



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:38 AM UTC

PDB ID : 8QKS / pdb_00008qks
Title : Plasmodium falciparum reticulocyte-binding protein homologue 5 (PfRH5) bound to R5.034
Authors : Wright, N.D.; Barrett, J.R.; Bradshaw, W.J.; Paterson, N.G.; MacLean, E.M.; Ferreira, L.; McHugh, K.; Von Delft, F.; Koekemoer, L.; Draper, S.J.
Deposited on : 2023-09-16
Resolution : 3.99 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

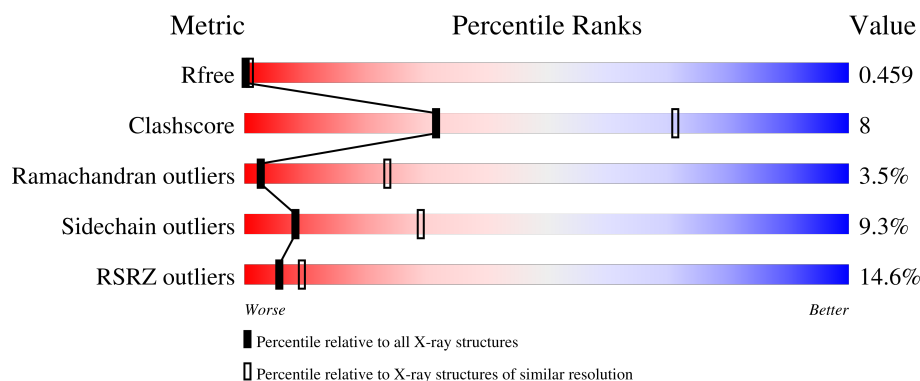
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.99 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	1082 (4.20-3.80)
Clashscore	190562	1129 (4.20-3.80)
Ramachandran outliers	187476	1064 (4.20-3.80)
Sidechain outliers	187428	1055 (4.20-3.80)
RSRZ outliers	180081	1082 (4.20-3.80)

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	308	11% 67% 21% 5% 5%
1	D	308	8% 65% 19% 11%
1	G	308	10% 73% 20% 6%
1	H	308	10% 63% 19% 14%
1	M	308	11% 74% 16% 6%

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Mol	Chain	Length	Quality of chain
1	N	308	
1	S	308	
1	T	308	
2	B	103	
2	E	103	
2	I	103	
2	K	103	
2	O	103	
2	Q	103	
2	U	103	
2	W	103	
3	C	125	
3	F	125	
3	J	125	
3	L	125	
3	P	125	
3	R	125	
3	V	125	
3	X	125	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 32284 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 Reticulocyte-binding protein-like protein 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	294	Total	C	N	O	S	0	0	0
			2503	1614	422	452	15			
1	D	273	Total	C	N	O	S	0	0	0
			2309	1488	389	418	14			
1	G	308	Total	C	N	O	S	0	0	0
			2618	1686	443	474	15			
1	H	266	Total	C	N	O	S	0	0	0
			2251	1447	379	412	13			
1	M	288	Total	C	N	O	S	0	0	0
			2450	1581	413	441	15			
1	N	283	Total	C	N	O	S	0	0	0
			2397	1539	406	438	14			
1	S	288	Total	C	N	O	S	0	0	0
			2442	1569	416	442	15			
1	T	270	Total	C	N	O	S	0	0	0
			2288	1473	384	417	14			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	77	ALA	THR	conflict	UNP A0A8F2YHP6
A	111	ALA	THR	conflict	UNP A0A8F2YHP6
D	77	ALA	THR	conflict	UNP A0A8F2YHP6
D	111	ALA	THR	conflict	UNP A0A8F2YHP6
G	77	ALA	THR	conflict	UNP A0A8F2YHP6
G	111	ALA	THR	conflict	UNP A0A8F2YHP6
H	77	ALA	THR	conflict	UNP A0A8F2YHP6
H	111	ALA	THR	conflict	UNP A0A8F2YHP6
M	77	ALA	THR	conflict	UNP A0A8F2YHP6
M	111	ALA	THR	conflict	UNP A0A8F2YHP6
N	77	ALA	THR	conflict	UNP A0A8F2YHP6
N	111	ALA	THR	conflict	UNP A0A8F2YHP6
S	77	ALA	THR	conflict	UNP A0A8F2YHP6

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Chain	Residue	Modelled	Actual	Comment	Reference
S	111	ALA	THR	conflict	UNP A0A8F2YHP6
T	77	ALA	THR	conflict	UNP A0A8F2YHP6
T	111	ALA	THR	conflict	UNP A0A8F2YHP6

- Molecule 2 is a protein called Immunoglobulin lambda variable 1-36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	96	Total	C	N	O	S	0	0	0
			721	445	124	150	2			
2	E	97	Total	C	N	O	S	0	1	0
			737	455	126	154	2			
2	I	97	Total	C	N	O	S	0	0	0
			728	450	125	151	2			
2	K	97	Total	C	N	O	S	0	0	0
			728	450	125	151	2			
2	O	96	Total	C	N	O	S	0	0	0
			713	442	120	149	2			
2	Q	93	Total	C	N	O	S	0	0	0
			702	434	121	145	2			
2	U	94	Total	C	N	O	S	0	0	0
			696	428	122	144	2			
2	W	97	Total	C	N	O	S	0	0	0
			725	449	125	149	2			

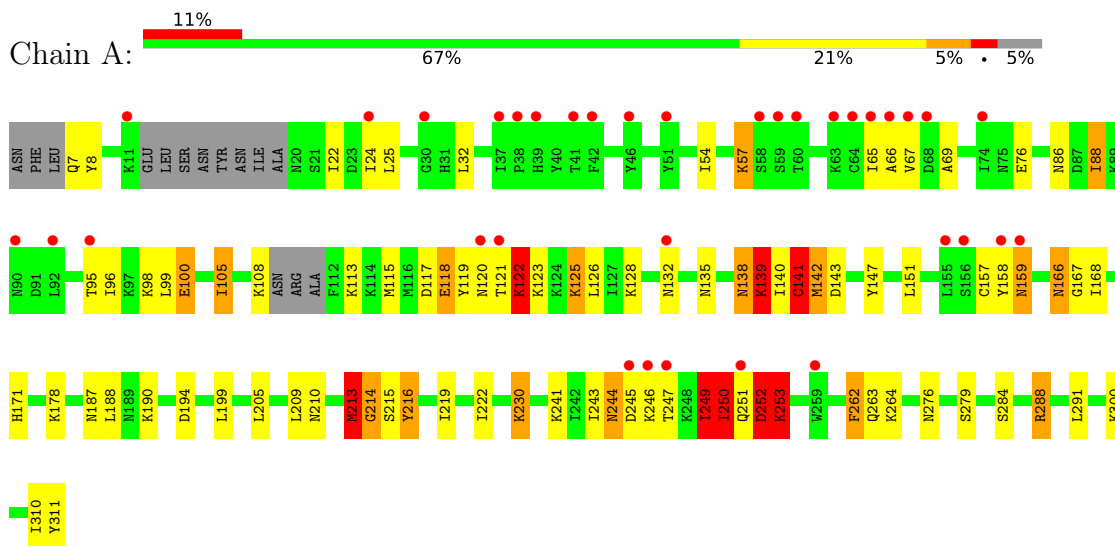
- Molecule 3 is a protein called R5034HV.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	120	Total	C	N	O	S	0	0	0
			910	570	159	176	5			
3	F	120	Total	C	N	O	S	0	0	0
			907	566	160	176	5			
3	J	120	Total	C	N	O	S	0	0	0
			903	564	159	175	5			
3	L	120	Total	C	N	O	S	0	0	0
			915	572	160	178	5			
3	P	120	Total	C	N	O	S	0	0	0
			914	572	160	177	5			
3	R	120	Total	C	N	O	S	0	0	0
			914	572	160	177	5			
3	V	120	Total	C	N	O	S	0	0	0
			908	566	160	177	5			
3	X	120	Total	C	N	O	S	0	0	0
			905	564	159	177	5			

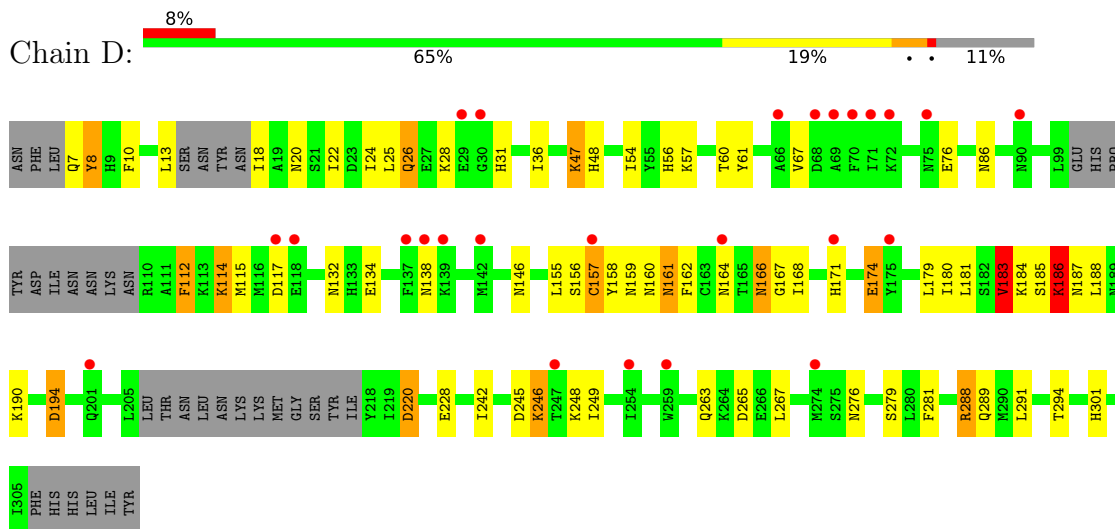
3 Residue-property plots [i](#)

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

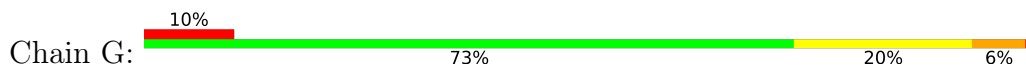
- Molecule 1: Reticulocyte-binding protein-like protein 5

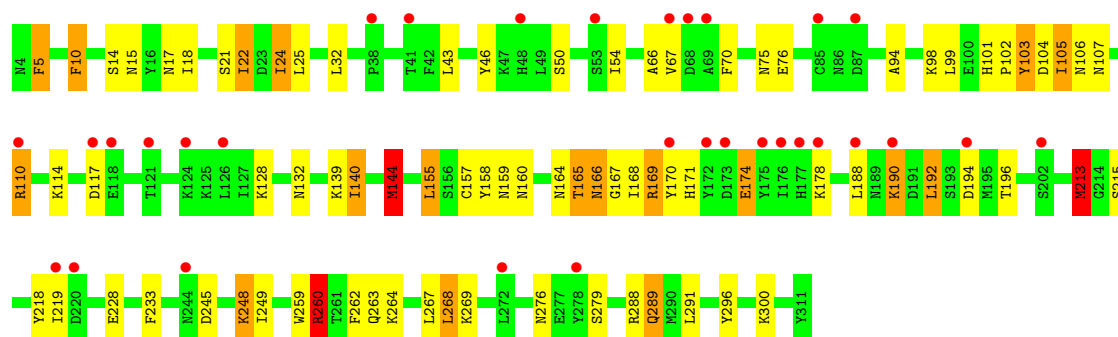


- Molecule 1: Reticulocyte-binding protein-like protein 5

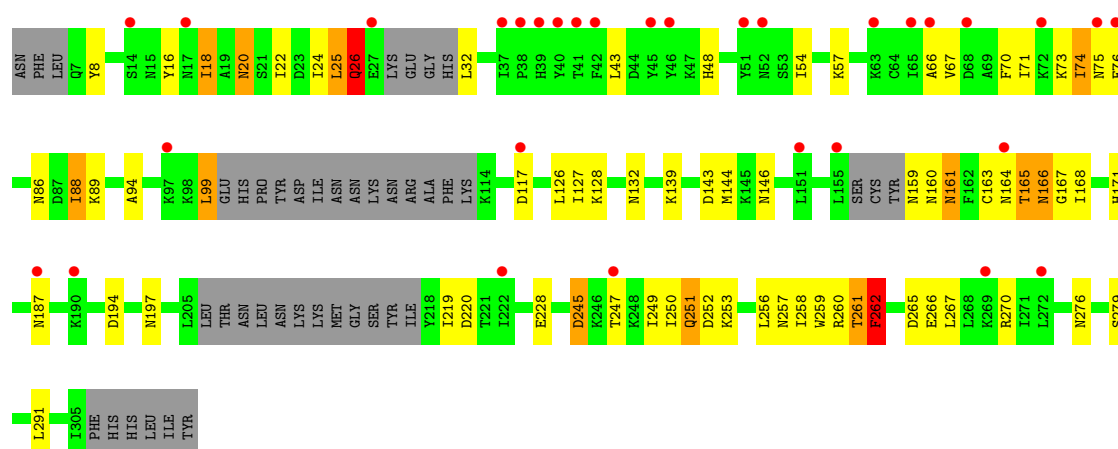


- Molecule 1: Reticulocyte-binding protein-like protein 5

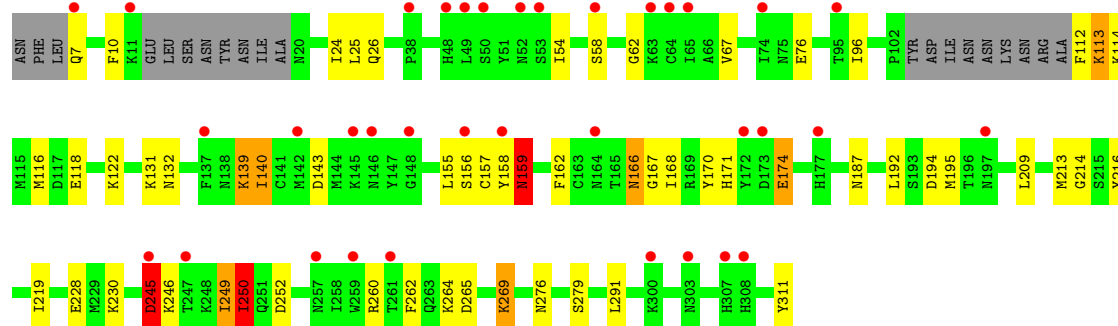
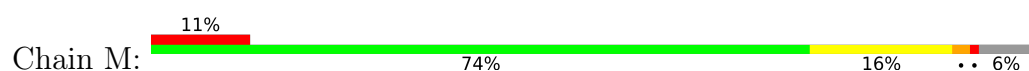




• Molecule 1: Reticulocyte-binding protein-like protein 5

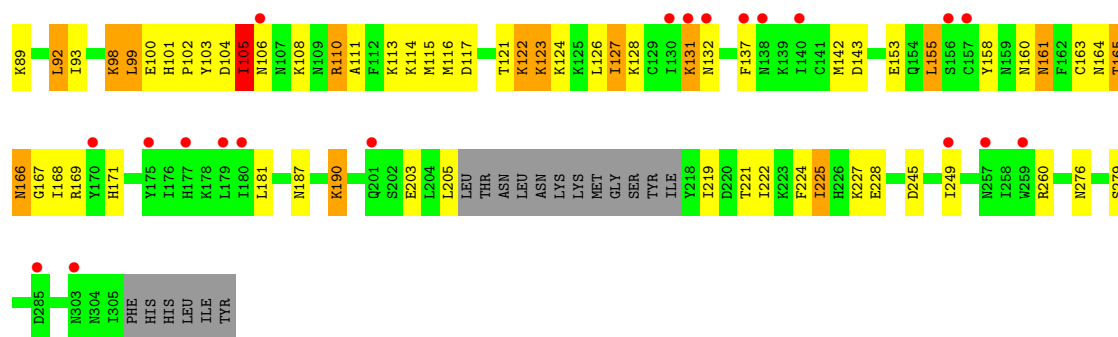


• Molecule 1: Reticulocyte-binding protein-like protein 5

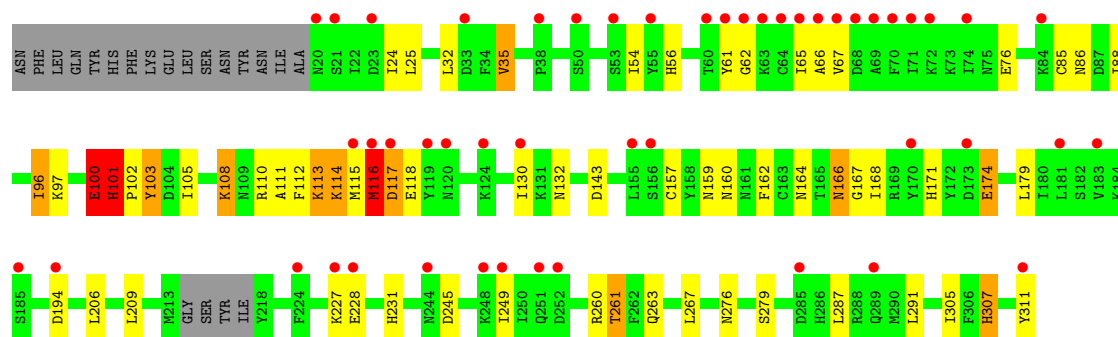


• Molecule 1: Reticulocyte-binding protein-like protein 5

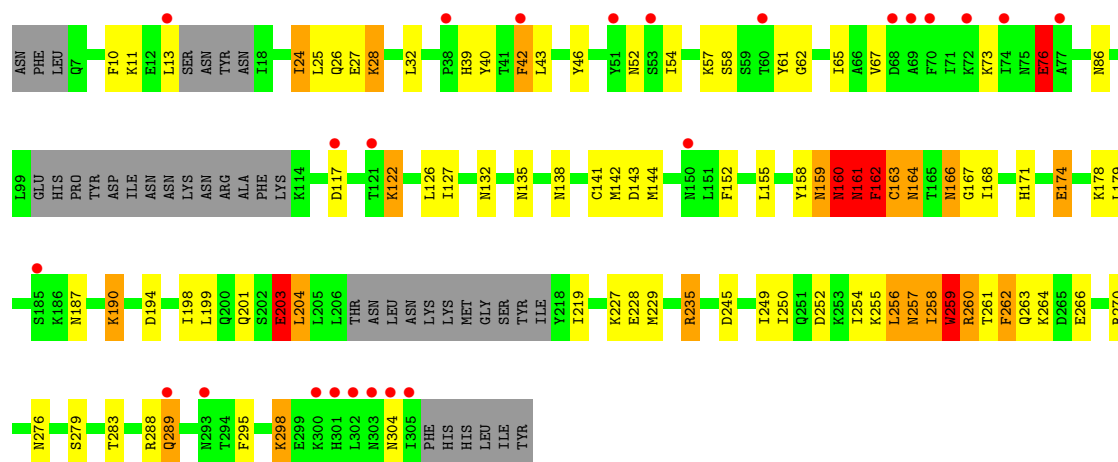




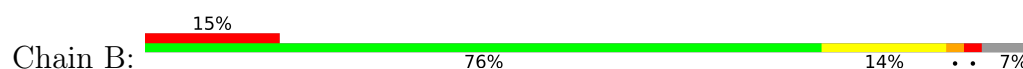
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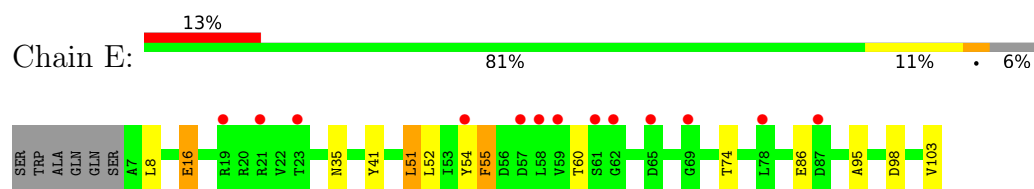
• Molecule 1: Reticulocyte-binding protein-like protein 5



