Full wwPDB X-ray Structure Validation Report ⓘ

Jul 21, 2024 – 01:35 am BST

PDB ID	:	8QKS
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:

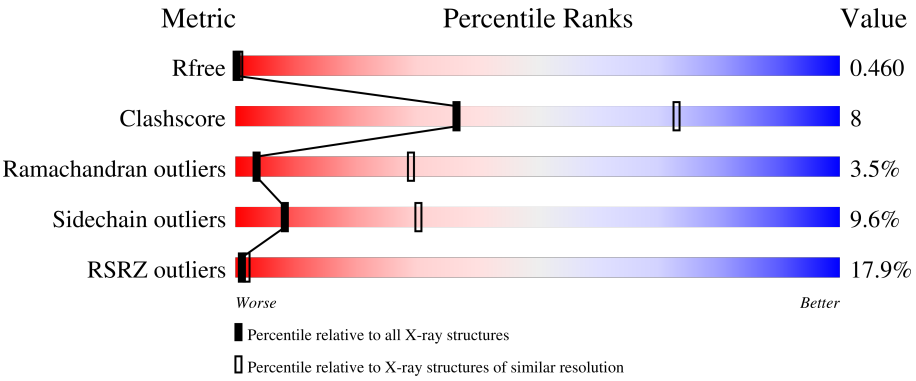
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 3.99 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}	130704	1087 (4.30-3.70)
Clashscore	141614	1148 (4.30-3.70)
Ramachandran outliers	138981	1108 (4.30-3.70)
Sidechain outliers	138945	1099 (4.30-3.70)
RSRZ outliers	127900	1028 (4.34-3.66)

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 <=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	12% 67% 20% 6% • 5%
1	D	308	14% 67% 18% • 11%
1	G	308	16% 74% 21% • •
1	H	308	13% 64% 18% • • 14%
1	M	308	11% 75% 17% • • 6%

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Mol	Chain	Length	Quality of chain
1	N	308	10% 65% 21% 5% 8%
1	S	308	12% 72% 18% 6%
1	T	308	8% 59% 20% 6% 12%
2	B	103	12% 77% 13% 7%
2	E	103	% 81% 13% 6%
2	I	103	17% 75% 17% 6%
2	K	103	23% 66% 22% 5% 6%
2	O	103	19% 66% 20% 7% 7%
2	Q	103	44% 75% 14% 10%
2	U	103	30% 73% 14% 9%
2	W	103	23% 61% 20% 11% 6%
3	C	125	20% 84% 10%
3	F	125	34% 78% 14%
3	J	125	18% 85% 9%
3	L	125	26% 66% 23% 5%
3	P	125	29% 71% 18%
3	R	125	25% 82% 13%
3	V	125	22% 78% 14%
3	X	125	20% 74% 16%

2 Entry composition (i)

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.

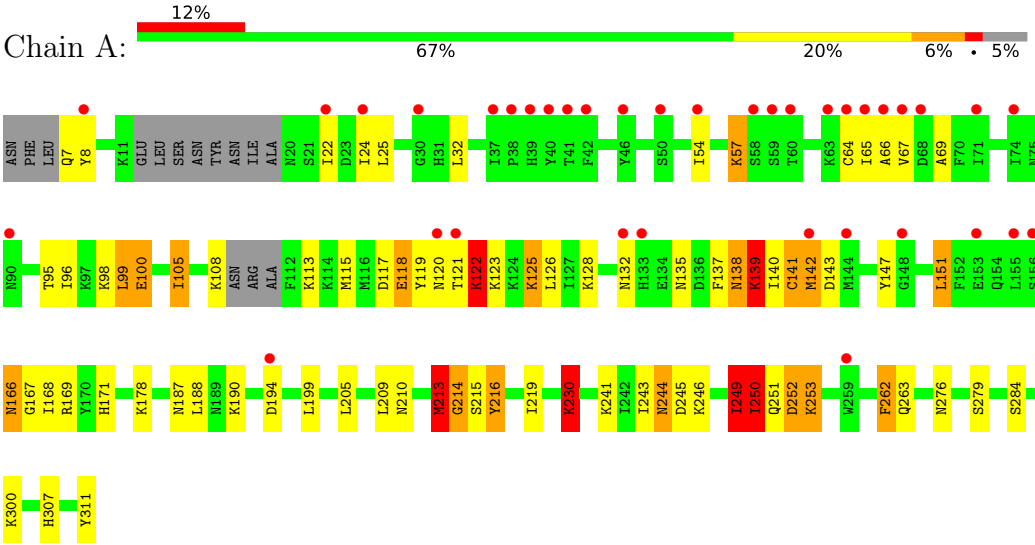
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	120	Total	C	N	O	S	0	0	0
			910	570	159	176	5			
3	F	120	Total	C	N	O	S	0	0	0
			907	566	160	176	5			
3	J	120	Total	C	N	O	S	0	0	0
			903	564	159	175	5			
3	L	120	Total	C	N	O	S	0	0	0
			915	572	160	178	5			
3	P	120	Total	C	N	O	S	0	0	0
			914	572	160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

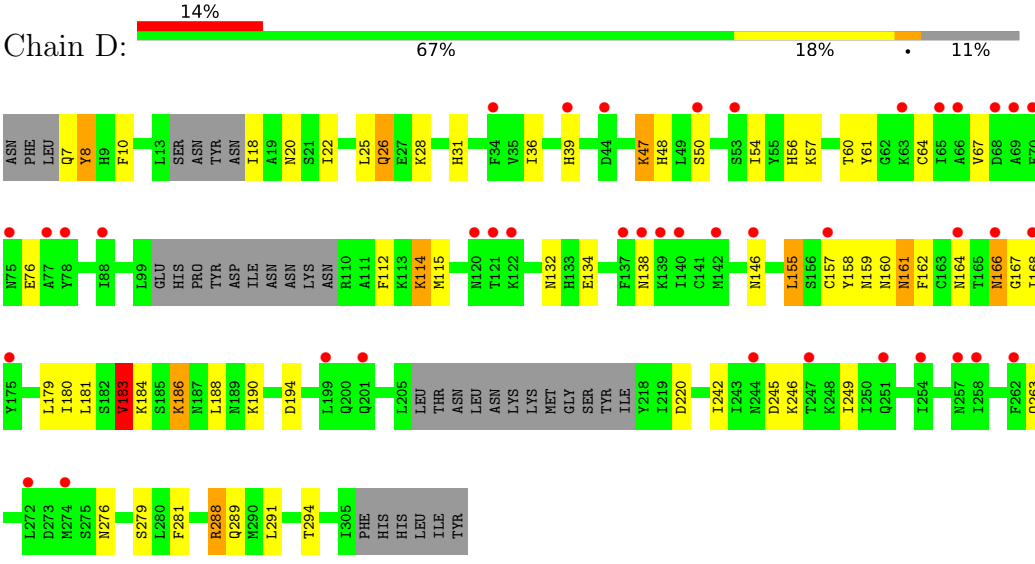
• Molecule 1: Reticulocyte-binding protein-like protein 5

Chain A:



