.40
1:M:403:PHE:HZ	1:M:481:LEU:HB3	1.86	0.40
1:M:485:THR:O	1:M:488:LYS:HB3	2.22	0.40
3:P:74:VAL:HG21	4:U:203:VAL:HG11	2.04	0.40
4:Q:334:LEU:HD23	4:Q:334:LEU:HA	1.86	0.40
4:S:22:ASP:OD1	4:S:22:ASP:N	2.55	0.40
4:T:328:ALA:HB1	4:T:356:TRP:CZ2	2.56	0.40
4:V:172:MET:CE	5:W:96:ARG:HD2	2.52	0.40
4:V:252:THR:HG22	4:V:357:VAL:HB	2.03	0.40
4:E:137:LYS:HE3	4:E:137:LYS:HB3	1.83	0.40
4:F:57:ASN:HB3	4:F:253:HIS:CE1	2.57	0.40
4:I:232:LEU:O	4:I:236:GLN:HG3	2.20	0.40
4:J:6:ASN:HD21	4:J:284:SER:HB3	1.85	0.40
5:K:99:LYS:H	5:K:99:LYS:HG2	1.71	0.40
4:Q:13:HIS:HB3	4:Q:272:ALA:HB1	2.03	0.40
4:Q:38:ARG:HA	4:Q:187:ALA:O	2.22	0.40
4:Q:151:ARG:HD3	4:Q:151:ARG:HA	1.95	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	470/502 (94%)	432 (92%)	36 (8%)	2 (0%)	30 65
1	M	485/502 (97%)	457 (94%)	24 (5%)	4 (1%)	16 50

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	155/160 (97%)	149 (96%)	6 (4%)	0	100	100
2	C	155/160 (97%)	147 (95%)	8 (5%)	0	100	100
2	N	148/160 (92%)	140 (95%)	7 (5%)	1 (1%)	18	53
2	O	154/160 (96%)	147 (96%)	7 (4%)	0	100	100
3	D	185/201 (92%)	178 (96%)	7 (4%)	0	100	100
3	P	185/201 (92%)	176 (95%)	9 (5%)	0	100	100
4	E	353/363 (97%)	333 (94%)	20 (6%)	0	100	100
4	F	355/363 (98%)	335 (94%)	20 (6%)	0	100	100
4	G	352/363 (97%)	335 (95%)	17 (5%)	0	100	100
4	H	361/363 (99%)	348 (96%)	12 (3%)	1 (0%)	36	70
4	I	351/363 (97%)	335 (95%)	16 (5%)	0	100	100
4	J	345/363 (95%)	324 (94%)	21 (6%)	0	100	100
4	Q	358/363 (99%)	347 (97%)	10 (3%)	1 (0%)	36	70
4	R	355/363 (98%)	335 (94%)	20 (6%)	0	100	100
4	S	357/363 (98%)	343 (96%)	13 (4%)	1 (0%)	36	70
4	T	356/363 (98%)	343 (96%)	13 (4%)	0	100	100
4	U	350/363 (96%)	325 (93%)	23 (7%)	2 (1%)	21	56
4	V	351/363 (97%)	331 (94%)	20 (6%)	0	100	100
5	K	216/224 (96%)	211 (98%)	5 (2%)	0	100	100
5	W	216/224 (96%)	210 (97%)	5 (2%)	1 (0%)	24	60
All	All	6613/6850 (96%)	6281 (95%)	319 (5%)	13 (0%)	43	76

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	U	336	ASP
5	W	45	GLY
1	M	160	GLY
1	M	321	ASN
1	M	488	LYS
4	Q	210	GLY
4	U	15	PRO
4	H	101	ASP
1	M	140	CYS
4	S	101	ASP