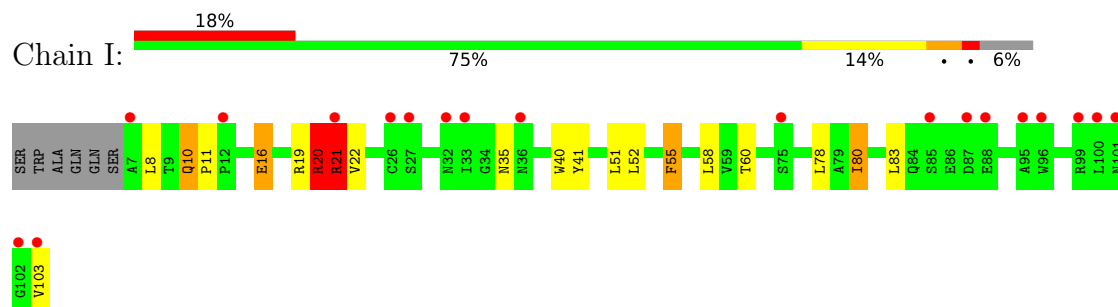
• Molecule 2: Immunoglobulin lambda variable 1-36



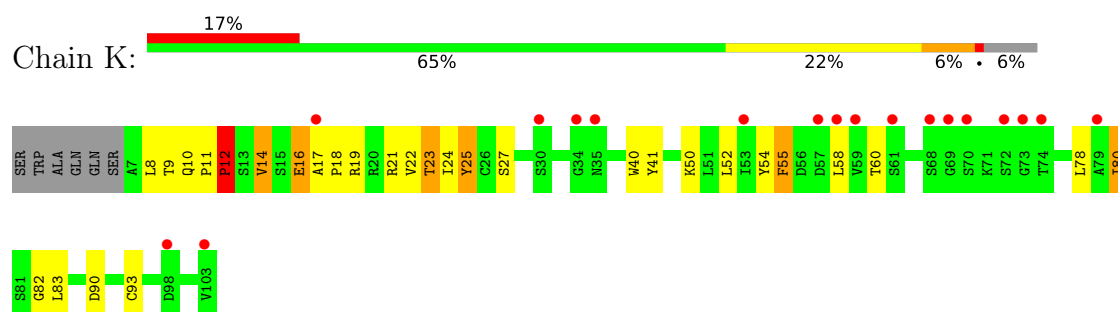
- Molecule 2: Immunoglobulin lambda variable 1-36



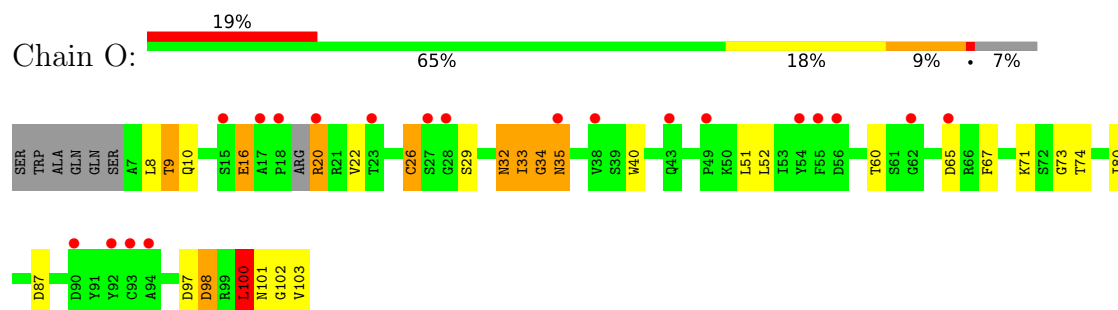
- Molecule 2: Immunoglobulin lambda variable 1-36



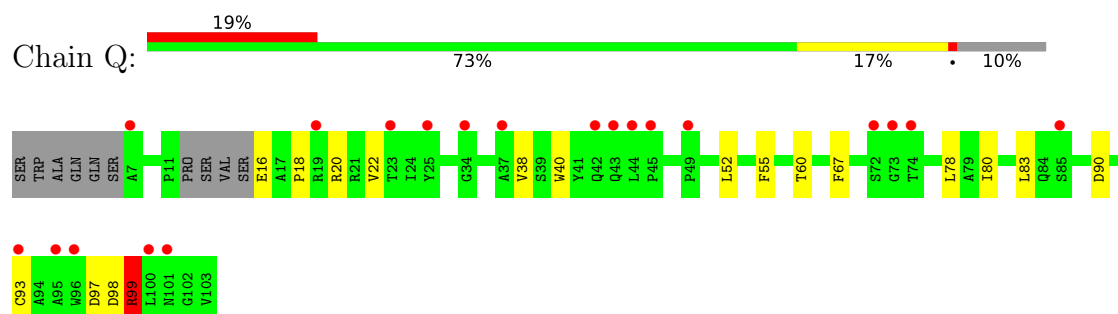
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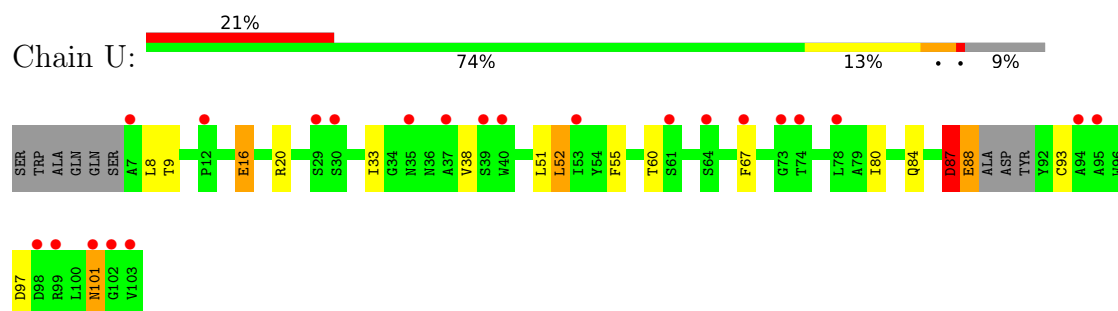
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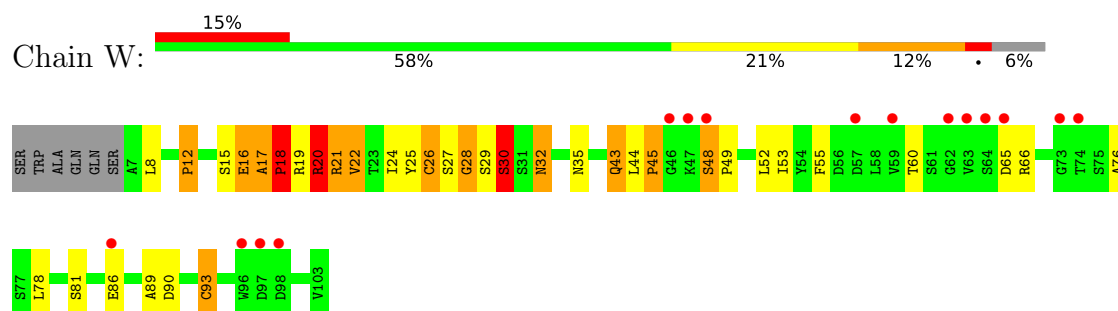
- Molecule 2: Immunoglobulin lambda variable 1-36



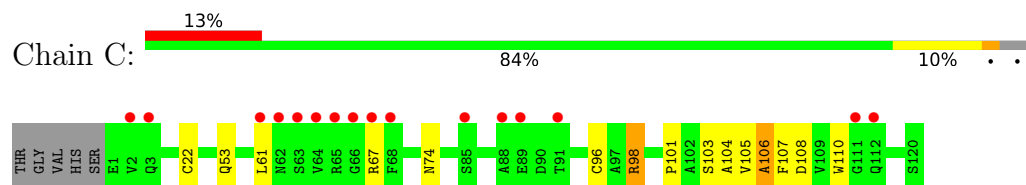
- Molecule 2: Immunoglobulin lambda variable 1-36



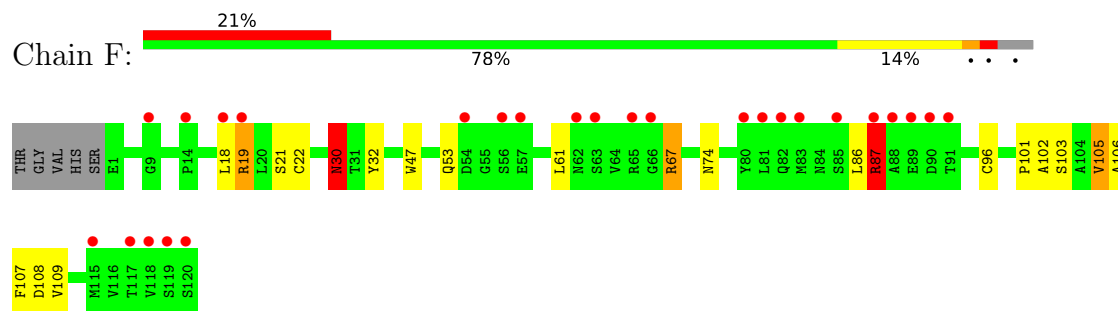
- Molecule 2: Immunoglobulin lambda variable 1-36



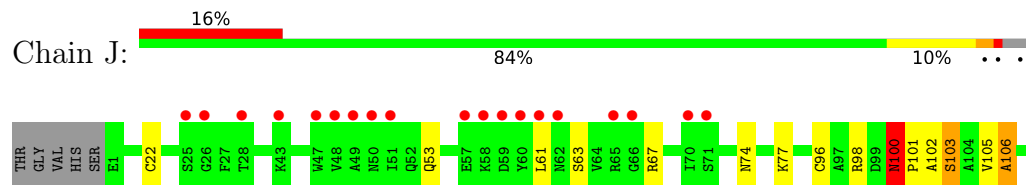
- Molecule 3: R5034HV



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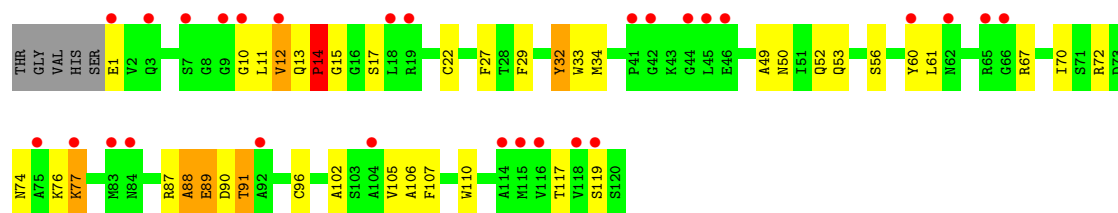


- Molecule 3: R5034HV

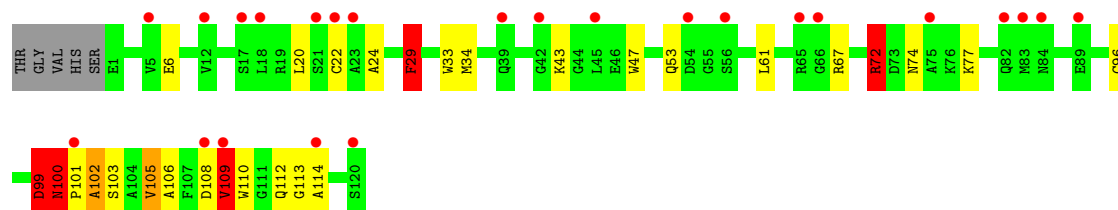


- Molecule 3: R5034HV

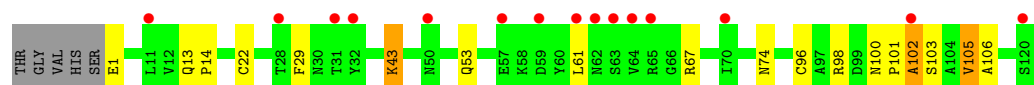
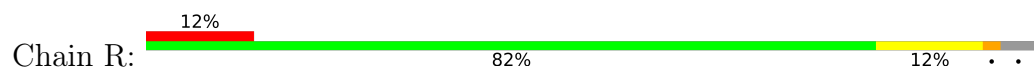




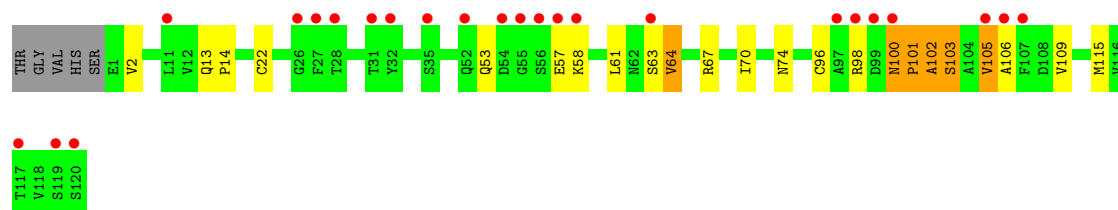
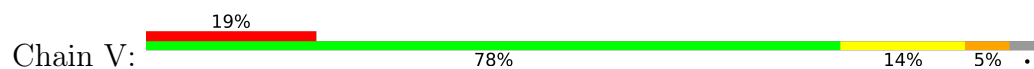
● Molecule 3: R5034HV



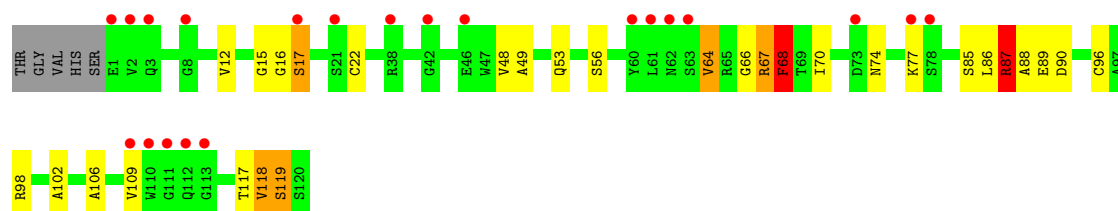
● Molecule 3: R5034HV



● Molecule 3: R5034HV



● Molecule 3: R5034HV



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	82.26Å 376.79Å 226.82Å 90.00° 90.06° 90.00°	Depositor
Resolution (Å)	65.60 – 3.99 65.60 – 3.99	Depositor EDS
% Data completeness (in resolution range)	98.9 (65.60-3.99) 98.9 (65.60-3.99)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.02 (at 4.01Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.441 , 0.458 0.442 , 0.459	Depositor DCC
R_{free} test set	1918 reflections (1.66%)	wwPDB-VP
Wilson B-factor (Å ²)	130.5	Xtriage
Anisotropy	0.442	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 337.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.22$, $\langle L^2 \rangle = 0.10$	Xtriage
Estimated twinning fraction	0.419 for h,-k,-l	Xtriage
F_o, F_c correlation	0.69	EDS
Total number of atoms	32284	wwPDB-VP
Average B, all atoms (Å ²)	166.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.53% 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	0.50	0/2556	1.37	17/3425 (0.5%)
1	D	0.49	0/2353	1.28	11/3149 (0.3%)
1	G	0.49	0/2675	1.33	11/3590 (0.3%)
1	H	0.52	0/2291	1.41	16/3067 (0.5%)
1	M	0.47	0/2502	1.28	8/3352 (0.2%)
1	N	0.51	0/2445	1.35	15/3276 (0.5%)
1	S	0.47	0/2492	1.28	11/3341 (0.3%)
1	T	0.51	0/2331	1.44	24/3121 (0.8%)
2	B	0.57	0/736	1.27	8/999 (0.8%)
2	E	0.55	0/752	1.12	3/1021 (0.3%)
2	I	0.55	0/743	1.15	5/1009 (0.5%)
2	K	0.65	0/743	1.32	6/1009 (0.6%)
2	O	0.56	0/727	1.19	4/987 (0.4%)
2	Q	0.53	0/715	1.12	4/968 (0.4%)
2	U	0.57	0/708	1.20	6/959 (0.6%)
2	W	0.78	0/740	1.66	22/1005 (2.2%)
3	C	0.48	0/929	0.97	0/1256
3	F	0.48	0/925	1.07	4/1250 (0.3%)
3	J	0.48	0/921	0.98	1/1245 (0.1%)
3	L	0.66	3/934 (0.3%)	1.41	15/1261 (1.2%)
3	P	0.54	0/933	1.28	9/1261 (0.7%)
3	R	0.50	0/933	1.06	2/1261 (0.2%)
3	V	0.49	0/926	1.04	1/1252 (0.1%)
3	X	0.56	0/922	1.25	8/1245 (0.6%)
All	All	0.52	3/32932 (0.0%)	1.29	211/44309 (0.5%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1
1	G	0	2
1	H	0	1
1	N	0	1
1	T	0	6
2	B	0	1
2	K	0	2
2	W	0	5
3	C	0	2
3	L	0	1
3	P	0	2
3	R	0	2
3	X	0	1
All	All	0	32