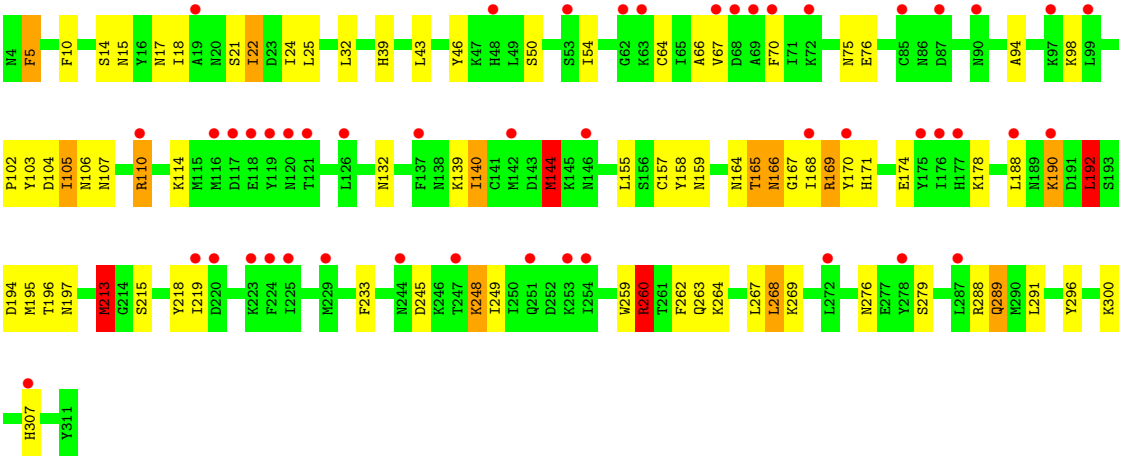
• Molecule 1: Reticulocyte-binding protein-like protein 5

Chain D:



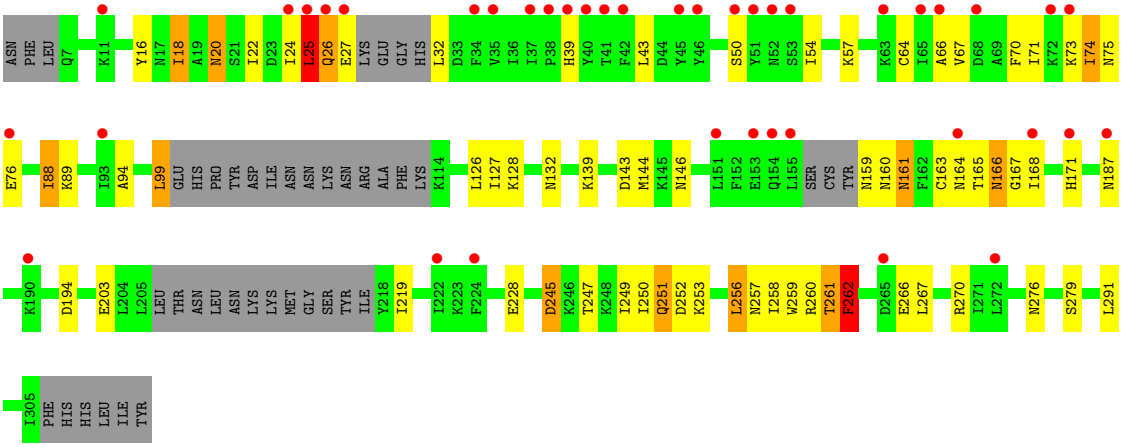
• Molecule 1: Reticulocyte-binding protein-like protein 5

Chain G:



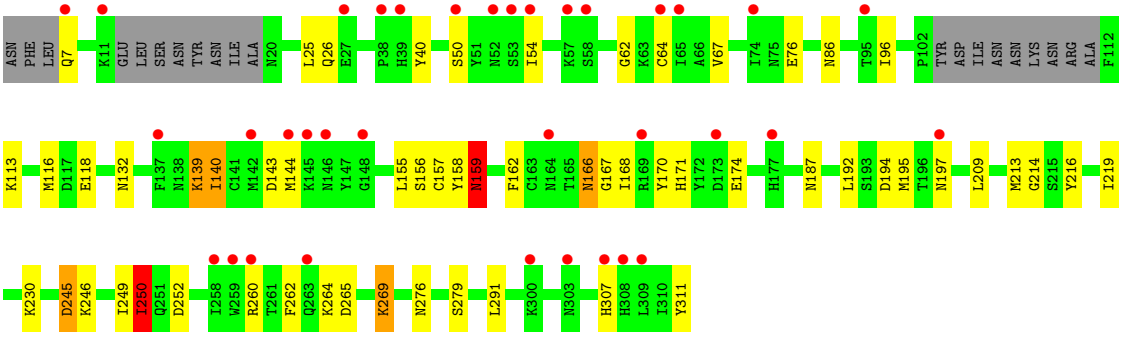
• Molecule 1: Reticulocyte-binding protein-like protein 5

Chain H:



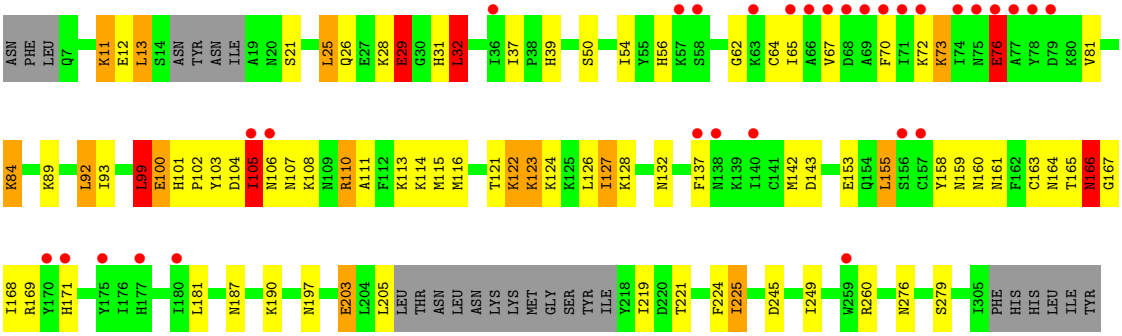
• Molecule 1: Reticulocyte-binding protein-like protein 5

Chain M:

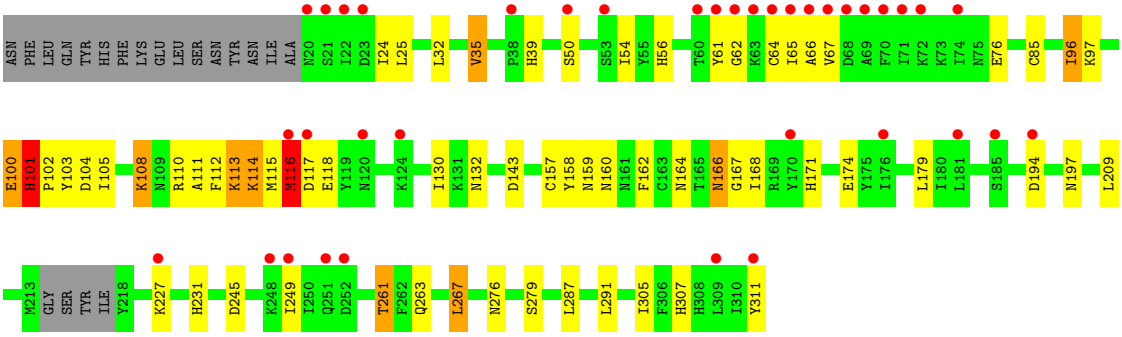


• Molecule 1: Reticulocyte-binding protein-like protein 5

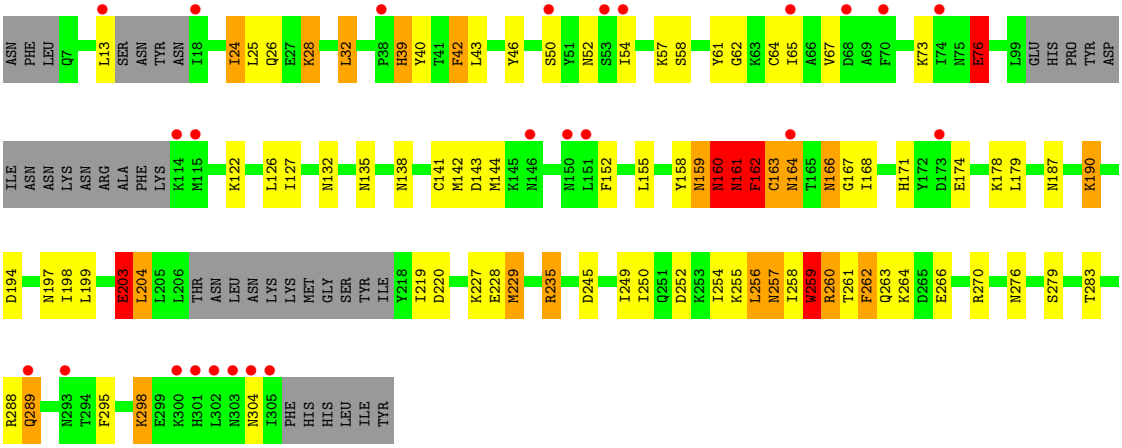
Chain N:



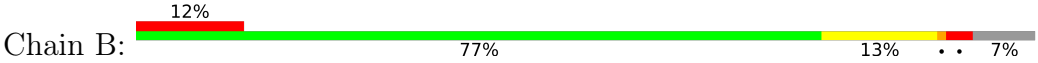
• Molecule 1: Reticulocyte-binding protein-like protein 5

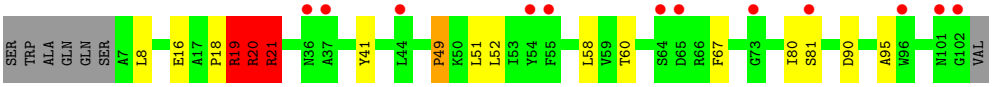


• Molecule 1: Reticulocyte-binding protein-like protein 5



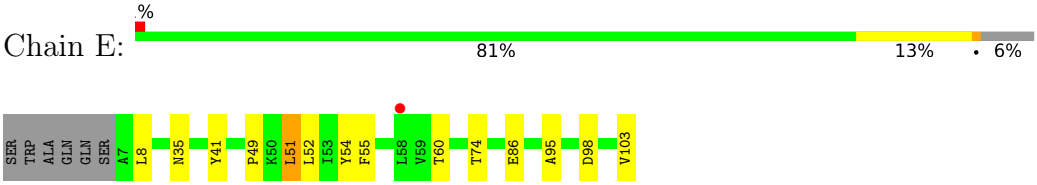
• Molecule 2: Immunoglobulin lambda variable 1-36





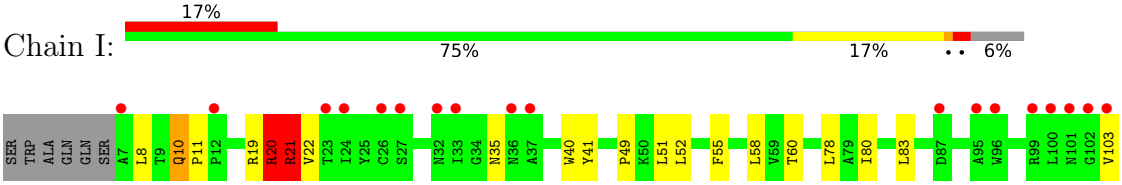
• Molecule 2: Immunoglobulin lambda variable 1-36

Chain E:



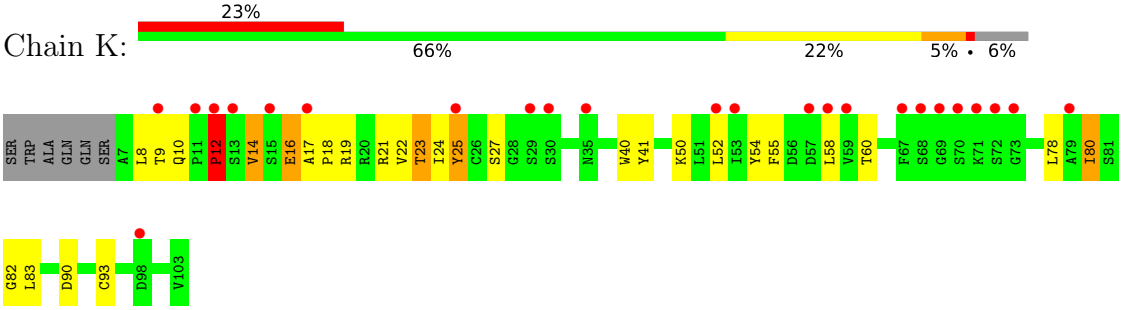
• Molecule 2: Immunoglobulin lambda variable 1-36

Chain I:



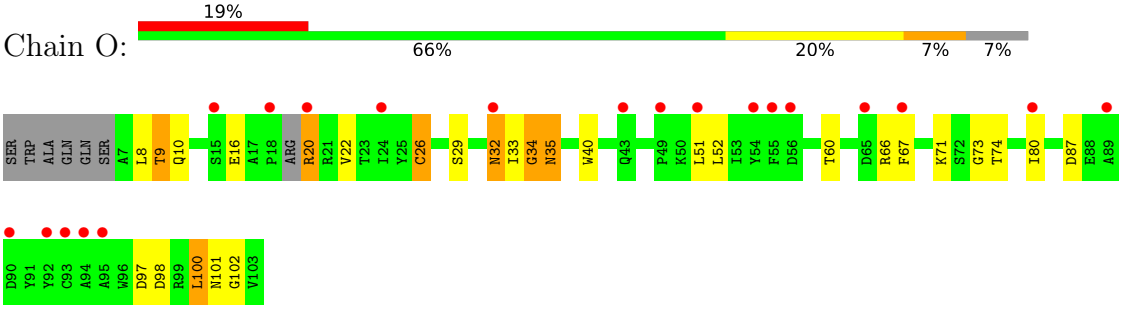
• Molecule 2: Immunoglobulin lambda variable 1-36

Chain K:



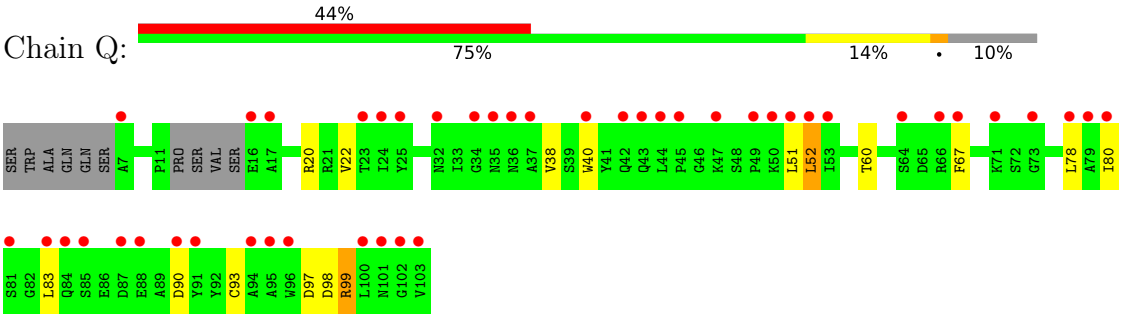
• Molecule 2: Immunoglobulin lambda variable 1-36

Chain O:



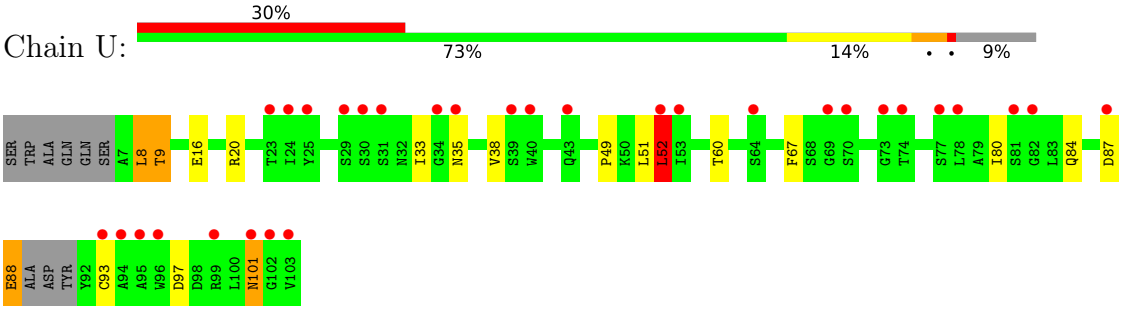
• Molecule 2: Immunoglobulin lambda variable 1-36

Chain Q:



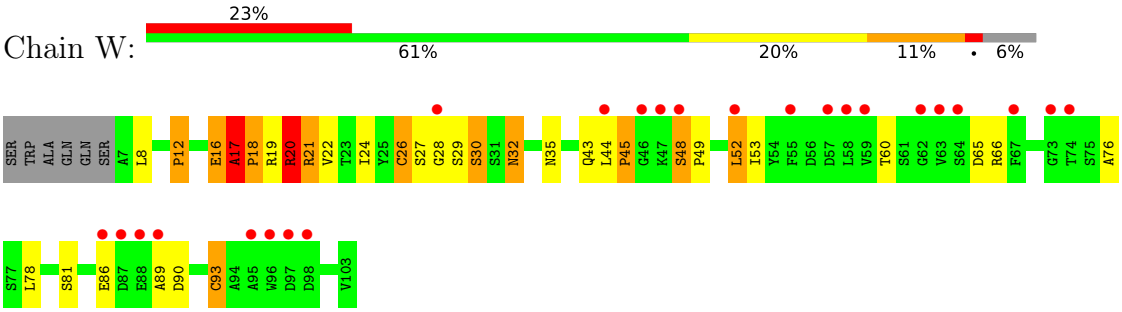
• Molecule 2: Immunoglobulin lambda variable 1-36

Chain U:



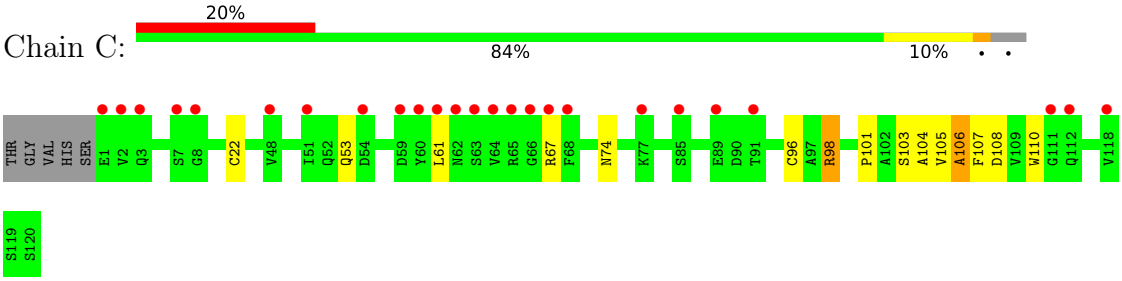
• Molecule 2: Immunoglobulin lambda variable 1-36

Chain W:



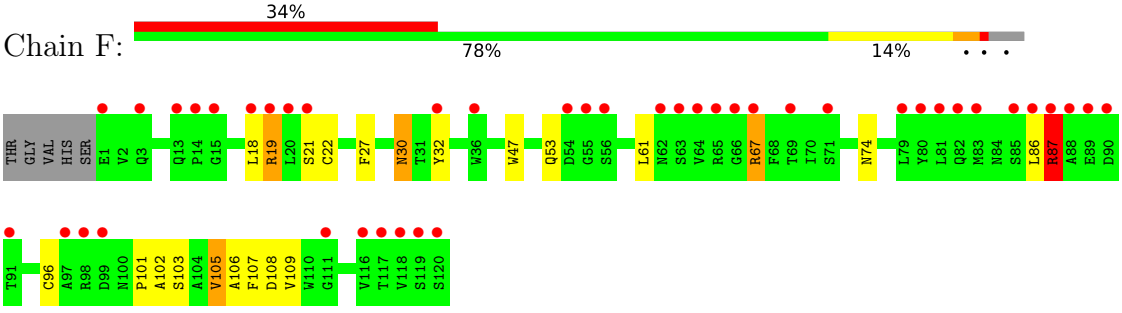
• Molecule 3: R5034HV

Chain C:



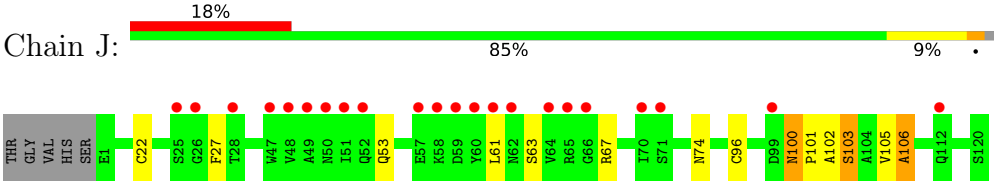
• Molecule 3: R5034HV

Chain F:



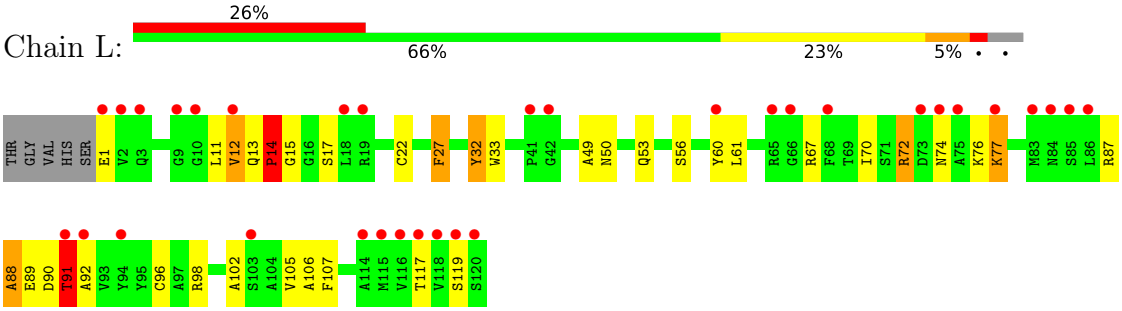
• Molecule 3: R5034HV

Chain J:



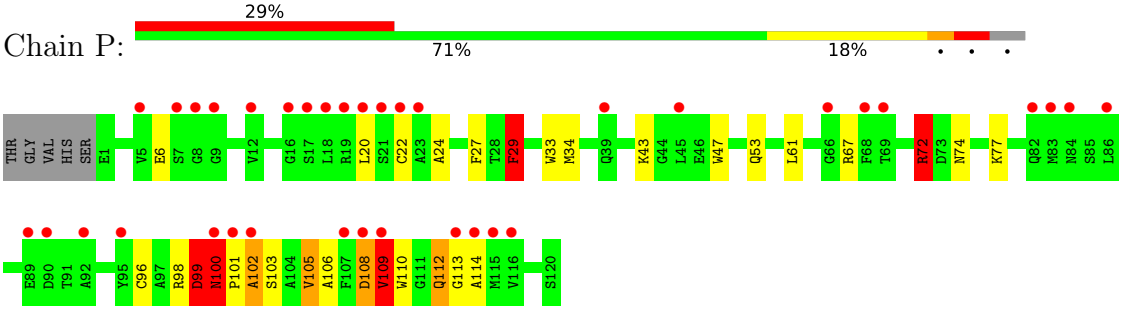
• Molecule 3: R5034HV

Chain L:



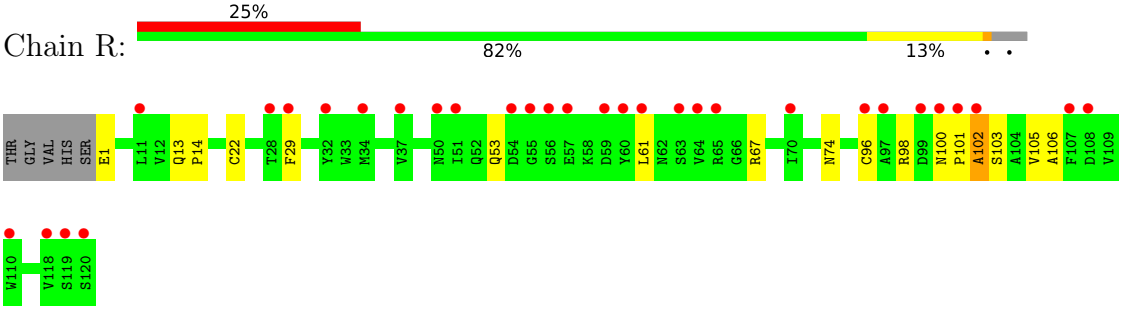
• Molecule 3: R5034HV

Chain P:



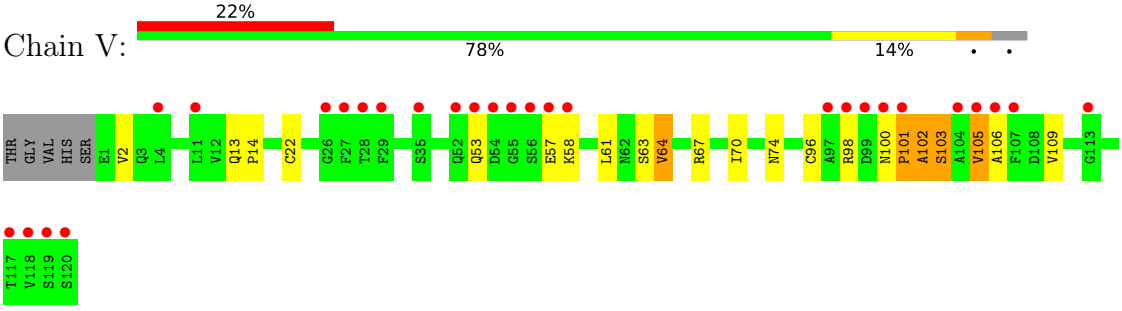
• Molecule 3: R5034HV

Chain R:



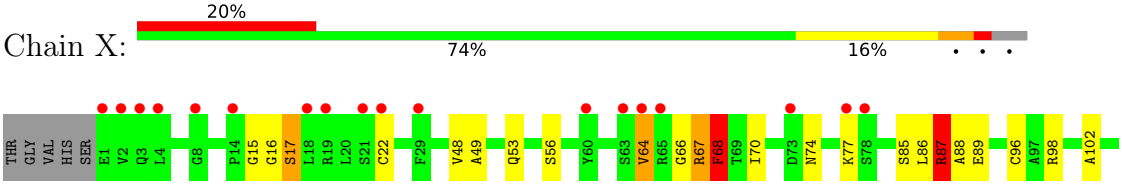
• Molecule 3: R5034HV

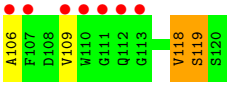
Chain V:



• Molecule 3: R5034HV

Chain X:




A106
F107
D108
V109
W110
G111
Q112
G113
V118
S119
S120

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	1.02 (at 4.01Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.441 , 0.458 0.441 , 0.460	Depositor DCC
R_{free} test set	1918 reflections (1.67%)	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 , 315.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.22$, $< L^2 > = 0.10$	Xtriage
Estimated twinning fraction	0.419 for h,-k,-l	Xtriage
F_o,F_c correlation	0.68	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.35	0/2556	0.96	13/3425 (0.4%)
1	D	0.34	0/2353	0.86	5/3149 (0.2%)
1	G	0.33	0/2675	0.91	8/3590 (0.2%)
1	H	0.36	0/2291	0.96	9/3067 (0.3%)
1	M	0.33	0/2502	0.84	5/3352 (0.1%)
1	N	0.35	0/2445	0.95	13/3276 (0.4%)
1	S	0.31	0/2492	0.82	5/3341 (0.1%)
1	T	0.36	0/2331	1.03	15/3121 (0.5%)
2	B	0.37	0/736	1.00	7/999 (0.7%)
2	E	0.36	0/752	0.83	1/1021 (0.1%)
2	I	0.37	0/743	0.89	3/1009 (0.3%)
2	K	0.43	0/743	1.07	6/1009 (0.6%)
2	O	0.39	0/727	0.91	2/987 (0.2%)
2	Q	0.37	0/715	0.89	1/968 (0.1%)
2	U	0.37	0/708	0.93	3/959 (0.3%)
2	W	0.53	0/740	1.30	12/1005 (1.2%)
3	C	0.33	0/929	0.74	0/1256
3	F	0.32	0/925	0.85	3/1250 (0.2%)
3	J	0.33	0/921	0.76	0/1245
3	L	0.48	0/934	1.13	9/1261 (0.7%)
3	P	0.39	0/933	1.05	7/1261 (0.6%)
3	R	0.35	0/933	0.83	0/1261
3	V	0.34	0/926	0.79	0/1252
3	X	0.40	0/922	1.04	3/1245 (0.2%)
All	All	0.36	0/32932	0.93	130/44309 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	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

There are no bond length outliers.