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Mol	Chain	Res	Type
2	N	26	ARG
1	A	160	GLY
1	A	370	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	401/426 (94%)	385 (96%)	16 (4%)	28	62
1	M	409/426 (96%)	395 (97%)	14 (3%)	32	66
2	B	136/138 (99%)	135 (99%)	1 (1%)	76	86
2	C	136/138 (99%)	132 (97%)	4 (3%)	37	70
2	N	130/138 (94%)	125 (96%)	5 (4%)	29	63
2	O	128/138 (93%)	123 (96%)	5 (4%)	28	62
3	D	151/171 (88%)	141 (93%)	10 (7%)	15	46
3	P	152/171 (89%)	143 (94%)	9 (6%)	18	50
4	E	289/298 (97%)	281 (97%)	8 (3%)	38	70
4	F	290/298 (97%)	280 (97%)	10 (3%)	32	66
4	G	291/298 (98%)	286 (98%)	5 (2%)	53	78
4	H	288/298 (97%)	282 (98%)	6 (2%)	47	75
4	I	287/298 (96%)	283 (99%)	4 (1%)	59	80
4	J	279/298 (94%)	273 (98%)	6 (2%)	45	74
4	Q	294/298 (99%)	286 (97%)	8 (3%)	39	71
4	R	282/298 (95%)	277 (98%)	5 (2%)	51	77
4	S	290/298 (97%)	283 (98%)	7 (2%)	43	73
4	T	293/298 (98%)	290 (99%)	3 (1%)	68	84
4	U	287/298 (96%)	267 (93%)	20 (7%)	14	44
4	V	286/298 (96%)	274 (96%)	12 (4%)	26	61
5	K	185/192 (96%)	179 (97%)	6 (3%)	34	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	W	186/192 (97%)	178 (96%)	8 (4%)	26	60
All	All	5470/5706 (96%)	5298 (97%)	172 (3%)	35	68

All (172) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ASN
1	A	18	LYS
1	A	19	VAL
1	A	78	ASP
1	A	79	GLU
1	A	82	GLN
1	A	104	LYS
1	A	111	VAL
1	A	197	LYS
1	A	198	GLN
1	A	289	LYS
1	A	293	VAL
1	A	314	VAL
1	A	420	GLU
1	A	441	SER
1	A	474	LYS
2	B	81	GLN
2	C	42	ARG
2	C	111	THR
2	C	119	ARG
2	C	143	ARG
3	D	2	TYR
3	D	6	VAL
3	D	45	ASN
3	D	65	VAL
3	D	73	GLN
3	D	93	ILE
3	D	119	GLU
3	D	135	ARG
3	D	140	HIS
3	D	180	GLN
4	E	66	ILE
4	E	77	GLN
4	E	112	THR
4	E	145	GLU
4	E	211	SER

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Mol	Chain	Res	Type
4	E	245	GLU
4	E	326	ASN
4	E	362	GLU
4	F	84	ASP
4	F	90	LYS
4	F	147	ILE
4	F	152	VAL
4	F	174	GLU
4	F	269	THR
4	F	282	ASN
4	F	305	LEU
4	F	337	VAL
4	F	362	GLU
4	G	60	GLU
4	G	86	LYS
4	G	104	GLU
4	G	147	ILE
4	G	282	ASN
4	H	101	ASP
4	H	104	GLU
4	H	177	LYS
4	H	183	SER
4	H	282	ASN
4	H	299	LYS
4	I	1	MET
4	I	249	GLU
4	I	269	THR
4	I	282	ASN
4	J	1	MET
4	J	77	GLN
4	J	87	ILE
4	J	254	VAL
4	J	282	ASN
4	J	341	THR
5	K	24	THR
5	K	51	THR
5	K	103	THR
5	K	123	THR
5	K	125	HIS
5	K	192	LEU
1	M	19	VAL
1	M	38	LEU

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Mol	Chain	Res	Type
1	M	97	GLU
1	M	115	GLU
1	M	140	CYS
1	M	179	ILE
1	M	253	CYS
1	M	276	LEU
1	M	288	VAL
1	M	294	GLU
1	M	322	GLU
1	M	327	VAL
1	M	380	GLU
1	M	441	SER
2	N	5	ILE
2	N	15	GLN
2	N	16	GLN
2	N	56	GLN
2	N	110	ARG
2	O	42	ARG
2	O	83	THR
2	O	111	THR
2	O	143	ARG
2	O	158	LYS
3	P	4	SER
3	P	41	VAL
3	P	55	GLN
3	P	61	VAL
3	P	93	ILE
3	P	96	ILE
3	P	132	ASN
3	P	140	HIS
3	P	177	ASP
4	Q	13	HIS
4	Q	60	GLU
4	Q	62	SER
4	Q	101	ASP
4	Q	147	ILE
4	Q	150	ILE
4	Q	220	SER
4	Q	305	LEU
4	R	134	LEU
4	R	137	LYS
4	R	183	SER

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Mol	Chain	Res	Type
4	R	282	ASN
4	R	314	GLN
4	S	81	GLU
4	S	84	ASP
4	S	130	GLU
4	S	221	SER
4	S	269	THR
4	S	278	MET
4	S	362	GLU
4	T	100	VAL
4	T	269	THR
4	T	321	ASN
4	U	5	ILE
4	U	19	ASN
4	U	60	GLU
4	U	70	GLN
4	U	76	ARG
4	U	83	PHE
4	U	86	LYS
4	U	87	ILE
4	U	94	LEU
4	U	102	GLU
4	U	125	GLN
4	U	126	VAL
4	U	128	LYS
4	U	169	SER
4	U	172	MET
4	U	203	VAL
4	U	249	GLU
4	U	282	ASN
4	U	335	SER
4	U	336	ASP
4	V	13	HIS
4	V	41	SER
4	V	42	GLN
4	V	65	THR
4	V	87	ILE
4	V	146	ASP
4	V	158	VAL
4	V	179	ASP
4	V	211	SER
4	V	268	ARG