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	88	ALA	CA-C	6.05	1.60	1.52
3	L	14	PRO	C-N	5.09	1.41	1.33
3	L	14	PRO	CA-C	5.05	1.59	1.52

All (211) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	262	PHE	CA-CB-CG	15.95	129.75	113.80
3	L	14	PRO	N-CA-C	14.98	143.33	112.47
3	P	108	ASP	CB-CA-C	-14.23	91.01	112.07
1	H	262	PHE	N-CA-CB	13.72	133.67	110.49
3	X	87	ARG	CA-CB-CG	13.54	141.18	114.10
1	H	245	ASP	CB-CA-C	12.71	130.91	115.79
1	T	162	PHE	CB-CA-C	-12.10	87.45	111.17
1	M	10	PHE	CA-CB-CG	11.85	125.65	113.80
1	T	190	LYS	CB-CG-CD	11.08	136.79	111.30
3	P	29	PHE	CA-CB-CG	10.58	124.38	113.80
2	K	12	PRO	N-CA-CB	-10.58	92.14	103.25
3	P	109	VAL	N-CA-CB	10.07	127.84	111.23
1	H	99	LEU	N-CA-CB	9.40	126.49	110.50
2	B	20	ARG	CB-CG-CD	9.21	132.49	111.30
3	P	99	ASP	CA-CB-CG	8.78	121.38	112.60
2	B	18	PRO	N-CA-C	8.60	125.48	113.53
1	G	169	ARG	CA-CB-CG	8.46	131.01	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	T	257	ASN	CB-CA-C	8.43	127.19	110.42
2	W	21	ARG	CA-C-N	8.38	133.19	121.96
2	W	21	ARG	C-N-CA	8.38	133.19	121.96
2	W	21	ARG	CA-CB-CG	-8.34	97.42	114.10
1	T	255	LYS	CB-CG-CD	8.32	130.44	111.30
2	E	74	THR	OG1-CB-CG2	-8.27	92.76	109.30
3	P	100	ASN	CB-CA-C	8.25	126.42	110.17
1	N	155	LEU	N-CA-CB	8.21	124.36	110.49
1	G	5	PHE	CA-CB-CG	8.13	121.94	113.80
2	W	20	ARG	CA-CB-CG	8.11	130.31	114.10
2	O	32	ASN	CA-CB-CG	8.07	120.67	112.60
2	K	12	PRO	N-CA-C	7.92	128.78	112.47
2	E	55	PHE	CA-CB-CG	7.91	121.70	113.80
1	M	245	ASP	CA-CB-CG	7.89	120.49	112.60
1	T	161	ASN	CA-CB-CG	7.81	120.41	112.60
1	H	48	HIS	CB-CG-CD2	-7.75	121.12	131.20
1	A	244	ASN	CB-CA-C	-7.69	99.01	110.62
1	H	197	ASN	CA-CB-CG	7.68	120.28	112.60
2	K	23	THR	CA-CB-OG1	7.53	120.90	109.60
2	W	20	ARG	CB-CA-C	7.53	125.40	110.42
1	S	174	GLU	CB-CG-CD	7.50	125.34	112.60
1	D	174	GLU	CB-CG-CD	7.46	125.28	112.60
1	D	10	PHE	CA-CB-CG	7.44	121.24	113.80
1	G	174	GLU	CB-CG-CD	7.42	125.22	112.60
1	M	174	GLU	CB-CG-CD	7.39	125.17	112.60
2	B	20	ARG	CA-CB-CG	7.34	128.79	114.10
1	T	174	GLU	CB-CG-CD	7.34	125.08	112.60
3	F	30	ASN	CA-CB-CG	7.33	119.93	112.60
1	H	261	THR	OG1-CB-CG2	-7.28	94.74	109.30
2	W	12	PRO	N-CA-C	7.26	127.43	112.47
3	L	12	VAL	N-CA-CB	7.21	123.13	111.23
2	K	25	TYR	CA-CB-CG	7.20	126.85	113.90
1	S	101	HIS	CA-CB-CG	7.18	120.98	113.80
2	I	21	ARG	CB-CG-CD	7.17	127.79	111.30
1	N	86	ASN	CA-CB-CG	7.12	119.72	112.60
1	A	122	LYS	CB-CA-C	7.05	124.46	110.42
2	W	20	ARG	CB-CG-CD	7.04	127.49	111.30
1	T	304	ASN	CB-CA-C	6.99	124.09	110.67
3	L	14	PRO	CA-C-N	6.95	135.03	121.41
3	L	14	PRO	C-N-CA	6.95	135.03	121.41
2	W	12	PRO	N-CA-CB	-6.90	96.00	103.25
3	L	77	LYS	CB-CG-CD	6.89	127.16	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	104	ASP	CB-CA-C	6.89	122.34	111.39
3	P	72	ARG	NE-CZ-NH1	-6.87	114.63	121.50
3	X	12	VAL	CA-C-O	-6.87	113.45	120.25
1	M	269	LYS	CA-CB-CG	6.86	127.82	114.10
3	F	67	ARG	CA-CB-CG	6.86	127.81	114.10
1	T	160	ASN	CB-CA-C	6.79	121.63	110.90
3	L	89	GLU	CB-CG-CD	6.78	124.13	112.60
2	W	93	CYS	CA-CB-SG	-6.73	98.92	114.40
3	L	110	TRP	N-CA-C	6.73	121.88	112.93
2	B	20	ARG	CB-CA-C	6.71	123.76	110.42
1	G	101	HIS	CA-CB-CG	6.70	120.50	113.80
1	S	101	HIS	CB-CA-C	-6.70	98.49	109.27
1	D	301	HIS	CB-CG-CD2	6.66	139.86	131.20
1	S	112	PHE	CB-CA-C	6.66	121.19	111.73
1	T	190	LYS	CG-CD-CE	6.66	126.62	111.30
2	K	11	PRO	N-CA-C	6.62	118.78	110.70
1	A	230	LYS	CB-CG-CD	6.61	126.51	111.30
1	H	48	HIS	CB-CG-ND1	6.60	132.59	122.70
3	L	87	ARG	CA-C-N	6.60	134.14	121.54
3	L	87	ARG	C-N-CA	6.60	134.14	121.54
2	W	28	GLY	CA-C-N	6.58	134.11	121.54
2	W	28	GLY	C-N-CA	6.58	134.11	121.54
2	I	20	ARG	CA-CB-CG	6.56	127.21	114.10
1	N	11	LYS	CA-CB-CG	6.51	127.11	114.10
1	G	144	MET	CB-CG-SD	6.49	132.16	112.70
1	A	141	CYS	CA-C-O	-6.45	111.29	120.51
1	G	5	PHE	CB-CA-C	6.41	121.58	111.39
3	V	100	ASN	CA-CB-CG	6.41	119.00	112.60
2	U	87	ASP	CA-CB-CG	6.40	119.00	112.60
3	F	87	ARG	CB-CG-CD	6.38	125.97	111.30
3	F	87	ARG	CG-CD-NE	6.37	126.02	112.00
3	R	29	PHE	CA-CB-CG	6.36	120.16	113.80
2	U	87	ASP	N-CA-C	-6.34	98.85	108.67
2	U	20	ARG	CA-CB-CG	6.33	126.76	114.10
1	S	112	PHE	CA-CB-CG	6.31	120.11	113.80
1	A	244	ASN	N-CA-CB	6.25	120.35	110.84
1	T	203	GLU	N-CA-CB	6.22	121.28	111.20
1	G	248	LYS	CB-CG-CD	6.20	125.56	111.30
2	K	55	PHE	CA-CB-CG	6.17	119.97	113.80
3	L	91	THR	OG1-CB-CG2	-6.16	96.98	109.30
2	W	48	SER	CB-CA-C	6.16	122.30	110.17
1	G	117	ASP	CA-CB-CG	6.13	118.73	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	139	LYS	CA-CB-CG	6.11	126.33	114.10
1	H	139	LYS	CA-CB-CG	6.11	126.31	114.10
2	W	30	SER	N-CA-C	6.10	123.79	110.80
2	O	32	ASN	CB-CA-C	6.09	122.54	110.42
1	N	32	LEU	N-CA-CB	6.07	121.33	111.74
1	A	57	LYS	CB-CG-CD	6.05	125.21	111.30
2	W	15	SER	CA-C-O	-6.04	115.58	121.02
2	Q	55	PHE	CA-CB-CG	6.04	119.84	113.80
1	D	112	PHE	CA-CB-CG	6.04	119.84	113.80
2	B	16	GLU	CB-CG-CD	6.03	122.85	112.60
1	A	262	PHE	CA-CB-CG	6.01	119.81	113.80
3	X	90	ASP	CA-CB-CG	6.00	118.61	112.60
1	N	165	THR	N-CA-CB	-5.99	101.44	110.91
1	N	76	GLU	N-CA-CB	5.97	120.57	110.49
3	R	43	LYS	CG-CD-CE	5.96	125.00	111.30
2	U	88	GLU	N-CA-CB	5.95	120.61	110.50
1	G	10	PHE	CA-CB-CG	5.94	119.74	113.80
2	W	43	GLN	N-CA-CB	5.94	118.80	110.90
1	D	183	VAL	N-CA-CB	5.89	123.27	111.24
1	H	165	THR	N-CA-CB	5.89	119.16	110.49
1	M	230	LYS	CB-CG-CD	5.86	124.78	111.30
1	T	76	GLU	N-CA-CB	5.83	120.34	110.49
1	A	253	LYS	CA-CB-CG	5.82	125.75	114.10
1	G	190	LYS	CB-CG-CD	5.82	124.69	111.30
2	B	19	ARG	CB-CA-C	-5.81	98.85	110.42
1	N	98	LYS	CB-CG-CD	5.76	124.56	111.30
1	A	250	ILE	N-CA-CB	5.76	120.73	111.23
2	W	55	PHE	CA-CB-CG	5.76	119.56	113.80
1	M	122	LYS	CB-CG-CD	5.73	124.49	111.30
1	N	84	LYS	CA-CB-CG	5.71	125.52	114.10
3	P	67	ARG	CG-CD-NE	5.70	124.53	112.00
3	X	87	ARG	CB-CG-CD	5.68	124.37	111.30
1	T	229	MET	CB-CG-SD	5.67	129.72	112.70
3	X	87	ARG	CD-NE-CZ	5.63	132.29	124.40
3	L	87	ARG	O-C-N	5.61	130.77	122.97
1	A	247	THR	N-CA-CB	5.59	119.54	110.32
3	X	68	PHE	N-CA-CB	-5.58	101.06	110.49
1	D	301	HIS	CB-CG-ND1	-5.56	114.35	122.70
2	B	19	ARG	N-CA-CB	5.56	119.89	110.49
1	T	10	PHE	CA-CB-CG	5.56	119.36	113.80
1	T	235	ARG	NE-CZ-NH1	-5.55	115.94	121.50
3	L	88	ALA	O-C-N	-5.55	115.21	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	252	ASP	CA-CB-CG	5.53	118.13	112.60
1	N	108	LYS	CB-CA-C	5.53	121.42	110.42
1	S	117	ASP	CA-CB-CG	5.53	118.13	112.60
1	T	235	ARG	NE-CZ-NH2	5.53	124.18	119.20
2	U	16	GLU	CB-CG-CD	5.53	122.00	112.60
3	J	100	ASN	CA-CB-CG	5.53	118.13	112.60
3	X	12	VAL	N-CA-CB	-5.53	103.81	111.99
1	D	220	ASP	CA-CB-CG	5.47	118.07	112.60
1	A	250	ILE	N-CA-C	-5.46	97.98	109.34
1	T	255	LYS	CA-C-N	5.46	131.97	121.54
1	T	255	LYS	C-N-CA	5.46	131.97	121.54
2	W	22	VAL	CA-C-O	-5.46	116.38	120.96
1	H	165	THR	CA-CB-OG1	-5.45	101.43	109.60
3	P	108	ASP	CA-CB-CG	5.44	118.04	112.60
3	L	10	GLY	CA-C-N	5.43	131.53	122.73
3	L	10	GLY	C-N-CA	5.43	131.53	122.73
1	A	122	LYS	CA-CB-CG	5.43	124.96	114.10
1	A	253	LYS	CB-CA-C	-5.42	99.63	110.42
2	I	55	PHE	CA-CB-CG	5.42	119.22	113.80
2	I	16	GLU	CB-CG-CD	5.39	121.76	112.60
1	T	117	ASP	CA-CB-CG	5.37	117.97	112.60
1	N	131	LYS	CB-CG-CD	5.37	123.64	111.30
1	S	307	HIS	CA-CB-CG	5.37	119.17	113.80
1	N	103	TYR	CB-CA-C	5.36	121.09	110.42
2	W	32	ASN	CB-CA-C	5.36	121.09	110.42
2	W	25	TYR	N-CA-CB	5.36	118.10	110.44
1	S	100	GLU	N-CA-CB	5.35	118.23	110.26
2	O	16	GLU	CB-CG-CD	5.33	121.66	112.60
2	W	22	VAL	O-C-N	-5.33	118.33	122.97
2	B	55	PHE	CA-CB-CG	5.28	119.08	113.80
2	Q	16	GLU	CB-CG-CD	5.27	121.56	112.60
1	A	166	ASN	CB-CA-C	5.26	120.89	110.42
1	T	163	CYS	CB-CA-C	-5.26	99.94	110.42
2	E	16	GLU	CB-CG-CD	5.25	121.53	112.60
3	L	89	GLU	N-CA-CB	5.25	117.58	110.59
1	A	253	LYS	N-CA-CB	5.24	119.35	110.49
1	H	166	ASN	CB-CA-C	5.24	120.85	110.42
2	W	18	PRO	N-CA-C	5.24	119.54	111.57
1	G	160	ASN	CA-CB-CG	5.23	117.83	112.60
1	H	265	ASP	CA-CB-CG	5.22	117.82	112.60
1	T	122	LYS	CB-CG-CD	5.22	123.31	111.30
1	T	304	ASN	N-CA-CB	5.22	118.38	110.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	W	8	LEU	CA-C-O	-5.22	115.31	121.16
1	N	117	ASP	CA-CB-CG	5.21	117.81	112.60
1	D	117	ASP	CA-CB-CG	5.20	117.80	112.60
2	I	21	ARG	CA-CB-CG	5.20	124.49	114.10
1	D	246	LYS	CG-CD-CE	5.19	123.24	111.30
1	H	8	TYR	CB-CA-C	5.18	119.80	111.66
1	T	258	ILE	CB-CA-C	5.18	120.50	111.18
1	T	298	LYS	CA-CB-CG	5.17	124.44	114.10
3	X	117	THR	CA-CB-OG1	-5.16	101.87	109.60
1	S	116	MET	CB-CA-C	-5.15	100.18	110.42
1	M	166	ASN	CB-CA-C	5.12	120.61	110.42
1	N	190	LYS	CA-CB-CG	5.12	124.34	114.10
2	Q	99	ARG	CA-CB-CG	5.11	124.31	114.10
1	D	194	ASP	CA-CB-CG	5.10	117.70	112.60
1	S	166	ASN	CB-CA-C	5.10	120.57	110.42
3	P	100	ASN	CA-CB-CG	5.06	117.66	112.60
1	H	117	ASP	CA-CB-CG	5.05	117.65	112.60
2	U	55	PHE	CA-CB-CG	5.05	118.85	113.80
1	N	161	ASN	CA-CB-CG	5.05	117.65	112.60
1	H	220	ASP	CA-CB-CG	5.04	117.64	112.60
1	T	166	ASN	CB-CA-C	5.04	120.45	110.42
1	S	260	ARG	CA-CB-CG	5.03	124.17	114.10
2	O	98	ASP	CA-CB-CG	5.03	117.63	112.60
1	D	166	ASN	CB-CA-C	5.03	120.42	110.42
2	Q	18	PRO	N-CA-C	5.02	120.07	111.68
1	A	262	PHE	N-CA-CB	5.01	119.73	111.62

There are no chirality outliers.