All (130) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	262	PHE	N-CA-CB	12.82	133.67	110.60
3	X	87	ARG	CA-CB-CG	12.62	141.18	113.40
3	L	14	PRO	N-CA-C	12.01	143.33	112.10
1	T	162	PHE	CB-CA-C	-11.48	87.45	110.40
3	P	72	ARG	NE-CZ-NH1	-11.35	114.63	120.30
1	H	245	ASP	CB-CA-C	10.26	130.91	110.40
3	P	108	ASP	CB-CA-C	-9.70	91.01	110.40
1	T	190	LYS	CB-CG-CD	9.69	136.79	111.60
2	K	12	PRO	N-CA-CB	-9.30	92.14	103.30
1	T	235	ARG	NE-CZ-NH1	-8.71	115.94	120.30
2	Q	52	LEU	CB-CG-CD1	8.62	125.66	111.00
1	N	99	LEU	CB-CG-CD1	8.52	125.48	111.00
2	K	25	TYR	CB-CG-CD1	8.47	126.08	121.00
1	T	257	ASN	CB-CA-C	8.39	127.19	110.40
2	W	93	CYS	CA-CB-SG	-8.38	98.92	114.00
1	H	25	LEU	CB-CG-CD2	8.11	124.78	111.00
1	H	99	LEU	N-CA-CB	8.04	126.49	110.40
2	B	20	ARG	CB-CG-CD	8.04	132.49	111.60
3	P	100	ASN	CB-CA-C	8.01	126.42	110.40
1	G	169	ARG	CA-CB-CG	8.00	131.01	113.40
1	T	235	ARG	NE-CZ-NH2	7.75	124.18	120.30
2	W	20	ARG	CA-CB-CG	7.69	130.31	113.40
1	T	32	LEU	CB-CG-CD1	7.57	123.87	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	W	20	ARG	CB-CA-C	7.50	125.40	110.40
2	E	74	THR	OG1-CB-CG2	-7.49	92.76	110.00
1	N	25	LEU	CB-CG-CD2	-7.44	98.35	111.00
3	P	109	VAL	N-CA-CB	7.43	127.84	111.50
2	W	52	LEU	CB-CG-CD1	7.39	123.56	111.00
2	W	21	ARG	CA-CB-CG	-7.26	97.42	113.40
1	T	255	LYS	CB-CG-CD	7.25	130.44	111.60
1	D	267	LEU	CB-CG-CD1	-7.22	98.73	111.00
2	K	25	TYR	CA-CB-CG	7.08	126.85	113.40
1	A	122	LYS	CB-CA-C	7.03	124.46	110.40
2	B	20	ARG	CA-CB-CG	6.99	128.79	113.40
1	N	155	LEU	N-CA-CB	6.98	124.36	110.40
2	U	52	LEU	CB-CG-CD1	6.98	122.86	111.00
1	T	304	ASN	CB-CA-C	6.85	124.09	110.40
3	F	87	ARG	CG-CD-NE	6.77	126.02	111.80
2	B	20	ARG	CB-CA-C	6.68	123.76	110.40
1	H	261	THR	OG1-CB-CG2	-6.63	94.74	110.00
1	H	262	PHE	CA-CB-CG	6.60	129.75	113.90
3	L	72	ARG	NE-CZ-NH1	6.59	123.60	120.30
1	G	144	MET	CB-CG-SD	6.58	132.16	112.40
1	M	269	LYS	CA-CB-CG	6.55	127.82	113.40
3	F	67	ARG	CA-CB-CG	6.55	127.81	113.40
1	M	144	MET	CG-SD-CE	6.51	110.62	100.20
2	W	8	LEU	CB-CG-CD2	-6.44	100.05	111.00
2	W	48	SER	CB-CA-C	6.42	122.30	110.10
2	K	12	PRO	N-CA-C	6.42	128.78	112.10
1	G	192	LEU	CB-CG-CD1	6.38	121.85	111.00
3	P	29	PHE	CB-CG-CD1	6.38	125.26	120.80
2	I	20	ARG	CA-CB-CG	6.28	127.21	113.40
1	N	11	LYS	CA-CB-CG	6.23	127.11	113.40
2	I	21	ARG	CB-CG-CD	6.23	127.79	111.60
3	X	87	ARG	CD-NE-CZ	6.20	132.29	123.60
1	A	151	LEU	CB-CG-CD1	-6.16	100.53	111.00
2	K	25	TYR	CB-CG-CD2	-6.15	117.31	121.00
2	W	20	ARG	CB-CG-CD	6.11	127.49	111.60
2	W	17	ALA	CB-CA-C	6.11	119.26	110.10
2	O	32	ASN	CB-CA-C	6.07	122.54	110.40
2	U	20	ARG	CA-CB-CG	6.07	126.76	113.40
3	L	14	PRO	C-N-CA	6.06	135.03	122.30
3	P	67	ARG	CG-CD-NE	6.06	124.53	111.80
2	W	12	PRO	N-CA-CB	-6.00	96.00	102.60
3	L	77	LYS	CB-CG-CD	5.98	127.16	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	N	104	ASP	CB-CA-C	5.97	122.34	110.40
1	S	101	HIS	CB-CA-C	-5.96	98.49	110.40
1	T	203	GLU	N-CA-CB	5.94	121.28	110.60
2	W	12	PRO	N-CA-C	5.90	127.43	112.10
1	M	139	LYS	CA-CB-CG	5.88	126.33	113.40
1	H	139	LYS	CA-CB-CG	5.87	126.31	113.40
1	A	99	LEU	CB-CG-CD2	5.83	120.90	111.00
3	P	112	GLN	CB-CA-C	5.82	122.04	110.40
2	B	19	ARG	CB-CA-C	-5.77	98.85	110.40
1	G	144	MET	CG-SD-CE	5.77	109.43	100.20
1	T	229	MET	CB-CG-SD	5.77	129.72	112.40
1	S	267	LEU	CB-CG-CD1	-5.77	101.19	111.00
1	A	230	LYS	CB-CG-CD	5.74	126.51	111.60
3	L	88	ALA	CB-CA-C	5.72	118.67	110.10
1	A	244	ASN	CB-CA-C	-5.69	99.01	110.40
2	K	23	THR	CA-CB-OG1	5.67	120.90	109.00
3	L	91	THR	OG1-CB-CG2	-5.66	96.98	110.00
1	N	100	GLU	CB-CA-C	5.62	121.64	110.40
1	T	160	ASN	CB-CA-C	5.62	121.63	110.40
1	A	253	LYS	CA-CB-CG	5.61	125.75	113.40
1	G	5	PHE	CB-CA-C	5.59	121.58	110.40
1	G	195	MET	CG-SD-CE	5.58	109.13	100.20
2	U	88	GLU	N-CA-CB	5.56	120.61	110.60
1	N	76	GLU	N-CA-CB	5.54	120.57	110.60
3	F	87	ARG	CB-CG-CD	5.53	125.97	111.60
1	H	256	LEU	CB-CG-CD2	-5.51	101.62	111.00
1	N	108	LYS	CB-CA-C	5.51	121.42	110.40
1	D	155	LEU	CB-CG-CD1	-5.51	101.64	111.00
1	N	84	LYS	CA-CB-CG	5.51	125.52	113.40
1	N	32	LEU	N-CA-CB	5.46	121.33	110.40
1	N	203	GLU	CG-CD-OE2	5.44	129.19	118.30
1	A	244	ASN	N-CA-CB	5.42	120.35	110.60
1	T	76	GLU	N-CA-CB	5.41	120.34	110.60
1	S	112	PHE	CB-CA-C	5.40	121.19	110.40
1	D	10	PHE	CB-CG-CD1	5.39	124.58	120.80
1	A	253	LYS	CB-CA-C	-5.38	99.63	110.40
1	G	248	LYS	CB-CG-CD	5.37	125.56	111.60
1	D	183	VAL	N-CA-CB	5.35	123.27	111.50
1	N	103	TYR	CB-CA-C	5.34	121.09	110.40
2	W	32	ASN	CB-CA-C	5.34	121.09	110.40
3	X	68	PHE	N-CA-CB	-5.30	101.06	110.60
3	L	12	VAL	N-CA-CB	5.29	123.13	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	O	66	ARG	CG-CD-NE	5.26	122.84	111.80
1	A	122	LYS	CA-CB-CG	5.25	124.96	113.40
1	A	166	ASN	CB-CA-C	5.25	120.89	110.40
1	A	57	LYS	CB-CG-CD	5.23	125.21	111.60
1	T	163	CYS	CB-CA-C	-5.23	99.94	110.40
1	H	166	ASN	CB-CA-C	5.23	120.85	110.40
2	B	19	ARG	N-CA-CB	5.16	119.89	110.60
1	A	137	PHE	N-CA-CB	5.16	119.89	110.60
1	N	166	ASN	CB-CA-C	5.15	120.70	110.40
2	B	18	PRO	N-CA-C	5.15	125.48	112.10
3	L	72	ARG	CG-CD-NE	5.12	122.56	111.80
1	S	116	MET	CB-CA-C	-5.11	100.18	110.40
1	M	166	ASN	CB-CA-C	5.11	120.61	110.40
1	S	166	ASN	CB-CA-C	5.08	120.57	110.40
1	A	262	PHE	N-CA-CB	5.07	119.73	110.60
1	M	230	LYS	CB-CG-CD	5.07	124.78	111.60
3	L	87	ARG	O-C-N	5.04	130.77	122.70
2	I	21	ARG	CA-CB-CG	5.04	124.49	113.40
1	G	190	LYS	CB-CG-CD	5.04	124.69	111.60
2	B	21	ARG	CB-CA-C	5.03	120.46	110.40
1	T	166	ASN	CB-CA-C	5.03	120.45	110.40
1	T	298	LYS	CA-CB-CG	5.02	124.44	113.40
1	D	166	ASN	CB-CA-C	5.01	120.42	110.40