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Mol	Chain	Res	Type
4	V	269	THR
4	V	282	ASN
5	W	20	THR
5	W	24	THR
5	W	44	LEU
5	W	87	THR
5	W	99	LYS
5	W	123	THR
5	W	143	THR
5	W	163	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (72) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	ASN
1	A	15	ASN
1	A	82	GLN
1	A	464	GLN
2	B	75	GLN
2	B	123	HIS
2	B	159	ASN
3	D	20	HIS
3	D	73	GLN
3	D	132	ASN
3	D	140	HIS
4	E	67	HIS
4	E	125	GLN
4	E	156	GLN
4	F	6	ASN
4	F	13	HIS
4	F	156	GLN
4	F	274	ASN
4	F	352	GLN
4	F	359	ASN
4	G	13	HIS
4	G	67	HIS
4	G	125	GLN
4	G	246	GLN
4	G	274	ASN
4	G	306	GLN
4	H	13	HIS
4	H	156	GLN

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Mol	Chain	Res	Type
4	I	156	GLN
4	I	217	GLN
4	J	13	HIS
4	J	57	ASN
4	J	253	HIS
4	J	256	HIS
4	J	274	ASN
1	M	94	ASN
1	M	218	ASN
1	M	426	GLN
2	N	54	HIS
3	P	45	ASN
3	P	132	ASN
3	P	140	HIS
4	Q	6	ASN
4	Q	13	HIS
4	Q	156	GLN
4	Q	217	GLN
4	Q	282	ASN
4	Q	352	GLN
4	Q	359	ASN
4	R	19	ASN
4	R	314	GLN
4	R	359	ASN
4	S	19	ASN
4	S	67	HIS
4	S	85	GLN
4	S	156	GLN
4	S	274	ASN
4	S	359	ASN
4	T	57	ASN
4	T	67	HIS
4	T	156	GLN
4	T	359	ASN
4	U	19	ASN
4	U	24	ASN
4	U	274	ASN
4	V	13	HIS
4	V	207	GLN
4	V	282	ASN
4	V	326	ASN
4	V	352	GLN

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Mol	Chain	Res	Type
5	W	101	HIS
5	W	163	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
6	L	60/61 (98%)	20 (33%)	2 (3%)
6	X	60/61 (98%)	20 (33%)	2 (3%)
All	All	120/122 (98%)	40 (33%)	4 (3%)

All (40) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
6	L	2	U
6	L	4	A
6	L	9	G
6	L	10	G
6	L	15	C
6	L	21	G
6	L	22	U
6	L	27	A
6	L	28	U
6	L	33	A
6	L	34	A
6	L	38	U
6	L	39	G
6	L	40	A
6	L	43	G
6	L	45	U
6	L	46	C
6	L	54	C
6	L	55	A
6	L	56	G
6	X	4	A
6	X	9	G
6	X	10	G
6	X	15	C
6	X	21	G
6	X	22	U
6	X	27	A
6	X	28	U

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Mol	Chain	Res	Type
6	X	33	A
6	X	34	A
6	X	38	U
6	X	39	G
6	X	40	A
6	X	43	G
6	X	44	U
6	X	45	U
6	X	46	C
6	X	53	C
6	X	54	C
6	X	56	G

All (4) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
6	L	27	A
6	L	45	U
6	X	15	C
6	X	45	U