All (32) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	117	ASP	Peptide
1	A	122	LYS	Peptide
1	A	216	TYR	Peptide
1	A	246	LYS	Peptide
1	A	249	ILE	Peptide
2	B	20	ARG	Sidechain
3	C	67	ARG	Sidechain
3	C	98	ARG	Sidechain
1	D	183	VAL	Peptide
1	G	158	TYR	Peptide
1	G	260	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	H	257	ASN	Peptide
2	K	14	VAL	Peptide
2	K	8	LEU	Peptide
3	L	67	ARG	Sidechain
1	N	163	CYS	Peptide
3	P	72	ARG	Sidechain
3	P	99	ASP	Peptide
3	R	1	GLU	Peptide
3	R	67	ARG	Sidechain
1	T	155	LEU	Peptide
1	T	160	ASN	Peptide
1	T	162	PHE	Peptide
1	T	235	ARG	Sidechain
1	T	257	ASN	Peptide
1	T	259	TRP	Peptide
2	W	16	GLU	Peptide
2	W	18	PRO	Peptide
2	W	28	GLY	Peptide
2	W	30	SER	Peptide
2	W	66	ARG	Sidechain
3	X	15	GLY	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	2503	0	2518	47	0
1	D	2309	0	2331	32	0
1	G	2618	0	2629	35	0
1	H	2251	0	2271	43	5
1	M	2450	0	2469	30	0
1	N	2397	0	2405	44	0
1	S	2442	0	2457	39	0
1	T	2288	0	2312	64	1
2	B	721	0	679	15	0
2	E	737	0	693	12	0
2	I	728	0	688	10	0
2	K	728	0	688	24	5

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	O	713	0	668	29	0
2	Q	702	0	661	6	0
2	U	696	0	662	8	0
2	W	725	0	686	31	4
3	C	910	0	864	8	0
3	F	907	0	863	16	0
3	J	903	0	857	8	0
3	L	915	0	870	21	12
3	P	914	0	870	26	0
3	R	914	0	870	6	0
3	V	908	0	863	15	0
3	X	905	0	862	14	2
All	All	32284	0	31736	517	23