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
1	H	257	ASN	Peptide
2	K	14	VAL	Peptide
2	K	8	LEU	Peptide

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Mol	Chain	Res	Type	Group
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 (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2503	0	2518	45	0
1	D	2309	0	2331	29	0
1	G	2618	0	2629	34	0
1	H	2251	0	2271	42	5
1	M	2450	0	2469	28	0
1	N	2397	0	2405	44	0
1	S	2442	0	2457	37	0
1	T	2288	0	2312	62	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
2	O	713	0	668	28	0
2	Q	702	0	661	6	0
2	U	696	0	662	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	20	12
3	P	914	0	870	25	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	503	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 (503) 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
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
2:E:86[B]:GLU:OE2	2:E:86[B]:GLU:C	2.17	0.81
3:J:100:ASN:HB3	3:J:101:PRO:CD	2.10	0.81
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
3:P:6:GLU:CD	3:P:114:ALA:HB2	2.14	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
1:H:143:ASP:OD2	3:J:103:SER:OG	2.14	0.65
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:S:115:MET:C	1:S:117:ASP:H	2.01	0.64
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
1:H:160:ASN:CG	1:H:161:ASN:OD1	2.35	0.63
1:T:58:SER:HG	2:W:65:ASP:CG	2.02	0.63
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: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:A:140:ILE:C	1:A:141:CYS:O	2.34	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
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
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
1:H:165:THR:HG1	1:H:259:TRP:HA	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
3:F:18:LEU:HB2	3:F:86:LEU:HD11	1.82	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
3:R:22:CYS:HG	3:R:96:CYS:HG	1.49	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
1:T:58:SER:OG	2:W:65:ASP:CG	2.43	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
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:W:43:GLN:C	2:W:45:PRO:HD3	2.26	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:L:50:ASN:O	3:L:70:ILE:CD1	2.53	0.56
1:N:143:ASP:OD1	3:P:103:SER:OG	2.21	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:S:143:ASP:CG	3:X:102:ALA:HA	2.27	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:P:33:TRP:HB3	3:P:99:ASP:CG	2.28	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
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: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:N:110:ARG:HA	1:N:114:LYS:HD2	1.91	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
3:V:63:SER:O	3:V:64:VAL:C	2.49	0.51
1:A:118:GLU:CB	1:A:120:ASN:HD22	2.22	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
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
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:W:24:ILE:HD12	2:W:78:LEU:HD23	1.94	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:70:PHE:CZ	3:L:102:ALA:HB2	2.47	0.50
1:A:69:ALA:HB3	2:B:58:LEU:HD13	1.94	0.50
1:G:168:ILE:O	1:G:170:TYR:N	2.45	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: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
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
2:W:18:PRO:HB2	2:W:19:ARG:HG3	1.95	0.48
2:O:26:CYS:SG	2:O:40:TRP:CZ2	3.06	0.48
2:O:71:LYS:NZ	2:O:73:GLY:O	2.47	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:K:54:TYR:CD2	3:L:105:VAL:HG21	2.49	0.47
1:S:54:ILE:HD13	1:S:67:VAL:HG21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:58:SER:OG	2:W:65:ASP:OD1	2.26	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
1:H:250:ILE:C	1:H:252:ASP:H	2.18	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
2:E:86[B]:GLU:C	2:E:86[B]:GLU:CD	2.72	0.47
1:G:102:PRO:O	1:G:104:ASP:N	2.48	0.47
1:T:262:PHE:HB2	1:T:266:GLU:HB2	1.97	0.47
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
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:A:108:LYS:C	1:A:216:TYR:OH	2.53	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
1:H:250:ILE:C	1:H:252:ASP:N	2.68	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
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:D:158:TYR:O	1:D:159:ASN:C	2.54	0.46
1:H:25:LEU:CD1	1:H:291:LEU:HD23	2.45	0.46
1:T:28:LYS:HD2	1:T:298:LYS:HZ1	1.79	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:T:258:ILE:C	1:T:260:ARG:HG3	2.37	0.46
1:A:147:TYR:CE2	1:A:151:LEU:HD11	2.51	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:A:252:ASP:OD1	1:A:252:ASP:C	2.55	0.45
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: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
1:M:249:ILE:C	1:M:250:ILE:O	2.55	0.45
2:Q:38:VAL:HG13	2:Q:93:CYS:SG	2.57	0.45