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	480/502 (95%)	0.02	4 (0%) 82 64	37, 80, 111, 135	0
1	M	489/502 (97%)	-0.39	1 (0%) 91 83	26, 42, 68, 122	0
2	B	157/160 (98%)	-0.36	2 (1%) 75 53	30, 44, 84, 120	0
2	C	157/160 (98%)	-0.17	2 (1%) 75 53	32, 52, 85, 115	0
2	N	152/160 (95%)	-0.20	0 100 100	40, 56, 85, 114	0
2	O	156/160 (97%)	0.21	4 (2%) 57 34	53, 84, 124, 146	0
3	D	191/201 (95%)	0.31	9 (4%) 36 19	41, 70, 112, 122	0
3	P	191/201 (95%)	0.37	9 (4%) 36 19	52, 78, 111, 127	0
4	E	357/363 (98%)	-0.29	6 (1%) 69 45	30, 48, 78, 104	0
4	F	359/363 (98%)	-0.29	3 (0%) 82 64	28, 48, 86, 121	0
4	G	356/363 (98%)	-0.40	2 (0%) 85 69	24, 44, 76, 101	0
4	H	363/363 (100%)	-0.21	5 (1%) 73 51	25, 47, 93, 116	0
4	I	355/363 (97%)	-0.33	0 100 100	26, 47, 79, 104	0
4	J	351/363 (96%)	-0.08	4 (1%) 78 57	35, 62, 110, 129	0
4	Q	362/363 (99%)	-0.37	5 (1%) 73 51	23, 39, 72, 114	0
4	R	359/363 (98%)	-0.11	10 (2%) 55 32	27, 50, 119, 155	0
4	S	361/363 (99%)	-0.24	4 (1%) 78 57	30, 52, 99, 118	0
4	T	360/363 (99%)	-0.32	3 (0%) 82 64	32, 50, 75, 121	0
4	U	354/363 (97%)	-0.01	3 (0%) 82 64	41, 68, 129, 146	0
4	V	355/363 (97%)	-0.40	4 (1%) 78 57	21, 38, 85, 120	0
5	K	218/224 (97%)	-0.07	2 (0%) 81 61	44, 67, 90, 106	0
5	W	218/224 (97%)	-0.49	0 100 100	22, 35, 53, 81	0
6	L	61/61 (100%)	-0.68	0 100 100	31, 47, 101, 118	0
6	X	61/61 (100%)	-0.55	0 100 100	25, 50, 120, 150	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
All	All	6823/6972 (97%)	-0.21	82 (1%)	76 55	21, 52, 103, 155	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	T	336	ASP	5.4
4	F	213	HIS	5.1
4	R	209	GLN	4.9
4	T	209	GLN	4.4
1	A	200	PRO	4.1
4	S	336	ASP	4.0
4	T	339	PRO	3.8
4	S	341	THR	3.7
3	D	28	PRO	3.5
4	R	208	GLU	3.5
4	Q	211	SER	3.4
3	P	27	PHE	3.3
3	P	-1	ALA	3.3
4	E	212	ALA	3.3
3	D	-1	ALA	3.2
4	Q	212	ALA	3.2
4	R	337	VAL	3.2
4	F	337	VAL	3.1
1	A	318	ILE	3.1
3	P	97	LEU	3.1
4	E	336	ASP	3.0
5	K	1	MET	3.0
3	D	12	TRP	2.9
4	R	84	ASP	2.9
5	K	45	GLY	2.8
4	E	211	SER	2.7
4	Q	210	GLY	2.7
1	A	289	LYS	2.7
4	H	133	ASN	2.7
2	B	82	THR	2.7
2	C	160	ALA	2.7
4	H	338	ASP	2.6
3	P	77	GLN	2.6
4	H	363	ALA	2.6
3	D	24	TRP	2.6
4	R	336	ASP	2.6
3	D	154	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
4	Q	363	ALA	2.5
2	O	81	GLN	2.5
3	D	65	VAL	2.5
4	J	209	GLN	2.5
3	P	12	TRP	2.4
4	E	209	GLN	2.4
4	R	103	ALA	2.4
2	O	50	GLU	2.4
4	U	94	LEU	2.4
4	G	209	GLN	2.4
3	P	188	SER	2.4
4	J	97	GLY	2.3
3	D	11	ALA	2.3
4	E	363	ALA	2.3
1	A	293	VAL	2.3
3	P	65	VAL	2.3
2	C	112	ALA	2.3
3	P	17	TYR	2.3
4	V	209	GLN	2.3
4	S	340	ILE	2.3
2	O	80	GLU	2.3
1	M	204	HIS	2.2
4	R	106	ILE	2.2
4	J	208	GLU	2.2
3	D	64	ALA	2.2
4	R	339	PRO	2.2
4	U	194	ASP	2.2
4	H	90	LYS	2.1
4	R	342	ALA	2.1
4	V	212	ALA	2.1
3	P	109	ILE	2.1
3	D	106	LYS	2.1
4	G	208	GLU	2.1
4	S	208	GLU	2.1
4	E	213	HIS	2.1
4	V	98	LYS	2.1
4	V	211	SER	2.1
4	U	163	SER	2.1
4	J	338	ASP	2.1
2	B	81	GLN	2.1
4	H	339	PRO	2.1
4	R	86	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
2	O	52	PRO	2.0
4	F	363	ALA	2.0
4	Q	341	THR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.