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 (517) 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)
2:E:86[B]:GLU:OE2	2:E:86[B]:GLU:O	1.70	1.09
2:W:17:ALA:HB1	2:W:18:PRO:HD3	1.35	1.05
1:N:143:ASP:HB3	3:P:102:ALA:HB1	1.39	1.00
1:T:258:ILE:HG23	1:T:260:ARG:CG	1.94	0.98
3:F:19:ARG:NH2	3:F:21:SER:HB2	1.83	0.94
2:O:33:ILE:HD13	2:O:74:THR:HA	1.48	0.92
1:A:65:ILE:HD13	1:D:61:TYR:HB3	1.51	0.92
2:W:17:ALA:CB	2:W:18:PRO:HD3	1.99	0.92
1:H:160:ASN:OD1	1:H:161:ASN:OD1	1.89	0.91
1:A:122:LYS:HB2	1:A:125:LYS:HB2	1.54	0.89
1:N:221:THR:O	1:N:225:ILE:HD13	1.71	0.89
2:O:8:LEU:O	2:O:10:GLN:N	2.07	0.88
1:S:61:TYR:HB3	1:T:65:ILE:HD13	1.56	0.88
3:J:100:ASN:HB3	3:J:101:PRO:HD2	1.54	0.87
2:E:86[B]:GLU:OE2	2:E:86[B]:GLU:C	2.17	0.86
1:S:108:LYS:HA	1:S:111:ALA:HB2	1.54	0.86
3:F:19:ARG:HH22	3:F:21:SER:HB2	1.42	0.84
1:T:258:ILE:HG23	1:T:260:ARG:HG2	1.60	0.83
1:A:141:CYS:O	1:A:143:ASP:N	2.11	0.83
1:D:25:LEU:O	1:D:31:HIS:HA	1.79	0.81
3:J:100:ASN:HB3	3:J:101:PRO:CD	2.10	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:ILE:O	1:A:250:ILE:HG12	1.80	0.81
1:H:165:THR:OG1	1:H:260:ARG:N	2.14	0.80
1:S:160:ASN:O	1:S:263:GLN:HB2	1.82	0.80
1:N:70:PHE:CZ	3:P:102:ALA:HB2	2.17	0.79
1:T:161:ASN:ND2	1:T:162:PHE:CE2	2.51	0.78
2:K:54:TYR:HB2	3:L:105:VAL:HG23	1.65	0.78
1:G:215:SER:O	1:G:219:ILE:HD11	1.84	0.78
1:N:165:THR:HB	1:N:260:ARG:O	1.84	0.78
3:V:64:VAL:HG23	3:V:67:ARG:HD3	1.65	0.77
2:O:32:ASN:HD22	2:O:97:ASP:HB2	1.47	0.76
1:A:118:GLU:HB3	1:A:120:ASN:HD22	1.51	0.76
1:T:250:ILE:O	1:T:254:ILE:HD12	1.86	0.74
2:K:17:ALA:HB1	2:K:18:PRO:CD	2.17	0.74
1:H:165:THR:OG1	1:H:259:TRP:HA	1.88	0.74
2:E:41:TYR:OH	3:F:107:PHE:N	2.21	0.74
1:A:118:GLU:HB3	1:A:120:ASN:ND2	2.03	0.73
2:O:34:GLY:O	2:O:35:ASN:HB2	1.88	0.73
1:H:250:ILE:O	1:H:252:ASP:N	2.22	0.72
3:P:6:GLU:CD	3:P:114:ALA:HB2	2.14	0.72
1:D:114:LYS:O	1:D:115:MET:HB2	1.90	0.72
1:T:42:PHE:CE1	1:T:141:CYS:HA	2.25	0.71
1:T:162:PHE:CE2	2:W:20:ARG:HG2	2.25	0.71
3:P:100:ASN:HB2	3:P:103:SER:HA	1.70	0.71
1:D:242:ILE:HG22	1:D:246:LYS:HD2	1.73	0.71
1:S:85:CYS:SG	1:S:130:ILE:HD13	2.31	0.71
1:H:66:ALA:HA	2:I:58:LEU:HD11	1.72	0.71
2:B:67:PHE:HD1	2:B:80:ILE:HD12	1.56	0.70
2:W:20:ARG:HD2	2:W:21:ARG:O	1.92	0.70
1:D:25:LEU:HD21	1:D:291:LEU:HD23	1.72	0.70
2:K:41:TYR:OH	3:L:107:PHE:N	2.24	0.70
1:S:25:LEU:HD21	1:S:291:LEU:HD23	1.73	0.70
1:M:155:LEU:HD23	1:M:264:LYS:HE2	1.74	0.70
3:L:72:ARG:HD2	3:L:74:ASN:OD1	1.92	0.70
1:N:143:ASP:CB	3:P:102:ALA:HB1	2.21	0.69
2:Q:67:PHE:HD1	2:Q:80:ILE:HD12	1.56	0.69
3:X:64:VAL:HG11	3:X:68:PHE:CZ	2.27	0.69
1:S:115:MET:C	1:S:117:ASP:H	2.01	0.69
1:G:188:LEU:O	1:G:192:LEU:HD22	1.93	0.69
1:M:25:LEU:HD21	1:M:291:LEU:HD23	1.74	0.69
2:U:67:PHE:HD1	2:U:80:ILE:HD12	1.57	0.68
1:A:25:LEU:HD21	1:A:291:LEU:HD23	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:35:VAL:HG11	1:S:287:LEU:HD21	1.75	0.68
1:A:213:MET:SD	1:A:214:GLY:N	2.67	0.68
1:G:25:LEU:HD21	1:G:291:LEU:HD23	1.74	0.68
2:K:24:ILE:HD12	2:K:78:LEU:HD23	1.74	0.68
2:O:22:VAL:CG2	2:O:80:ILE:HG23	2.22	0.68
2:W:21:ARG:NH2	2:W:81:SER:HB2	2.08	0.68
1:S:162:PHE:HA	1:S:261:THR:OG1	1.94	0.68
1:H:160:ASN:CG	1:H:161:ASN:OD1	2.35	0.68
1:M:143:ASP:OD1	3:R:102:ALA:HB3	1.94	0.68
1:N:32:LEU:HB2	1:N:89:LYS:HD2	1.76	0.67
1:T:39:HIS:HA	1:T:42:PHE:HD2	1.59	0.67
1:H:43:LEU:HD22	1:H:74:ILE:CD1	2.25	0.67
2:K:17:ALA:HB1	2:K:18:PRO:HD2	1.77	0.67
3:X:67:ARG:HG3	3:X:68:PHE:CD1	2.30	0.67
1:M:157:CYS:HB2	1:M:264:LYS:HE3	1.77	0.66
2:K:19:ARG:HA	2:K:82:GLY:HA2	1.78	0.66
1:T:42:PHE:CZ	1:T:141:CYS:HA	2.31	0.66
2:B:41:TYR:OH	3:C:106:ALA:HA	1.96	0.66
1:S:85:CYS:SG	1:S:130:ILE:CD1	2.84	0.66
2:I:20:ARG:HD2	2:I:21:ARG:O	1.97	0.65
2:W:17:ALA:CB	2:W:18:PRO:CD	2.74	0.65
1:T:162:PHE:CG	2:W:21:ARG:HD2	2.32	0.64
1:D:181:LEU:HD23	1:D:184:LYS:HD2	1.78	0.64
2:O:34:GLY:O	2:O:35:ASN:CB	2.45	0.63
1:T:162:PHE:HE2	2:W:20:ARG:HG2	1.64	0.63
2:K:24:ILE:HD12	2:K:78:LEU:HB3	1.80	0.63
3:V:13:GLN:HG3	3:V:14:PRO:HD2	1.81	0.63
2:W:19:ARG:O	2:W:20:ARG:HB2	1.98	0.62
1:A:140:ILE:C	1:A:141:CYS:O	2.34	0.62
1:T:259:TRP:CE3	1:T:259:TRP:HA	2.34	0.62
1:D:263:GLN:O	1:D:267:LEU:HD12	1.99	0.62
1:M:62:GLY:HA2	1:N:62:GLY:HA2	1.82	0.62
1:N:101:HIS:N	1:N:102:PRO:HD3	2.13	0.62
1:H:165:THR:HG1	1:H:259:TRP:HA	1.64	0.62
1:N:143:ASP:HB3	3:P:102:ALA:CB	2.22	0.62
3:P:29:PHE:HD2	3:P:77:LYS:HB3	1.65	0.62
1:T:58:SER:OG	2:W:65:ASP:CG	2.43	0.62
2:W:24:ILE:HD12	2:W:78:LEU:HB3	1.82	0.62
1:H:165:THR:OG1	1:H:259:TRP:CA	2.48	0.61
3:X:16:GLY:O	3:X:17:SER:HB3	2.00	0.61
1:M:249:ILE:O	1:M:250:ILE:O	2.19	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:92:LEU:HD21	1:N:122:LYS:O	2.00	0.61
1:S:96:ILE:O	1:S:100:GLU:HG3	2.01	0.61
2:W:43:GLN:C	2:W:45:PRO:HD3	2.26	0.61
2:O:22:VAL:HG23	2:O:80:ILE:CG2	2.30	0.61
1:A:213:MET:SD	1:A:215:SER:N	2.71	0.61
1:S:35:VAL:CG1	1:S:287:LEU:HD21	2.30	0.60
1:T:254:ILE:O	1:T:259:TRP:CD2	2.55	0.60
1:D:246:LYS:HD3	1:D:281:PHE:HA	1.82	0.60
2:K:54:TYR:CB	3:L:105:VAL:HG23	2.32	0.60
1:M:113:LYS:HA	1:M:116:MET:HB3	1.83	0.60
2:Q:97:ASP:O	2:Q:99:ARG:N	2.31	0.60
1:T:58:SER:HG	2:W:65:ASP:CG	2.10	0.60
1:T:73:LYS:HA	1:T:76:GLU:HG2	1.83	0.60
1:T:162:PHE:HA	1:T:261:THR:OG1	2.01	0.60
1:H:143:ASP:OD2	3:J:103:SER:OG	2.14	0.59
3:F:18:LEU:HB2	3:F:86:LEU:HD11	1.82	0.59
1:A:213:MET:HE1	1:A:215:SER:O	2.01	0.59
1:S:143:ASP:CG	3:X:102:ALA:HA	2.27	0.59
1:T:258:ILE:HG23	1:T:260:ARG:HG3	1.82	0.59
1:A:213:MET:HB3	1:A:219:ILE:HD11	1.84	0.59
1:N:70:PHE:HZ	3:P:102:ALA:HB2	1.68	0.59
1:N:73:LYS:HA	1:N:76:GLU:HG2	1.84	0.59
2:I:10:GLN:NE2	2:I:11:PRO:O	2.36	0.59
2:K:22:VAL:HG23	2:K:80:ILE:HD13	1.83	0.59
1:S:35:VAL:HG11	1:S:287:LEU:CD2	2.33	0.58
3:P:20:LEU:HD12	3:P:20:LEU:N	2.18	0.58
1:H:262:PHE:HE1	1:H:266:GLU:HB3	1.68	0.58
1:N:105:ILE:HG23	1:N:110:ARG:HB3	1.86	0.58
1:G:46:TYR:HB2	1:G:144:MET:HG3	1.86	0.57
1:T:52:ASN:HD21	1:T:168:ILE:HG13	1.70	0.57
1:A:199:LEU:HD13	1:A:230:LYS:HE3	1.85	0.57
2:B:8:LEU:HD11	2:B:95:ALA:HB3	1.86	0.57
1:H:25:LEU:HD11	1:H:291:LEU:HD23	1.86	0.57
2:U:87:ASP:O	2:U:88:GLU:HG3	2.03	0.57
1:A:243:ILE:HD11	1:A:284:SER:HB2	1.86	0.57
1:G:268:LEU:HD23	1:G:269:LYS:N	2.19	0.57
1:H:250:ILE:O	1:H:253:LYS:N	2.33	0.57
1:M:159:ASN:OD1	2:O:20:ARG:HA	2.05	0.57
1:G:105:ILE:HG23	1:G:106:ASN:H	1.69	0.57
1:N:165:THR:CB	1:N:260:ARG:O	2.53	0.57
3:P:33:TRP:HB3	3:P:99:ASP:CG	2.28	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:52:ASN:HD21	1:T:168:ILE:CG1	2.18	0.57
1:G:219:ILE:HD12	1:G:219:ILE:H	1.70	0.56
1:A:249:ILE:O	1:A:250:ILE:CG1	2.53	0.56
2:E:86[B]:GLU:C	2:E:86[B]:GLU:CD	2.72	0.56
2:B:41:TYR:OH	3:C:107:PHE:N	2.39	0.56
1:T:13:LEU:HD21	1:T:138:ASN:HD22	1.70	0.56
1:G:165:THR:HG21	1:G:262:PHE:CD2	2.41	0.56
2:I:41:TYR:OH	3:J:106:ALA:HB3	2.05	0.56
1:T:143:ASP:OD1	3:V:102:ALA:N	2.39	0.56
1:S:166:ASN:O	1:S:168:ILE:N	2.39	0.56
1:T:13:LEU:HD12	1:T:142:MET:HG2	1.87	0.56
1:A:241:LYS:O	1:A:245:ASP:HA	2.06	0.56
2:K:80:ILE:H	2:K:80:ILE:HD12	1.70	0.56
2:O:26:CYS:HG	2:O:40:TRP:HH2	1.48	0.56
3:P:24:ALA:HB3	3:P:29:PHE:CD2	2.40	0.56
1:S:24:ILE:CG2	1:S:32:LEU:HD21	2.36	0.56
3:V:63:SER:O	3:V:64:VAL:C	2.49	0.56
3:L:50:ASN:O	3:L:70:ILE:CD1	2.53	0.56
2:K:18:PRO:HA	2:K:83:LEU:O	2.06	0.55
1:N:113:LYS:H	1:N:116:MET:HB3	1.70	0.55
1:T:13:LEU:HD21	1:T:138:ASN:ND2	2.21	0.55
1:H:70:PHE:O	1:H:74:ILE:HG23	2.06	0.55
2:K:24:ILE:CD1	2:K:78:LEU:HD23	2.36	0.55
2:O:26:CYS:SG	2:O:40:TRP:CH2	2.99	0.55
1:M:166:ASN:O	1:M:168:ILE:N	2.40	0.55
1:D:180:ILE:O	1:D:184:LYS:HB3	2.07	0.55
1:H:249:ILE:HG23	1:H:251:GLN:HB2	1.89	0.54
2:W:53:ILE:CD1	2:W:78:LEU:CD1	2.85	0.54
2:O:22:VAL:HG23	2:O:80:ILE:HG23	1.86	0.54
1:T:258:ILE:HG23	1:T:260:ARG:CD	2.36	0.54
2:O:22:VAL:HG22	2:O:80:ILE:HG23	1.87	0.54
1:A:166:ASN:O	1:A:168:ILE:N	2.40	0.54
3:P:72:ARG:HE	3:P:74:ASN:HD21	1.55	0.54
3:V:64:VAL:CG2	3:V:67:ARG:HD3	2.37	0.54
1:T:259:TRP:HA	1:T:259:TRP:HE3	1.70	0.54
2:K:16:GLU:HB3	2:K:83:LEU:CD1	2.38	0.54
2:O:20:ARG:HH12	2:O:22:VAL:HG12	1.73	0.54
1:H:74:ILE:HG13	1:H:75:ASN:N	2.23	0.54
1:A:95:THR:HG22	1:A:120:ASN:OD1	2.09	0.53
1:D:166:ASN:O	1:D:168:ILE:N	2.40	0.53
3:L:11:LEU:O	3:L:12:VAL:CG2	2.56	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:24:ILE:HG12	1:T:32:LEU:HD11	1.90	0.53
1:A:205:LEU:O	1:A:209:LEU:HG	2.07	0.53
1:M:139:LYS:HB3	3:R:103:SER:HB2	1.89	0.53
3:V:13:GLN:CG	3:V:14:PRO:HD2	2.38	0.53
1:N:166:ASN:O	1:N:168:ILE:N	2.38	0.53
1:A:158:TYR:O	1:A:159:ASN:ND2	2.37	0.53
1:T:259:TRP:O	1:T:260:ARG:HB2	2.09	0.53
2:B:67:PHE:CD1	2:B:80:ILE:HD12	2.43	0.53
1:G:14:SER:HA	1:G:22:ILE:HD11	1.90	0.53
3:F:30:ASN:HB3	3:F:74:ASN:HB3	1.91	0.53
1:H:166:ASN:O	1:H:168:ILE:N	2.41	0.52
3:P:100:ASN:ND2	3:P:102:ALA:O	2.42	0.52
1:N:56:HIS:CE1	1:N:164:ASN:HB2	2.44	0.52
1:G:104:ASP:O	1:G:107:ASN:N	2.37	0.52
1:T:39:HIS:HA	1:T:42:PHE:CD2	2.42	0.52
1:H:262:PHE:CE1	1:H:266:GLU:CB	2.93	0.52
1:H:250:ILE:C	1:H:252:ASP:H	2.18	0.52
2:U:67:PHE:CD1	2:U:80:ILE:HD12	2.44	0.52
1:T:13:LEU:CD1	1:T:142:MET:HG2	2.39	0.52
1:T:162:PHE:CZ	2:W:20:ARG:HG2	2.45	0.51
1:T:166:ASN:O	1:T:168:ILE:N	2.41	0.51
1:A:69:ALA:HB3	2:B:58:LEU:CD1	2.40	0.51
1:A:108:LYS:C	1:A:216:TYR:OH	2.53	0.51
1:G:66:ALA:HA	2:K:58:LEU:HD11	1.91	0.51
1:N:32:LEU:CD2	1:N:93:ILE:HD11	2.40	0.51
1:T:42:PHE:CG	1:T:43:LEU:N	2.77	0.51
1:T:163:CYS:SG	1:T:164:ASN:N	2.80	0.51
1:H:250:ILE:C	1:H:252:ASP:N	2.68	0.51
1:N:110:ARG:HA	1:N:114:LYS:HD2	1.91	0.51
3:L:29:PHE:CD1	3:L:34:MET:HE3	2.45	0.51
2:K:22:VAL:HG23	2:K:80:ILE:CD1	2.41	0.51
1:N:224:PHE:CD2	1:N:225:ILE:HD12	2.46	0.51
2:O:33:ILE:HD13	2:O:74:THR:CA	2.31	0.51
1:G:213:MET:O	1:G:213:MET:SD	2.69	0.51
2:K:9:THR:O	2:K:10:GLN:HG3	2.11	0.51
1:N:29:GLU:HG2	1:N:93:ILE:HD13	1.91	0.51
2:O:67:PHE:CE1	2:O:80:ILE:HD12	2.46	0.51
1:A:118:GLU:CB	1:A:120:ASN:HD22	2.22	0.51
1:D:158:TYR:O	1:D:159:ASN:C	2.54	0.51
1:A:96:ILE:HG23	1:A:100:GLU:CG	2.41	0.51
1:H:18:ILE:HG22	1:H:22:ILE:HD11	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:105:ILE:HG23	1:N:105:ILE:O	2.11	0.51
1:T:254:ILE:O	1:T:259:TRP:CE3	2.64	0.51
1:T:58:SER:OG	2:W:65:ASP:OD1	2.26	0.50
1:T:258:ILE:C	1:T:260:ARG:HG3	2.37	0.50
1:N:143:ASP:OD1	3:P:103:SER:OG	2.21	0.50
2:O:22:VAL:CG2	2:O:80:ILE:CG2	2.87	0.50
1:H:43:LEU:HD22	1:H:74:ILE:HD12	1.94	0.50
2:O:8:LEU:C	2:O:10:GLN:H	2.19	0.50
2:W:24:ILE:HD12	2:W:78:LEU:HD23	1.94	0.50
3:X:87:ARG:HG2	3:X:89:GLU:CD	2.36	0.50
2:W:20:ARG:HD2	2:W:21:ARG:H	1.75	0.50
2:W:21:ARG:HH21	2:W:81:SER:HB2	1.76	0.50
1:H:71:ILE:O	1:H:74:ILE:HG13	2.11	0.50
1:G:70:PHE:CZ	3:L:102:ALA:HB2	2.47	0.50
3:P:29:PHE:HD1	3:P:34:MET:HE3	1.76	0.50
1:A:69:ALA:HB3	2:B:58:LEU:HD13	1.94	0.50
1:M:249:ILE:C	1:M:250:ILE:O	2.55	0.50
1:G:168:ILE:O	1:G:170:TYR:N	2.45	0.49
3:R:22:CYS:HG	3:R:96:CYS:HG	1.57	0.49
1:S:110:ARG:O	1:S:113:LYS:HG3	2.13	0.49
2:W:43:GLN:HG3	2:W:90:ASP:HB2	1.93	0.49
2:W:44:LEU:H	2:W:89:ALA:HB1	1.76	0.49
1:A:252:ASP:OD1	1:A:252:ASP:C	2.55	0.49
1:T:162:PHE:CB	2:W:21:ARG:HD2	2.42	0.49
1:G:259:TRP:CZ3	1:G:260:ARG:NH2	2.81	0.49
3:P:110:TRP:O	3:P:112:GLN:OE1	2.31	0.49
2:W:26:CYS:SG	2:W:76:ALA:HB3	2.52	0.49
3:P:20:LEU:N	3:P:20:LEU:CD1	2.76	0.49
3:R:13:GLN:CG	3:R:14:PRO:HD2	2.43	0.49
3:C:22:CYS:SG	3:C:96:CYS:SG	3.10	0.49
3:X:16:GLY:O	3:X:17:SER:CB	2.60	0.49
1:T:245:ASP:O	1:T:249:ILE:HG12	2.13	0.49
1:T:260:ARG:HH11	1:T:262:PHE:HE2	1.60	0.49
2:E:54:TYR:CD2	3:F:105:VAL:CG1	2.96	0.49
1:G:66:ALA:CA	2:K:58:LEU:HD11	2.43	0.49
2:O:67:PHE:CD1	2:O:80:ILE:HD12	2.47	0.49
1:A:66:ALA:HA	2:B:58:LEU:HD11	1.94	0.48
1:G:155:LEU:HD23	1:G:264:LYS:HE3	1.95	0.48
1:S:96:ILE:HD13	1:S:96:ILE:N	2.28	0.48
1:D:146:ASN:HB3	3:F:32:TYR:HE1	1.78	0.48
1:M:155:LEU:HD23	1:M:264:LYS:CE	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:13:LEU:HD22	1:N:142:MET:SD	2.53	0.48
2:U:52:LEU:N	2:U:52:LEU:HD12	2.28	0.48
2:O:80:ILE:HD11	2:O:87:ASP:OD2	2.13	0.48
3:L:27:PHE:CD2	3:L:32:TYR:CZ	3.02	0.48
1:T:28:LYS:HD2	1:T:298:LYS:HZ1	1.78	0.48
2:W:18:PRO:HB2	2:W:19:ARG:HG3	1.95	0.48
1:A:263:GLN:CD	1:A:263:GLN:H	2.22	0.48
2:O:26:CYS:SG	2:O:40:TRP:CZ2	3.06	0.48
1:T:288:ARG:HH21	1:T:289:GLN:CD	2.22	0.48
2:O:71:LYS:NZ	2:O:73:GLY:O	2.47	0.48
1:S:62:GLY:HA2	1:T:61:TYR:C	2.38	0.48
1:S:115:MET:O	1:S:117:ASP:N	2.47	0.48
1:A:139:LYS:HG3	1:A:142:MET:HB2	1.96	0.48
1:G:245:ASP:O	1:G:249:ILE:HG12	2.14	0.48
3:P:6:GLU:OE1	3:P:114:ALA:HB2	2.13	0.48
3:C:98:ARG:NH1	3:C:108:ASP:OD2	2.47	0.47
1:T:258:ILE:HG23	1:T:260:ARG:HD2	1.96	0.47
1:H:219:ILE:H	1:H:219:ILE:HD12	1.80	0.47
1:N:165:THR:HG23	1:N:169:ARG:NH2	2.29	0.47
2:O:8:LEU:C	2:O:10:GLN:N	2.70	0.47
1:A:143:ASP:CG	3:C:103:SER:H	2.21	0.47
2:K:54:TYR:CD2	3:L:105:VAL:HG21	2.49	0.47
2:O:8:LEU:O	2:O:9:THR:C	2.56	0.47
1:S:54:ILE:HD13	1:S:67:VAL:HG21	1.96	0.47
1:S:65:ILE:HD12	1:S:66:ALA:N	2.29	0.47
3:X:64:VAL:HA	3:X:67:ARG:NH1	2.29	0.47
2:B:20:ARG:NH2	2:B:21:ARG:NH2	2.62	0.47
1:S:108:LYS:HD2	1:S:111:ALA:HB2	1.96	0.47
1:T:39:HIS:CA	1:T:42:PHE:HD2	2.25	0.47
1:T:143:ASP:HA	3:V:101:PRO:CB	2.45	0.47
2:W:21:ARG:CZ	2:W:81:SER:HB2	2.44	0.47
2:I:21:ARG:HD3	2:I:80:ILE:O	2.15	0.47
1:G:54:ILE:HD13	1:G:67:VAL:HG21	1.97	0.47
2:K:22:VAL:HG11	2:K:83:LEU:HD11	1.96	0.47
1:N:245:ASP:O	1:N:249:ILE:HG12	2.14	0.47
1:A:213:MET:CE	1:A:215:SER:O	2.62	0.47
1:D:22:ILE:CD1	1:D:36:ILE:HG23	2.45	0.47
1:D:54:ILE:HD13	1:D:67:VAL:HG21	1.96	0.47
1:G:102:PRO:O	1:G:104:ASP:N	2.48	0.47
1:T:43:LEU:C	1:T:43:LEU:HD12	2.40	0.47
1:T:262:PHE:HB2	1:T:266:GLU:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:U:38:VAL:HG13	2:U:93:CYS:SG	2.55	0.47
3:L:53:GLN:O	3:L:74:ASN:ND2	2.48	0.47
1:N:32:LEU:HD23	1:N:89:LYS:HE3	1.97	0.47
2:O:97:ASP:CG	2:O:102:GLY:HA2	2.40	0.47
1:T:203:GLU:HB3	1:T:204:LEU:HD12	1.97	0.47
2:U:84:GLN:O	2:U:87:ASP:O	2.32	0.47
1:H:146:ASN:ND2	3:J:101:PRO:O	2.48	0.47
1:M:159:ASN:HB3	1:M:162:PHE:O	2.15	0.47
1:N:54:ILE:HD13	1:N:67:VAL:HG21	1.96	0.47
1:A:54:ILE:HD13	1:A:67:VAL:HG21	1.96	0.46
1:H:54:ILE:HD13	1:H:67:VAL:HG21	1.96	0.46
2:I:8:LEU:HD11	2:I:103:VAL:HG12	1.97	0.46
2:B:19:ARG:O	2:B:20:ARG:CB	2.62	0.46
1:M:156:SER:O	1:M:157:CYS:C	2.58	0.46
2:O:26:CYS:SG	2:O:40:TRP:HH2	2.35	0.46
1:T:54:ILE:HD13	1:T:67:VAL:HG21	1.96	0.46
1:A:96:ILE:HG23	1:A:100:GLU:CD	2.40	0.46
1:H:25:LEU:CD1	1:H:291:LEU:HD23	2.45	0.46
1:H:249:ILE:CG2	1:H:251:GLN:HB2	2.46	0.46
1:N:127:ILE:HD13	1:N:127:ILE:HA	1.88	0.46
2:W:43:GLN:N	2:W:90:ASP:O	2.48	0.46
3:P:24:ALA:HB3	3:P:29:PHE:CE2	2.50	0.46
1:G:110:ARG:HB2	1:G:114:LYS:HB2	1.98	0.46
1:M:139:LYS:HB2	1:M:140:ILE:HD13	1.97	0.46
2:B:20:ARG:NE	2:B:21:ARG:O	2.49	0.46
1:S:110:ARG:HB3	1:S:114:LYS:NZ	2.31	0.46
1:S:245:ASP:O	1:S:249:ILE:HG13	2.16	0.46
1:A:147:TYR:CE2	1:A:151:LEU:HD11	2.51	0.46
2:E:86[A]:GLU:CD	2:E:86[A]:GLU:N	2.74	0.46
1:N:21:SER:HB3	1:N:37:ILE:HD12	1.98	0.46
3:R:13:GLN:HG2	3:R:14:PRO:HD2	1.97	0.46
2:W:24:ILE:CD1	2:W:78:LEU:HD23	2.46	0.46
1:D:26:GLN:NE2	1:D:294:THR:OG1	2.50	0.45
1:G:140:ILE:CD1	1:G:140:ILE:N	2.79	0.45
1:M:62:GLY:CA	1:N:62:GLY:HA2	2.46	0.45
1:S:115:MET:C	1:S:117:ASP:N	2.67	0.45
1:D:245:ASP:O	1:D:249:ILE:HG13	2.16	0.45
2:E:8:LEU:HD11	2:E:95:ALA:HB3	1.98	0.45
1:M:54:ILE:HD13	1:M:67:VAL:HG21	1.96	0.45
2:Q:38:VAL:HG13	2:Q:93:CYS:SG	2.57	0.45
1:N:121:THR:OG1	1:N:122:LYS:NZ	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:18:ILE:O	1:D:18:ILE:HG13	2.16	0.45
1:H:74:ILE:HG13	1:H:75:ASN:H	1.82	0.45
3:L:60:TYR:CE1	3:L:70:ILE:HG12	2.51	0.45
1:M:250:ILE:C	1:M:252:ASP:H	2.24	0.45
2:Q:67:PHE:CD1	2:Q:80:ILE:HD12	2.43	0.45
1:N:123:LYS:HD3	1:N:124:LYS:HD2	1.98	0.45
1:T:24:ILE:HD11	1:T:126:LEU:HD23	1.97	0.45
1:H:73:LYS:HG2	2:I:55:PHE:HB3	1.99	0.45
1:A:24:ILE:HG13	1:A:32:LEU:HD21	1.99	0.45
1:A:139:LYS:O	1:A:141:CYS:O	2.35	0.45
1:G:288:ARG:HH21	1:G:289:GLN:CD	2.24	0.45
1:G:296:TYR:O	1:G:300:LYS:HG2	2.16	0.45
1:M:170:TYR:HE2	1:N:65:ILE:HG23	1.82	0.45
1:T:143:ASP:HA	3:V:101:PRO:HB3	1.99	0.45
1:N:99:LEU:HD21	1:N:224:PHE:HE2	1.82	0.45
1:M:140:ILE:CD1	1:M:140:ILE:N	2.80	0.44
3:P:53:GLN:O	3:P:74:ASN:ND2	2.50	0.44
1:T:254:ILE:HD12	1:T:254:ILE:H	1.81	0.44
3:F:87:ARG:HH11	3:F:87:ARG:HG2	1.83	0.44
1:H:74:ILE:CD1	1:H:144:MET:SD	3.06	0.44
1:H:262:PHE:CE1	1:H:266:GLU:HB3	2.49	0.44
1:M:155:LEU:CD2	1:M:264:LYS:HE2	2.47	0.44
1:M:192:LEU:HA	1:M:195:MET:HE3	1.97	0.44
1:N:100:GLU:C	1:N:102:PRO:HD3	2.42	0.44
1:S:108:LYS:HA	1:S:108:LYS:HD2	1.77	0.44
3:X:53:GLN:O	3:X:74:ASN:ND2	2.51	0.44
1:S:110:ARG:HB3	1:S:114:LYS:HZ1	1.82	0.44
1:D:146:ASN:HB3	3:F:32:TYR:CE1	2.53	0.44
2:E:55:PHE:HE1	3:F:103:SER:HB2	1.83	0.44
3:J:53:GLN:O	3:J:74:ASN:ND2	2.50	0.44
3:V:53:GLN:O	3:V:74:ASN:ND2	2.51	0.44
1:D:7:GLN:HG2	1:D:8:TYR:H	1.82	0.44
1:D:57:LYS:HE3	1:D:60:THR:CG2	2.47	0.44
1:D:185:SER:C	1:D:187:ASN:H	2.25	0.44
1:H:66:ALA:CA	2:I:58:LEU:HD11	2.45	0.44
3:J:22:CYS:HB2	3:J:96:CYS:SG	2.58	0.44
3:X:48:VAL:HG13	3:X:68:PHE:CZ	2.53	0.44
1:D:134:GLU:O	1:D:138:ASN:ND2	2.48	0.44
2:K:55:PHE:CZ	3:L:102:ALA:HB1	2.52	0.44
2:O:29:SER:O	2:O:33:ILE:HD12	2.17	0.44
1:S:24:ILE:HG23	1:S:32:LEU:HD21	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:22:CYS:CB	3:X:96:CYS:HG	2.30	0.44
1:H:26:GLN:HA	1:H:32:LEU:HA	2.00	0.44
1:H:74:ILE:HD13	1:H:144:MET:SD	2.57	0.44
1:S:159:ASN:ND2	1:S:162:PHE:O	2.51	0.44
2:U:33:ILE:HD12	2:U:97:ASP:OD1	2.18	0.44
2:W:43:GLN:OE1	2:W:49:PRO:HA	2.18	0.44
1:A:188:LEU:HD22	1:A:288:ARG:CZ	2.48	0.44
1:N:56:HIS:CE1	1:N:166:ASN:OD1	2.71	0.44
3:P:22:CYS:CB	3:P:96:CYS:HG	2.31	0.44
3:R:53:GLN:O	3:R:74:ASN:ND2	2.51	0.44
1:D:156:SER:O	1:D:157:CYS:C	2.61	0.43
1:N:110:ARG:HG2	1:N:114:LYS:HD2	2.01	0.43
3:V:103:SER:HB2	3:V:105:VAL:HG13	1.99	0.43
1:A:250:ILE:C	1:A:252:ASP:H	2.25	0.43
1:A:121:THR:O	1:A:123:LYS:N	2.49	0.43
1:D:188:LEU:HD22	1:D:288:ARG:CZ	2.48	0.43
1:G:139:LYS:HD3	3:L:33:TRP:CZ2	2.53	0.43
3:P:112:GLN:HG2	3:P:113:GLY:N	2.33	0.43
2:B:49:PRO:HG2	3:C:110:TRP:CD2	2.53	0.43
1:H:163:CYS:SG	1:H:164:ASN:N	2.89	0.43
3:L:22:CYS:CB	3:L:96:CYS:HG	2.30	0.43
1:T:24:ILE:HD11	1:T:126:LEU:CD2	2.49	0.43
1:A:135:ASN:HD22	1:A:139:LYS:HE2	1.84	0.43
1:G:164:ASN:OD1	1:G:165:THR:N	2.51	0.43
3:V:58:LYS:HD2	3:V:70:ILE:HG23	1.99	0.43
1:A:138:ASN:O	1:A:139:LYS:HE3	2.19	0.43
3:C:22:CYS:CB	3:C:96:CYS:HG	2.31	0.43
3:F:53:GLN:O	3:F:74:ASN:ND2	2.52	0.43
1:G:166:ASN:O	1:G:168:ILE:N	2.51	0.43
2:K:10:GLN:OE1	2:K:93:CYS:SG	2.73	0.43
1:N:219:ILE:HD12	1:N:219:ILE:N	2.34	0.43
1:S:102:PRO:HG3	1:S:305:ILE:CD1	2.48	0.43
3:C:53:GLN:O	3:C:74:ASN:ND2	2.51	0.43
2:W:19:ARG:O	2:W:20:ARG:CB	2.66	0.43
3:X:49:ALA:HB3	3:X:70:ILE:HG21	1.99	0.43
1:D:186:LYS:C	1:D:188:LEU:N	2.76	0.43
2:E:41:TYR:HE1	3:F:107:PHE:O	2.01	0.43
1:G:140:ILE:N	1:G:140:ILE:HD13	2.34	0.43
1:H:219:ILE:HD12	1:H:219:ILE:N	2.33	0.43
3:L:49:ALA:HB3	3:L:70:ILE:HG21	2.01	0.43
1:A:119:TYR:HB2	1:A:122:LYS:HE3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:7:GLN:HE22	1:M:265:ASP:HB3	1.83	0.43
3:P:100:ASN:HA	3:P:103:SER:HA	2.00	0.43
1:A:7:GLN:HG2	1:A:8:TYR:N	2.34	0.42
1:D:159:ASN:O	1:D:161:ASN:N	2.51	0.42
1:H:256:LEU:O	1:H:260:ARG:NH1	2.52	0.42
1:M:58:SER:HB2	2:O:65:ASP:CG	2.44	0.42
1:M:62:GLY:HA2	1:N:62:GLY:CA	2.48	0.42
1:N:56:HIS:HE1	1:N:164:ASN:HB2	1.83	0.42
1:S:105:ILE:HD12	1:S:110:ARG:HH12	1.84	0.42
3:V:22:CYS:HB2	3:V:96:CYS:SG	2.58	0.42
3:L:53:GLN:HA	3:L:72:ARG:NH2	2.33	0.42
1:G:165:THR:HG21	1:G:262:PHE:CE2	2.54	0.42
1:S:85:CYS:SG	1:S:130:ILE:HD11	2.57	0.42
1:T:135:ASN:ND2	3:V:57:GLU:OE2	2.51	0.42
1:T:159:ASN:HB2	1:T:264:LYS:HB2	2.02	0.42
1:T:198:ILE:HD11	1:T:295:PHE:HE1	1.84	0.42
2:B:21:ARG:HB2	2:B:81:SER:HA	2.01	0.42
3:F:22:CYS:CB	3:F:96:CYS:HG	2.32	0.42
2:U:87:ASP:O	2:U:88:GLU:CB	2.67	0.42
1:H:261:THR:HG21	2:K:21:ARG:CD	2.50	0.42
1:N:81:VAL:HG11	1:N:137:PHE:CZ	2.54	0.42
1:S:116:MET:SD	1:S:116:MET:C	3.02	0.42
2:W:44:LEU:N	2:W:89:ALA:HB1	2.34	0.42
1:G:24:ILE:HG21	1:G:32:LEU:HD21	2.01	0.42
1:G:43:LEU:HD23	1:G:75:ASN:OD1	2.20	0.42
1:N:153:GLU:OE1	1:N:153:GLU:HA	2.20	0.42
3:X:64:VAL:HG12	3:X:67:ARG:HD2	2.00	0.42
1:A:105:ILE:HG22	1:A:105:ILE:O	2.19	0.42
1:A:138:ASN:O	1:A:139:LYS:HB2	2.20	0.42
1:D:7:GLN:HG2	1:D:8:TYR:N	2.35	0.42
1:G:102:PRO:O	1:G:103:TYR:C	2.62	0.42
1:D:288:ARG:HG3	1:D:289:GLN:N	2.35	0.42
2:O:20:ARG:HH12	2:O:22:VAL:CG1	2.33	0.42
1:T:39:HIS:O	1:T:42:PHE:CD2	2.73	0.42
1:M:118:GLU:OE1	1:M:118:GLU:N	2.53	0.42
3:X:87:ARG:HG3	3:X:89:GLU:OE1	2.19	0.42
2:E:103:VAL:HG21	3:F:47:TRP:HB3	2.02	0.41
1:M:26:GLN:HE21	1:M:96:ILE:HD13	1.85	0.41
1:M:260:ARG:HD2	1:M:262:PHE:CZ	2.55	0.41
1:T:42:PHE:CD1	1:T:42:PHE:C	2.97	0.41
1:A:199:LEU:HD13	1:A:230:LYS:CE	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:20:ASN:O	1:H:20:ASN:CG	2.62	0.41
3:L:52:GLN:C	3:L:72:ARG:HH21	2.28	0.41
1:S:62:GLY:N	1:T:62:GLY:HA2	2.34	0.41
1:T:39:HIS:O	1:T:42:PHE:CE2	2.74	0.41
2:B:20:ARG:HB2	1:D:162:PHE:CE2	2.54	0.41
1:D:47:LYS:HG3	1:D:48:HIS:HD2	1.84	0.41
1:D:56:HIS:HE1	1:D:164:ASN:HB2	1.85	0.41
1:G:94:ALA:O	1:G:98:LYS:HD3	2.20	0.41
1:N:110:ARG:HA	1:N:114:LYS:CD	2.50	0.41
1:S:97:LYS:HA	1:S:101:HIS:CE1	2.55	0.41
1:T:40:TYR:CE1	1:T:283:THR:HA	2.55	0.41
2:B:19:ARG:O	2:B:20:ARG:HB3	2.19	0.41
1:S:113:LYS:HD2	1:S:113:LYS:O	2.19	0.41
1:D:263:GLN:HE21	1:D:265:ASP:HB2	1.86	0.41
1:H:88:ILE:HD11	1:H:126:LEU:HA	2.02	0.41
2:O:100:LEU:HG	3:P:47:TRP:CZ3	2.56	0.41
2:I:22:VAL:HG11	2:I:83:LEU:HD11	2.02	0.41
3:V:100:ASN:HB2	3:V:105:VAL:CB	2.51	0.41
2:I:40:TRP:CD2	2:I:78:LEU:HB2	2.56	0.41
1:M:219:ILE:HG22	1:M:219:ILE:O	2.20	0.41
2:E:51:LEU:HD23	3:F:108:ASP:O	2.21	0.41
2:K:54:TYR:CD2	3:L:105:VAL:CG2	3.04	0.41
1:M:112:PHE:C	1:M:114:LYS:H	2.29	0.41
1:S:96:ILE:N	1:S:96:ILE:CD1	2.84	0.41
2:W:53:ILE:CD1	2:W:78:LEU:HD13	2.51	0.41
1:A:88:ILE:HD11	1:A:126:LEU:HA	2.02	0.41
1:H:32:LEU:HD22	1:H:89:LYS:HE2	2.03	0.41
3:J:63:SER:O	3:J:67:ARG:NH2	2.54	0.41
3:P:29:PHE:CD2	3:P:77:LYS:C	2.99	0.41
1:S:56:HIS:HE1	1:S:164:ASN:HB2	1.86	0.41
3:V:101:PRO:O	3:V:102:ALA:HB2	2.20	0.41
3:X:49:ALA:CB	3:X:70:ILE:HG21	2.50	0.41
3:L:50:ASN:O	3:L:70:ILE:HD11	2.21	0.41
1:T:201:GLN:C	1:T:203:GLU:H	2.29	0.41
1:T:46:TYR:HB2	1:T:144:MET:HG3	2.03	0.40
3:L:11:LEU:O	3:L:12:VAL:HG22	2.20	0.40
3:P:100:ASN:CB	3:P:103:SER:HA	2.45	0.40
2:K:40:TRP:CD2	2:K:78:LEU:HB2	2.57	0.40
1:S:102:PRO:O	1:S:103:TYR:C	2.64	0.40
2:E:54:TYR:HD2	3:F:105:VAL:CG1	2.33	0.40
1:G:18:ILE:HG22	1:G:18:ILE:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:22:VAL:HG11	2:Q:83:LEU:HD11	2.03	0.40
2:Q:40:TRP:CD2	2:Q:78:LEU:HB2	2.57	0.40
1:G:159:ASN:HA	1:G:264:LYS:HB2	2.02	0.40
1:H:16:TYR:OH	1:H:20:ASN:OD1	2.37	0.40

All (23) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:15:GLY:N	3:L:88:ALA:CA[2_455]	1.26	0.94
3:L:15:GLY:N	3:L:88:ALA:C[2_455]	1.30	0.90
1:H:161:ASN:ND2	2:K:14:VAL:CG2[2_555]	1.35	0.85
1:H:161:ASN:ND2	2:K:14:VAL:CB[2_555]	1.54	0.66
3:L:14:PRO:C	3:L:88:ALA:C[2_455]	1.56	0.64
2:W:22:VAL:O	2:W:22:VAL:O[2_655]	1.56	0.64
3:L:14:PRO:C	3:L:89:GLU:N[2_455]	1.57	0.63
3:L:15:GLY:N	3:L:88:ALA:N[2_455]	1.59	0.61
3:L:14:PRO:C	3:L:88:ALA:CA[2_455]	1.66	0.54
1:H:160:ASN:O	2:K:90:ASP:OD1[2_555]	1.74	0.46
3:L:14:PRO:O	3:L:89:GLU:N[2_455]	1.74	0.46
3:X:85:SER:O	3:X:87:ARG:NE[2_755]	1.78	0.42
3:L:15:GLY:N	3:L:89:GLU:N[2_455]	1.85	0.35
3:L:14:PRO:CA	3:L:88:ALA:CA[2_455]	1.96	0.24
3:L:14:PRO:C	3:L:88:ALA:N[2_455]	1.98	0.22
2:W:22:VAL:N	2:W:22:VAL:O[2_655]	1.98	0.22
3:L:13:GLN:O	3:L:88:ALA:O[2_455]	2.02	0.18
3:L:14:PRO:O	3:L:90:ASP:N[2_455]	2.04	0.16
1:T:252:ASP:O	2:W:32:ASN:ND2[2_655]	2.05	0.15
1:H:159:ASN:N	2:K:14:VAL:N[2_555]	2.07	0.13
3:X:86:LEU:O	3:X:88:ALA:N[2_755]	2.11	0.09
2:W:22:VAL:C	2:W:22:VAL:O[2_655]	2.14	0.06
1:H:258:ILE:O	2:K:27:SER:OG[2_555]	2.15	0.05

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	288/308 (94%)	243 (84%)	29 (10%)	16 (6%)	1	17
1	D	265/308 (86%)	230 (87%)	27 (10%)	8 (3%)	3	26
1	G	306/308 (99%)	255 (83%)	41 (13%)	10 (3%)	3	24
1	H	256/308 (83%)	228 (89%)	19 (7%)	9 (4%)	3	23
1	M	282/308 (92%)	247 (88%)	25 (9%)	10 (4%)	3	23
1	N	277/308 (90%)	236 (85%)	30 (11%)	11 (4%)	2	21
1	S	284/308 (92%)	251 (88%)	28 (10%)	5 (2%)	6	34
1	T	262/308 (85%)	233 (89%)	21 (8%)	8 (3%)	3	25
2	B	94/103 (91%)	78 (83%)	14 (15%)	2 (2%)	5	32
2	E	96/103 (93%)	84 (88%)	12 (12%)	0	100	100
2	I	95/103 (92%)	83 (87%)	11 (12%)	1 (1%)	11	44
2	K	95/103 (92%)	83 (87%)	11 (12%)	1 (1%)	11	44
2	O	92/103 (89%)	75 (82%)	12 (13%)	5 (5%)	1	18
2	Q	89/103 (86%)	79 (89%)	9 (10%)	1 (1%)	11	44
2	U	90/103 (87%)	73 (81%)	15 (17%)	2 (2%)	5	31
2	W	95/103 (92%)	70 (74%)	19 (20%)	6 (6%)	1	15
3	C	118/125 (94%)	100 (85%)	14 (12%)	4 (3%)	3	24
3	F	118/125 (94%)	100 (85%)	14 (12%)	4 (3%)	3	24
3	J	118/125 (94%)	97 (82%)	16 (14%)	5 (4%)	2	21
3	L	118/125 (94%)	95 (80%)	20 (17%)	3 (2%)	4	29
3	P	118/125 (94%)	96 (81%)	15 (13%)	7 (6%)	1	16
3	R	118/125 (94%)	97 (82%)	16 (14%)	5 (4%)	2	21
3	V	118/125 (94%)	100 (85%)	11 (9%)	7 (6%)	1	16
3	X	118/125 (94%)	96 (81%)	14 (12%)	8 (7%)	1	14
All	All	3910/4288 (91%)	3329 (85%)	443 (11%)	138 (4%)	3	23

All (138) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	105	ILE
1	A	118	GLU
1	A	122	LYS

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Mol	Chain	Res	Type
1	A	138	ASN
1	A	142	MET
2	B	19	ARG
2	B	20	ARG
1	D	157	CYS
1	D	186	LYS
3	F	102	ALA
1	G	103	TYR
1	G	105	ILE
1	G	167	GLY
1	G	169	ARG
1	G	213	MET
1	H	251	GLN
3	L	106	ALA
1	M	245	ASP
1	M	250	ILE
1	N	29	GLU
1	N	106	ASN
1	N	160	ASN
1	N	167	GLY
2	O	9	THR
2	O	35	ASN
3	P	106	ALA
3	P	109	VAL
3	R	101	PRO
3	R	102	ALA
3	R	106	ALA
1	S	116	MET
1	T	256	LEU
1	T	260	ARG
2	U	9	THR
3	V	64	VAL
3	V	101	PRO
2	W	17	ALA
2	W	30	SER
2	W	48	SER
3	X	17	SER
3	X	64	VAL
3	X	67	ARG
3	X	68	PHE
3	X	106	ALA
1	A	76	GLU

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Mol	Chain	Res	Type
1	A	139	LYS
1	A	141	CYS
1	A	167	GLY
1	A	250	ILE
1	A	253	LYS
1	D	76	GLU
1	D	112	PHE
1	D	161	ASN
3	F	101	PRO
1	G	76	GLU
1	H	18	ILE
1	H	26	GLN
1	H	76	GLU
1	H	167	GLY
2	I	10	GLN
3	J	102	ALA
3	L	14	PRO
1	M	76	GLU
1	M	167	GLY
1	M	216	TYR
1	N	28	LYS
1	N	31	HIS
1	N	76	GLU
2	O	100	LEU
3	P	100	ASN
3	P	102	ALA
2	Q	98	ASP
1	S	76	GLU
1	S	167	GLY
1	T	76	GLU
1	T	167	GLY
3	V	2	VAL
3	V	102	ALA
2	W	29	SER
2	W	45	PRO
1	A	22	ILE
1	A	157	CYS
1	A	187	ASN
1	D	160	ASN
1	D	167	GLY
3	F	106	ALA
1	G	17	ASN

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Mol	Chain	Res	Type
1	G	21	SER
1	G	22	ILE
1	G	218	TYR
1	H	262	PHE
1	M	158	TYR
2	O	98	ASP
3	P	105	VAL
1	S	108	LYS
1	T	28	LYS
3	X	66	GLY
3	C	61	LEU
1	D	8	TYR
1	H	94	ALA
3	J	106	ALA
3	L	61	LEU
1	M	187	ASN
1	M	246	LYS
1	N	187	ASN
3	P	101	PRO
3	R	61	LEU
1	S	103	TYR
1	T	187	ASN
3	V	61	LEU
3	V	106	ALA
2	W	20	ARG
1	A	213	MET
1	A	214	GLY
3	C	106	ALA
3	F	61	LEU
1	H	187	ASN
3	J	61	LEU
2	K	12	PRO
1	N	105	ILE
1	N	111	ALA
1	N	158	TYR
3	P	61	LEU
3	R	105	VAL
1	T	161	ASN
2	U	101	ASN
3	V	103	SER
3	X	119	SER
3	C	101	PRO

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Mol	Chain	Res	Type
3	C	104	ALA
1	H	247	THR
3	J	103	SER
1	M	159	ASN
1	T	204	LEU
2	O	34	GLY
1	M	214	GLY
3	J	100	ASN
3	X	118	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	285/297 (96%)	251 (88%)	34 (12%)	5	21
1	D	261/297 (88%)	238 (91%)	23 (9%)	9	32
1	G	297/297 (100%)	264 (89%)	33 (11%)	6	23
1	H	257/297 (86%)	235 (91%)	22 (9%)	10	33
1	M	279/297 (94%)	260 (93%)	19 (7%)	14	39
1	N	272/297 (92%)	235 (86%)	37 (14%)	3	18
1	S	277/297 (93%)	250 (90%)	27 (10%)	8	27
1	T	261/297 (88%)	225 (86%)	36 (14%)	3	17
2	B	80/86 (93%)	72 (90%)	8 (10%)	7	26
2	E	82/86 (95%)	76 (93%)	6 (7%)	13	37
2	I	81/86 (94%)	72 (89%)	9 (11%)	6	23
2	K	80/86 (93%)	72 (90%)	8 (10%)	7	26
2	O	79/86 (92%)	69 (87%)	10 (13%)	4	20
2	Q	76/86 (88%)	71 (93%)	5 (7%)	15	40
2	U	78/86 (91%)	71 (91%)	7 (9%)	9	31
2	W	80/86 (93%)	71 (89%)	9 (11%)	5	22
3	C	94/100 (94%)	93 (99%)	1 (1%)	65	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	F	95/100 (95%)	89 (94%)	6 (6%)	16	41
3	J	93/100 (93%)	90 (97%)	3 (3%)	34	56
3	L	94/100 (94%)	85 (90%)	9 (10%)	8	28
3	P	96/100 (96%)	90 (94%)	6 (6%)	16	41
3	R	95/100 (95%)	91 (96%)	4 (4%)	26	49
3	V	95/100 (95%)	91 (96%)	4 (4%)	26	49
3	X	95/100 (95%)	88 (93%)	7 (7%)	13	36
All	All	3582/3864 (93%)	3249 (91%)	333 (9%)	8	29

All (333) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	LYS
1	A	86	ASN
1	A	88	ILE
1	A	98	LYS
1	A	99	LEU
1	A	100	GLU
1	A	113	LYS
1	A	115	MET
1	A	125	LYS
1	A	128	LYS
1	A	132	ASN
1	A	139	LYS
1	A	159	ASN
1	A	171	HIS
1	A	178	LYS
1	A	190	LYS
1	A	194	ASP
1	A	210	ASN
1	A	213	MET
1	A	222	ILE
1	A	244	ASN
1	A	249	ILE
1	A	250	ILE
1	A	251	GLN
1	A	252	ASP
1	A	253	LYS
1	A	262	PHE
1	A	264	LYS

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Mol	Chain	Res	Type
1	A	276	ASN
1	A	279	SER
1	A	288	ARG
1	A	300	LYS
1	A	310	ILE
1	A	311	TYR
2	B	16	GLU
2	B	19	ARG
2	B	20	ARG
2	B	21	ARG
2	B	51	LEU
2	B	52	LEU
2	B	60	THR
2	B	90	ASP
3	C	105	VAL
1	D	13	LEU
1	D	20	ASN
1	D	24	ILE
1	D	26	GLN
1	D	28	LYS
1	D	47	LYS
1	D	86	ASN
1	D	114	LYS
1	D	132	ASN
1	D	155	LEU
1	D	171	HIS
1	D	174	GLU
1	D	179	LEU
1	D	183	VAL
1	D	186	LYS
1	D	190	LYS
1	D	194	ASP
1	D	220	ASP
1	D	228	GLU
1	D	248	LYS
1	D	276	ASN
1	D	279	SER
1	D	288	ARG
2	E	16	GLU
2	E	35	ASN
2	E	51	LEU
2	E	52	LEU

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Mol	Chain	Res	Type
2	E	60	THR
2	E	98	ASP
3	F	19	ARG
3	F	30	ASN
3	F	67	ARG
3	F	87	ARG
3	F	105	VAL
3	F	109	VAL
1	G	5	PHE
1	G	10	PHE
1	G	15	ASN
1	G	24	ILE
1	G	50	SER
1	G	99	LEU
1	G	110	ARG
1	G	128	LYS
1	G	132	ASN
1	G	140	ILE
1	G	144	MET
1	G	155	LEU
1	G	157	CYS
1	G	165	THR
1	G	166	ASN
1	G	171	HIS
1	G	174	GLU
1	G	178	LYS
1	G	190	LYS
1	G	192	LEU
1	G	194	ASP
1	G	196	THR
1	G	213	MET
1	G	228	GLU
1	G	233	PHE
1	G	248	LYS
1	G	260	ARG
1	G	263	GLN
1	G	267	LEU
1	G	268	LEU
1	G	276	ASN
1	G	279	SER
1	G	289	GLN
1	H	20	ASN

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Mol	Chain	Res	Type
1	H	24	ILE
1	H	25	LEU
1	H	26	GLN
1	H	57	LYS
1	H	74	ILE
1	H	86	ASN
1	H	88	ILE
1	H	99	LEU
1	H	127	ILE
1	H	128	LYS
1	H	132	ASN
1	H	161	ASN
1	H	171	HIS
1	H	194	ASP
1	H	228	GLU
1	H	245	ASP
1	H	262	PHE
1	H	267	LEU
1	H	270	ARG
1	H	276	ASN
1	H	279	SER
2	I	16	GLU
2	I	19	ARG
2	I	20	ARG
2	I	21	ARG
2	I	35	ASN
2	I	51	LEU
2	I	52	LEU
2	I	60	THR
2	I	80	ILE
3	J	77	LYS
3	J	98	ARG
3	J	105	VAL
2	K	12	PRO
2	K	16	GLU
2	K	23	THR
2	K	25	TYR
2	K	50	LYS
2	K	52	LEU
2	K	60	THR
2	K	80	ILE
3	L	1	GLU

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Mol	Chain	Res	Type
3	L	17	SER
3	L	32	TYR
3	L	56	SER
3	L	76	LYS
3	L	77	LYS
3	L	91	THR
3	L	117	THR
3	L	119	SER
1	M	24	ILE
1	M	113	LYS
1	M	131	LYS
1	M	132	ASN
1	M	140	ILE
1	M	159	ASN
1	M	171	HIS
1	M	174	GLU
1	M	194	ASP
1	M	209	LEU
1	M	213	MET
1	M	228	GLU
1	M	245	ASP
1	M	249	ILE
1	M	250	ILE
1	M	269	LYS
1	M	276	ASN
1	M	279	SER
1	M	311	TYR
1	N	11	LYS
1	N	12	GLU
1	N	13	LEU
1	N	25	LEU
1	N	26	GLN
1	N	29	GLU
1	N	32	LEU
1	N	72	LYS
1	N	73	LYS
1	N	84	LYS
1	N	92	LEU
1	N	98	LYS
1	N	99	LEU
1	N	105	ILE
1	N	110	ARG

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Mol	Chain	Res	Type
1	N	115	MET
1	N	122	LYS
1	N	123	LYS
1	N	126	LEU
1	N	127	ILE
1	N	128	LYS
1	N	131	LYS
1	N	132	ASN
1	N	155	LEU
1	N	161	ASN
1	N	166	ASN
1	N	171	HIS
1	N	181	LEU
1	N	190	LYS
1	N	203	GLU
1	N	205	LEU
1	N	222	ILE
1	N	225	ILE
1	N	227	LYS
1	N	228	GLU
1	N	276	ASN
1	N	279	SER
2	O	16	GLU
2	O	20	ARG
2	O	26	CYS
2	O	33	ILE
2	O	51	LEU
2	O	52	LEU
2	O	60	THR
2	O	100	LEU
2	O	101	ASN
2	O	103	VAL
3	P	29	PHE
3	P	43	LYS
3	P	99	ASP
3	P	100	ASN
3	P	105	VAL
3	P	109	VAL
2	Q	20	ARG
2	Q	52	LEU
2	Q	60	THR
2	Q	90	ASP

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Mol	Chain	Res	Type
2	Q	99	ARG
3	R	43	LYS
3	R	98	ARG
3	R	100	ASN
3	R	105	VAL
1	S	35	VAL
1	S	86	ASN
1	S	88	ILE
1	S	96	ILE
1	S	100	GLU
1	S	101	HIS
1	S	113	LYS
1	S	114	LYS
1	S	116	MET
1	S	118	GLU
1	S	132	ASN
1	S	157	CYS
1	S	171	HIS
1	S	174	GLU
1	S	179	LEU
1	S	194	ASP
1	S	206	LEU
1	S	209	LEU
1	S	227	LYS
1	S	228	GLU
1	S	231	HIS
1	S	261	THR
1	S	267	LEU
1	S	276	ASN
1	S	279	SER
1	S	307	HIS
1	S	311	TYR
1	T	11	LYS
1	T	24	ILE
1	T	25	LEU
1	T	26	GLN
1	T	27	GLU
1	T	42	PHE
1	T	57	LYS
1	T	86	ASN
1	T	122	LYS
1	T	127	ILE

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Mol	Chain	Res	Type
1	T	132	ASN
1	T	152	PHE
1	T	158	TYR
1	T	159	ASN
1	T	160	ASN
1	T	161	ASN
1	T	164	ASN
1	T	171	HIS
1	T	174	GLU
1	T	178	LYS
1	T	179	LEU
1	T	190	LYS
1	T	194	ASP
1	T	199	LEU
1	T	203	GLU
1	T	219	ILE
1	T	227	LYS
1	T	228	GLU
1	T	256	LEU
1	T	259	TRP
1	T	262	PHE
1	T	263	GLN
1	T	270	ARG
1	T	276	ASN
1	T	279	SER
1	T	289	GLN
2	U	8	LEU
2	U	16	GLU
2	U	51	LEU
2	U	52	LEU
2	U	60	THR
2	U	87	ASP
2	U	101	ASN
3	V	98	ARG
3	V	105	VAL
3	V	109	VAL
3	V	115	MET
2	W	12	PRO
2	W	16	GLU
2	W	26	CYS
2	W	27	SER
2	W	35	ASN

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Mol	Chain	Res	Type
2	W	52	LEU
2	W	60	THR
2	W	86	GLU
2	W	93	CYS
3	X	56	SER
3	X	77	LYS
3	X	87	ARG
3	X	98	ARG
3	X	109	VAL
3	X	118	VAL
3	X	119	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (90) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	HIS
1	A	101	HIS
1	A	135	ASN
1	A	161	ASN
1	A	289	GLN
1	A	304	ASN
1	A	307	HIS
1	A	308	HIS
2	B	84	GLN
3	C	3	GLN
3	C	82	GLN
1	D	20	ASN
1	D	26	GLN
1	D	31	HIS
1	D	56	HIS
1	D	146	ASN
1	D	161	ASN
1	D	166	ASN
2	E	10	GLN
2	E	35	ASN
3	F	84	ASN
1	G	4	ASN
1	G	52	ASN
1	G	86	ASN
1	G	106	ASN
1	G	138	ASN
1	G	159	ASN

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Mol	Chain	Res	Type
1	G	197	ASN
1	G	234	ASN
1	G	257	ASN
1	H	7	GLN
1	H	9	HIS
1	H	52	ASN
1	H	56	HIS
1	H	132	ASN
1	H	138	ASN
1	H	146	ASN
1	H	234	ASN
2	I	35	ASN
2	I	36	ASN
2	I	43	GLN
2	I	84	GLN
3	J	39	GLN
2	K	84	GLN
1	M	26	GLN
1	M	39	HIS
1	M	138	ASN
1	M	146	ASN
1	M	161	ASN
1	M	177	HIS
1	M	234	ASN
1	N	56	HIS
1	N	138	ASN
1	N	146	ASN
1	N	159	ASN
1	N	177	HIS
1	N	197	ASN
1	N	201	GLN
1	N	234	ASN
2	O	32	ASN
2	O	84	GLN
3	P	82	GLN
3	P	100	ASN
2	Q	35	ASN
2	Q	84	GLN
3	R	82	GLN
1	S	26	GLN
1	S	56	HIS
1	S	120	ASN

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Mol	Chain	Res	Type
1	S	138	ASN
1	S	146	ASN
1	S	177	HIS
1	S	197	ASN
1	S	201	GLN
1	S	210	ASN
1	S	234	ASN
1	S	308	HIS
1	T	52	ASN
1	T	138	ASN
1	T	146	ASN
1	T	197	ASN
1	T	234	ASN
1	T	286	HIS
1	T	304	ASN
2	U	84	GLN
3	V	82	GLN
3	V	112	GLN
3	X	13	GLN
3	X	52	GLN
3	X	112	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	294/308 (95%)	0.45	35 (11%)	9 12	25, 112, 211, 269	0
1	D	273/308 (88%)	0.55	25 (9%)	14 17	32, 133, 218, 269	0
1	G	308/308 (100%)	0.58	31 (10%)	12 14	42, 143, 257, 359	0
1	H	266/308 (86%)	0.48	31 (11%)	9 12	20, 167, 290, 353	0
1	M	288/308 (93%)	0.48	35 (12%)	8 12	19, 108, 205, 282	0
1	N	283/308 (91%)	0.62	39 (13%)	6 10	22, 149, 253, 398	0
1	S	288/308 (93%)	0.69	49 (17%)	4 7	51, 141, 262, 391	0
1	T	270/308 (87%)	0.48	24 (8%)	15 17	36, 135, 255, 338	0
2	B	96/103 (93%)	0.79	15 (15%)	5 9	88, 199, 275, 316	0
2	E	97/103 (94%)	0.77	13 (13%)	7 10	89, 195, 327, 365	1 (1%)
2	I	97/103 (94%)	0.94	19 (19%)	3 5	118, 244, 386, 435	0
2	K	97/103 (94%)	0.97	18 (18%)	3 6	103, 248, 405, 484	0
2	O	96/103 (93%)	1.03	20 (20%)	2 5	106, 180, 281, 301	0
2	Q	93/103 (90%)	1.04	20 (21%)	2 4	84, 204, 294, 326	0
2	U	94/103 (91%)	1.15	22 (23%)	2 4	123, 225, 378, 400	0
2	W	97/103 (94%)	0.79	15 (15%)	5 9	131, 232, 436, 496	0
3	C	120/125 (96%)	0.65	16 (13%)	7 10	52, 168, 317, 438	0
3	F	120/125 (96%)	1.00	26 (21%)	2 4	38, 136, 259, 328	0
3	J	120/125 (96%)	0.78	20 (16%)	4 8	41, 176, 295, 361	0
3	L	120/125 (96%)	1.09	28 (23%)	2 4	62, 194, 310, 475	0
3	P	120/125 (96%)	1.10	24 (20%)	3 5	30, 162, 283, 322	0
3	R	120/125 (96%)	0.68	15 (12%)	8 12	68, 163, 328, 366	0
3	V	120/125 (96%)	1.00	24 (20%)	3 5	63, 181, 321, 443	0
3	X	120/125 (96%)	0.89	21 (17%)	4 7	88, 219, 330, 373	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	3997/4288 (93%)	0.70	585 (14%) 6 9	19, 159, 304, 496	1 (0%)

All (585) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	V	99	ASP	9.0
1	S	20	ASN	8.7
1	S	62	GLY	8.6
1	S	64	CYS	8.4
2	I	7	ALA	8.2
3	J	50	ASN	7.7
2	W	64	SER	7.6
1	M	307	HIS	7.6
1	S	120	ASN	7.6
3	V	106	ALA	7.6
3	C	66	GLY	7.5
3	L	92	ALA	7.4
3	V	55	GLY	7.3
1	S	117	ASP	7.2
1	T	68	ASP	7.1
3	X	78	SER	7.1
2	I	36	ASN	7.0
1	G	117	ASP	7.0
1	A	58	SER	6.9
1	G	170	TYR	6.8
1	N	66	ALA	6.7
2	E	19	ARG	6.7
2	K	69	GLY	6.7
2	I	12	PRO	6.7
1	N	157	CYS	6.7
2	O	56	ASP	6.6
1	A	59	SER	6.4
1	N	106	ASN	6.4
3	C	112	GLN	6.4
3	C	63	SER	6.4
1	S	68	ASP	6.4
3	J	26	GLY	6.2
3	P	82	GLN	6.1
1	G	121	THR	6.1
3	L	18	LEU	6.1
1	T	303	ASN	6.1
2	E	58	LEU	6.1

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Mol	Chain	Res	Type	RSRZ
2	O	54	TYR	6.1
1	N	72	LYS	6.0
1	M	53	SER	5.9
1	A	68	ASP	5.9
3	C	111	GLY	5.8
1	T	293	ASN	5.8
3	C	65	ARG	5.7
3	J	59	ASP	5.6
1	N	69	ALA	5.6
3	V	57	GLU	5.6
3	P	108	ASP	5.6
2	W	63	VAL	5.5
2	K	57	ASP	5.5
2	W	98	ASP	5.5
2	B	36	ASN	5.5
1	H	38	PRO	5.5
1	N	77	ALA	5.4
2	W	46	GLY	5.4
2	W	86	GLU	5.4
3	F	88	ALA	5.3
2	K	58	LEU	5.3
1	S	185	SER	5.3
3	V	98	ARG	5.3
3	J	49	ALA	5.3
1	D	139	LYS	5.3
2	E	62	GLY	5.2
3	C	62	ASN	5.2
1	G	69	ALA	5.2
1	A	156	SER	5.2
1	N	68	ASP	5.2
3	C	67	ARG	5.2
2	I	96	TRP	5.2
1	N	76	GLU	5.1
3	F	91	THR	5.1
1	A	67	VAL	5.0
1	D	69	ALA	5.0
1	M	303	ASN	5.0
3	P	83	MET	5.0
2	I	27	SER	5.0
3	L	116	VAL	5.0
1	S	65	ILE	5.0
2	U	102	GLY	4.9

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Mol	Chain	Res	Type	RSRZ
1	G	220	ASP	4.9
2	B	101	ASN	4.9
3	V	56	SER	4.9
3	R	28	THR	4.9
3	P	5	VAL	4.9
1	H	39	HIS	4.9
2	K	79	ALA	4.9
1	M	64	CYS	4.8
3	J	28	THR	4.8
2	K	68	SER	4.8
1	S	38	PRO	4.8
2	B	62	GLY	4.8
3	V	54	ASP	4.7
1	M	146	ASN	4.7
2	Q	42	GLN	4.7
3	J	58	LYS	4.7
2	Q	101	ASN	4.7
2	W	97	ASP	4.6
3	P	22	CYS	4.6
3	C	64	VAL	4.6
1	N	65	ILE	4.6
1	S	115	MET	4.6
2	U	94	ALA	4.6
1	A	159	ASN	4.6
3	J	60	TYR	4.6
1	A	38	PRO	4.5
2	O	90	ASP	4.5
1	S	53	SER	4.5
1	A	60	THR	4.5
3	V	107	PHE	4.5
3	P	23	ALA	4.5
1	A	41	THR	4.4
1	N	137	PHE	4.4
2	B	65	ASP	4.4
2	U	40	TRP	4.4
1	D	66	ALA	4.4
1	S	194	ASP	4.4
3	J	65	ARG	4.3
2	Q	95	ALA	4.3
3	L	9	GLY	4.3
1	S	116	MET	4.3
3	F	89	GLU	4.3

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Mol	Chain	Res	Type	RSRZ
1	N	74	ILE	4.3
3	X	77	LYS	4.3
1	S	70	PHE	4.3
3	J	25	SER	4.3
3	X	112	GLN	4.3
1	N	177	HIS	4.3
1	S	181	LEU	4.2
2	I	95	ALA	4.2
3	L	83	MET	4.2
3	P	21	SER	4.2
1	S	311	TYR	4.2
2	K	30	SER	4.2
1	G	175	TYR	4.1
1	H	164	ASN	4.1
1	A	30	GLY	4.1
2	U	74	THR	4.1
2	Q	37	ALA	4.1
3	J	47	TRP	4.1
1	G	172	TYR	4.1
3	V	117	THR	4.1
2	K	72	SER	4.1
2	W	48	SER	4.1
3	J	62	ASN	4.1
1	G	118	GLU	4.0
3	R	63	SER	4.0
2	I	100	LEU	4.0
1	S	170	TYR	4.0
3	X	1	GLU	4.0
3	J	66	GLY	4.0
1	N	156	SER	4.0
1	T	70	PHE	4.0
2	E	23	THR	4.0
1	A	132	ASN	4.0
3	V	26	GLY	4.0
3	V	28	THR	4.0
3	L	118	VAL	3.9
2	E	57	ASP	3.9
3	P	84	ASN	3.9
3	F	85	SER	3.9
3	F	66	GLY	3.9
1	S	63	LYS	3.9
3	F	62	ASN	3.9

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Mol	Chain	Res	Type	RSRZ
3	P	18	LEU	3.9
3	J	57	GLU	3.9
1	T	53	SER	3.9
3	C	85	SER	3.9
1	M	164	ASN	3.9
3	L	66	GLY	3.9
2	I	26	CYS	3.8
3	R	57	GLU	3.8
1	H	42	PHE	3.8
1	S	67	VAL	3.8
1	G	177	HIS	3.8
1	M	142	MET	3.8
1	D	137	PHE	3.8
3	R	59	ASP	3.8
3	V	105	VAL	3.8
3	X	21	SER	3.8
1	M	52	ASN	3.8
3	L	12	VAL	3.8
1	D	68	ASP	3.7
1	M	48	HIS	3.7
1	D	157	CYS	3.7
2	K	35	ASN	3.7
1	T	289	GLN	3.7
3	L	119	SER	3.7
1	N	303	ASN	3.7
1	M	300	LYS	3.7
3	F	81	LEU	3.7
1	M	65	ILE	3.7
3	L	115	MET	3.7
2	W	57	ASP	3.7
2	E	21	ARG	3.6
1	N	79	ASP	3.6
1	G	110	ARG	3.6
1	A	42	PHE	3.6
2	B	102	GLY	3.6
1	N	58	SER	3.6
3	V	120	SER	3.6
1	N	71	ILE	3.6
1	T	300	LYS	3.6
3	V	11	LEU	3.6
1	H	65	ILE	3.6
2	B	44	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
3	F	90	ASP	3.6
1	N	180	ILE	3.5
2	B	96	TRP	3.5
2	K	73	GLY	3.5
3	F	80	TYR	3.5
2	U	103	VAL	3.5
3	J	71	SER	3.5
3	P	114	ALA	3.5
3	X	111	GLY	3.5
3	L	104	ALA	3.5
2	E	65	ASP	3.5
1	H	63	LYS	3.5
3	R	64	VAL	3.5
2	U	35	ASN	3.5
1	A	37	ILE	3.4
1	N	67	VAL	3.4
3	F	118	VAL	3.4
1	D	72	LYS	3.4
1	A	66	ALA	3.4
2	Q	72	SER	3.4
1	H	46	TYR	3.4
3	F	87	ARG	3.4
1	H	72	LYS	3.3
3	P	17	SER	3.3
1	M	74	ILE	3.3
1	N	201	GLN	3.3
2	O	94	ALA	3.3
2	U	64	SER	3.3
3	L	84	ASN	3.3
3	R	65	ARG	3.3
1	T	51	TYR	3.3
3	P	75	ALA	3.3
1	H	272	LEU	3.3
1	G	85	CYS	3.3
2	B	100	LEU	3.3
3	X	62	ASN	3.3
2	I	103	VAL	3.3
3	J	112	GLN	3.3
1	G	219	ILE	3.2
1	S	23	ASP	3.2
1	S	252	ASP	3.2
1	D	30	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
1	H	52	ASN	3.2
2	Q	23	THR	3.2
1	H	37	ILE	3.2
1	H	45	TYR	3.2
1	D	29	GLU	3.2
3	J	70	ILE	3.2
3	L	1	GLU	3.2
3	L	41	PRO	3.2
1	H	190	LYS	3.2
1	D	117	ASP	3.2
2	O	55	PHE	3.2
3	C	61	LEU	3.2
3	P	101	PRO	3.2
2	K	53	ILE	3.2
3	X	8	GLY	3.2
3	C	89	GLU	3.2
1	H	66	ALA	3.2
3	F	19	ARG	3.1
1	A	64	CYS	3.1
1	T	150	ASN	3.1
1	H	40	TYR	3.1
1	G	68	ASP	3.1
2	U	95	ALA	3.1
2	K	70	SER	3.1
1	T	305	ILE	3.1
2	O	49	PRO	3.1
2	U	73	GLY	3.1
2	K	98	ASP	3.1
1	S	60	THR	3.1
1	S	72	LYS	3.1
3	F	83	MET	3.1
1	M	7	GLN	3.1
1	M	58	SER	3.1
2	E	61	SER	3.1
2	W	59	VAL	3.1
3	X	110	TRP	3.0
2	O	43	GLN	3.0
1	N	130	ILE	3.0
1	N	140	ILE	3.0
2	O	93	CYS	3.0
3	J	51	ILE	3.0
2	W	96	TRP	3.0

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Mol	Chain	Res	Type	RSRZ
1	N	63	LYS	3.0
2	O	17	ALA	3.0
3	L	75	ALA	3.0
1	T	13	LEU	3.0
2	E	54	TYR	3.0
3	X	3	GLN	3.0
2	E	59	VAL	3.0
2	U	39	SER	3.0
3	L	114	ALA	3.0
3	V	27	PHE	3.0
3	C	2	VAL	3.0
3	R	32	TYR	3.0
1	S	183	VAL	3.0
2	I	32	ASN	2.9
1	H	76	GLU	2.9
3	L	10	GLY	2.9
1	M	197	ASN	2.9
1	H	68	ASP	2.9
2	K	59	VAL	2.9
3	V	97	ALA	2.9
2	U	53	ILE	2.9
2	O	92	TYR	2.9
3	X	73	ASP	2.9
1	M	156	SER	2.9
3	V	52	GLN	2.9
2	O	65	ASP	2.9
1	N	259	TRP	2.9
1	M	145	LYS	2.9
1	H	247	THR	2.8
1	S	74	ILE	2.8
1	T	121	THR	2.8
1	A	120	ASN	2.8
1	S	21	SER	2.8
1	G	173	ASP	2.8
1	G	194	ASP	2.8
1	D	70	PHE	2.8
2	B	55	PHE	2.8
3	J	61	LEU	2.8
3	R	120	SER	2.8
3	L	42	GLY	2.8
3	P	54	ASP	2.8
1	S	124	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
2	B	54	TYR	2.8
2	U	99	ARG	2.8
3	P	120	SER	2.8
1	N	70	PHE	2.8
1	M	177	HIS	2.7
3	F	65	ARG	2.7
1	S	33	ASP	2.7
3	P	109	VAL	2.7
3	X	2	VAL	2.7
3	X	63	SER	2.7
2	B	25	TYR	2.7
2	W	47	LYS	2.7
1	S	228	GLU	2.7
1	M	257	ASN	2.7
2	K	74	THR	2.7
1	G	87	ASP	2.7
2	B	64	SER	2.7
2	Q	85	SER	2.7
3	F	115	MET	2.7
1	D	201	GLN	2.7
1	N	170	TYR	2.7
1	G	188	LEU	2.7
1	M	63	LYS	2.7
1	T	185	SER	2.7
3	P	12	VAL	2.7
3	X	42	GLY	2.7
1	D	90	ASN	2.7
1	H	222	ILE	2.7
1	G	38	PRO	2.7
1	T	302	LEU	2.7
1	A	46	TYR	2.7
1	H	269	LYS	2.7
3	F	63	SER	2.7
1	T	117	ASP	2.7
2	I	75	SER	2.7
2	O	62	GLY	2.6
1	D	247	THR	2.6
1	N	75	ASN	2.6
3	L	7	SER	2.6
3	F	54	ASP	2.6
3	L	60	TYR	2.6
2	E	78	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	N	132	ASN	2.6
1	G	176	ILE	2.6
1	D	175	TYR	2.6
1	H	51	TYR	2.6
1	D	254	ILE	2.6
1	N	131	LYS	2.6
1	D	171	HIS	2.6
2	Q	45	PRO	2.6
1	S	69	ALA	2.6
1	M	95	THR	2.6
1	S	119	TYR	2.6
2	W	74	THR	2.6
3	L	46	GLU	2.6
2	I	101	ASN	2.6
3	F	56	SER	2.6
3	F	120	SER	2.6
1	D	274	MET	2.6
1	A	247	THR	2.6
3	F	57	GLU	2.6
3	R	70	ILE	2.6
1	G	178	LYS	2.6
1	A	155	LEU	2.6
1	M	137	PHE	2.5
2	O	18	PRO	2.5
3	P	66	GLY	2.5
1	G	41	THR	2.5
1	S	71	ILE	2.5
1	S	55	TYR	2.5
2	Q	19	ARG	2.5
1	D	138	ASN	2.5
1	T	77	ALA	2.5
2	W	62	GLY	2.5
1	A	24	ILE	2.5
1	T	60	THR	2.5
1	S	61	TYR	2.5
2	O	20	ARG	2.5
3	V	119	SER	2.5
1	H	187	ASN	2.5
2	U	12	PRO	2.5
3	F	82	GLN	2.5
2	U	78	LEU	2.5
1	G	67	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
3	J	48	VAL	2.5
1	D	259	TRP	2.5
1	S	66	ALA	2.5
2	Q	43	GLN	2.5
1	T	69	ALA	2.5
3	L	45	LEU	2.5
1	M	172	TYR	2.5
1	D	75	ASN	2.4
1	M	38	PRO	2.4
1	H	41	THR	2.4
1	M	50	SER	2.4
2	I	85	SER	2.4
1	A	158	TYR	2.4
1	A	39	HIS	2.4
1	A	259	TRP	2.4
3	F	117	THR	2.4
3	V	58	LYS	2.4
1	G	126	LEU	2.4
1	T	301	HIS	2.4
3	P	89	GLU	2.4
3	R	11	LEU	2.4
1	N	20	ASN	2.4
1	A	74	ILE	2.4
1	A	92	LEU	2.4
1	H	151	LEU	2.4
2	Q	100	LEU	2.4
1	G	48	HIS	2.4
3	C	88	ALA	2.4
3	L	19	ARG	2.4
2	K	34	GLY	2.4
2	O	27	SER	2.4
1	M	49	LEU	2.4
2	Q	25	TYR	2.4
2	Q	96	TRP	2.4
3	F	14	PRO	2.4
1	S	50	SER	2.4
1	A	245	ASP	2.4
1	S	173	ASP	2.4
1	N	257	ASN	2.3
3	F	119	SER	2.3
3	P	56	SER	2.3
3	R	50	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
3	P	65	ARG	2.3
1	G	124	LYS	2.3
1	M	11	LYS	2.3
1	S	227	LYS	2.3
1	S	285	ASP	2.3
2	Q	7	ALA	2.3
2	K	61	SER	2.3
1	N	64	CYS	2.3
1	D	142	MET	2.3
1	N	249	ILE	2.3
3	F	18	LEU	2.3
1	G	202	SER	2.3
2	U	61	SER	2.3
3	R	102	ALA	2.3
2	E	69	GLY	2.3
2	Q	34	GLY	2.3
2	Q	49	PRO	2.3
2	Q	44	LEU	2.3
1	N	285	ASP	2.3
1	S	248	LYS	2.3
1	T	304	ASN	2.3
3	P	45	LEU	2.3
1	H	27	GLU	2.3
1	S	156	SER	2.3
3	L	44	GLY	2.3
2	U	98	ASP	2.3
1	S	130	ILE	2.2
1	T	74	ILE	2.2
2	U	37	ALA	2.2
1	M	158	TYR	2.2
3	L	3	GLN	2.2
2	W	65	ASP	2.2
3	V	31	THR	2.2
1	H	17	ASN	2.2
3	C	68	PHE	2.2
2	B	81	SER	2.2
1	D	118	GLU	2.2
1	N	179	LEU	2.2
3	C	91	THR	2.2
1	D	164	ASN	2.2
1	M	173	ASP	2.2
1	S	244	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	S	249	ILE	2.2
1	A	63	LYS	2.2
3	L	77	LYS	2.2
1	S	289	GLN	2.2
2	U	29	SER	2.2
3	V	63	SER	2.2
3	X	46	GLU	2.2
1	A	95	THR	2.2
1	M	261	THR	2.2
1	H	75	ASN	2.2
2	O	35	ASN	2.2
3	P	39	GLN	2.2
1	H	155	LEU	2.2
2	I	21	ARG	2.2
3	X	60	TYR	2.2
2	I	88	GLU	2.2
2	Q	73	GLY	2.2
1	D	71	ILE	2.2
1	T	42	PHE	2.2
1	A	90	ASN	2.2
2	I	87	ASP	2.2
1	A	251	GLN	2.2
2	I	99	ARG	2.2
3	L	65	ARG	2.2
1	G	272	LEU	2.2
1	G	53	SER	2.1
1	M	308	HIS	2.1
2	I	33	ILE	2.1
1	A	11	LYS	2.1
1	T	72	LYS	2.1
3	P	42	GLY	2.1
3	R	31	THR	2.1
3	L	62	ASN	2.1
1	S	251	GLN	2.1
1	A	65	ILE	2.1
1	T	38	PRO	2.1
3	R	62	ASN	2.1
2	O	15	SER	2.1
1	S	224	PHE	2.1
2	B	63	VAL	2.1
1	H	117	ASP	2.1
2	E	87	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
2	U	67	PHE	2.1
1	A	51	TYR	2.1
2	O	28	GLY	2.1
3	R	61	LEU	2.1
1	G	244	ASN	2.1
1	H	14	SER	2.1
1	N	138	ASN	2.1
2	U	101	ASN	2.1
1	M	148	GLY	2.1
3	V	32	TYR	2.1
1	M	247	THR	2.1
2	O	23	THR	2.1
2	Q	93	CYS	2.1
1	S	155	LEU	2.1
2	W	73	GLY	2.1
3	X	113	GLY	2.1
3	X	38	ARG	2.1
1	A	246	LYS	2.1
2	U	30	SER	2.1
3	V	35	SER	2.1
2	O	38	VAL	2.1
3	V	100	ASN	2.1
1	N	78	TYR	2.0
1	M	245	ASP	2.0
2	Q	74	THR	2.0
1	N	36	ILE	2.0
1	S	84	LYS	2.0
3	J	43	LYS	2.0
2	B	17	ALA	2.0
3	X	61	LEU	2.0
3	F	9	GLY	2.0
1	N	175	TYR	2.0
1	A	121	THR	2.0
2	K	17	ALA	2.0
3	X	17	SER	2.0
3	C	3	GLN	2.0
1	G	190	LYS	2.0
1	H	97	LYS	2.0
2	I	102	GLY	2.0
1	G	278	TYR	2.0
1	M	259	TRP	2.0
2	U	7	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
2	K	103	VAL	2.0
3	X	109	VAL	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.