3:X:87:ARG:HG2	3:X:89:GLU:CD	2.36	0.45
1:N:121:THR:OG1	1:N:122:LYS:NZ	2.48	0.45
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
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:S:115:MET:C	1:S:117:ASP:N	2.67	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
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
2:O:8:LEU:C	2:O:10:GLN:H	2.19	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:A:143:ASP:CG	3:C:103:SER:H	2.21	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:164:ASN:OD1	1:G:165:THR:N	2.51	0.43
1:M:192:LEU:HA	1:M:195:MET:HE3	1.99	0.43
1:T:288:ARG:HH21	1:T:289:GLN:CD	2.22	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:62:GLY:HA2	1:T:61:TYR:C	2.38	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
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
2:O:8:LEU:C	2:O:10:GLN:N	2.70	0.43
1:A:119:TYR:HB2	1:A:122:LYS:HE3	2.01	0.43
1:A:263:GLN:CD	1:A:263:GLN:H	2.22	0.43
1:M:7:GLN:HE22	1:M:265:ASP:HB3	1.83	0.43
2:O:8:LEU:O	2:O:9:THR:C	2.56	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:T:43:LEU:C	1:T:43:LEU:HD12	2.40	0.42
2:W:44:LEU:N	2:W:89:ALA:HB1	2.34	0.42
2:O:97:ASP:CG	2:O:102:GLY:HA2	2.40	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:D:288:ARG:HG3	1:D:289:GLN:N	2.35	0.42
1:M:156:SER:O	1:M:157:CYS:C	2.58	0.42
2:O:20:ARG:HH12	2:O:22:VAL:CG1	2.33	0.42
3:P:34:MET:HE3	3:P:72:ARG:HH22	1.85	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
1:A:96:ILE:HG23	1:A:100:GLU:CD	2.40	0.41
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:A:199:LEU:HD13	1:A:230:LYS:CE	2.51	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:L:91:THR:O	3:L:92:ALA:HB2	2.21	0.41
3:V:100:ASN:HB2	3:V:105:VAL:CB	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:86[A]:GLU:CD	2:E:86[A]:GLU:N	2.74	0.41
2:K:54:TYR:CD2	3:L:105:VAL:CG2	3.04	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
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: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
1:M:250:ILE:C	1:M:252:ASP:H	2.24	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
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
1:N:100:GLU:C	1:N:102:PRO:HD3	2.42	0.40
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
2:U:8:LEU:O	2:U:9:THR:CB	2.70	0.40
1:G:159:ASN:HA	1:G:264:LYS:HB2	2.02	0.40
1:G:288:ARG:HH21	1:G:289:GLN:CD	2.24	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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 (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	288/308 (94%)	243 (84%)	29 (10%)	16 (6%)	2 20
1	D	265/308 (86%)	230 (87%)	27 (10%)	8 (3%)	4 32
1	G	306/308 (99%)	255 (83%)	41 (13%)	10 (3%)	4 30
1	H	256/308 (83%)	228 (89%)	19 (7%)	9 (4%)	3 29
1	M	282/308 (92%)	247 (88%)	25 (9%)	10 (4%)	3 29
1	N	277/308 (90%)	236 (85%)	30 (11%)	11 (4%)	3 26
1	S	284/308 (92%)	251 (88%)	28 (10%)	5 (2%)	8 41
1	T	262/308 (85%)	233 (89%)	21 (8%)	8 (3%)	4 31
2	B	94/103 (91%)	78 (83%)	14 (15%)	2 (2%)	7 39

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	E	96/103 (93%)	84 (88%)	12 (12%)	0	100	100
2	I	95/103 (92%)	83 (87%)	11 (12%)	1 (1%)	14	51
2	K	95/103 (92%)	83 (87%)	11 (12%)	1 (1%)	14	51
2	O	92/103 (89%)	75 (82%)	12 (13%)	5 (5%)	2	21
2	Q	89/103 (86%)	79 (89%)	9 (10%)	1 (1%)	14	51
2	U	90/103 (87%)	73 (81%)	15 (17%)	2 (2%)	6	37
2	W	95/103 (92%)	70 (74%)	19 (20%)	6 (6%)	1	18
3	C	118/125 (94%)	100 (85%)	14 (12%)	4 (3%)	3	30
3	F	118/125 (94%)	100 (85%)	14 (12%)	4 (3%)	3	30
3	J	118/125 (94%)	97 (82%)	16 (14%)	5 (4%)	3	25
3	L	118/125 (94%)	95 (80%)	20 (17%)	3 (2%)	5	35
3	P	118/125 (94%)	96 (81%)	15 (13%)	7 (6%)	1	19
3	R	118/125 (94%)	97 (82%)	16 (14%)	5 (4%)	3	25
3	V	118/125 (94%)	100 (85%)	11 (9%)	7 (6%)	1	19
3	X	118/125 (94%)	96 (81%)	14 (12%)	8 (7%)	1	17
All	All	3910/4288 (91%)	3329 (85%)	443 (11%)	138 (4%)	3	29

All (138) Ramachandran outliers are listed below:

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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 (i)

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%)	252 (88%)	33 (12%)	5 24
1	D	261/297 (88%)	240 (92%)	21 (8%)	12 39
1	G	297/297 (100%)	265 (89%)	32 (11%)	6 27
1	H	257/297 (86%)	232 (90%)	25 (10%)	8 30
1	M	279/297 (94%)	259 (93%)	20 (7%)	14 42
1	N	272/297 (92%)	234 (86%)	38 (14%)	3 20
1	S	277/297 (93%)	248 (90%)	29 (10%)	7 27
1	T	261/297 (88%)	222 (85%)	39 (15%)	3 17
2	B	80/86 (93%)	71 (89%)	9 (11%)	6 25
2	E	82/86 (95%)	76 (93%)	6 (7%)	14 42
2	I	81/86 (94%)	73 (90%)	8 (10%)	8 29
2	K	80/86 (93%)	72 (90%)	8 (10%)	7 29
2	O	79/86 (92%)	72 (91%)	7 (9%)	9 34
2	Q	76/86 (88%)	70 (92%)	6 (8%)	12 39
2	U	78/86 (91%)	70 (90%)	8 (10%)	7 28
2	W	80/86 (93%)	70 (88%)	10 (12%)	4 22
3	C	94/100 (94%)	93 (99%)	1 (1%)	73 85
3	F	95/100 (95%)	88 (93%)	7 (7%)	13 41
3	J	93/100 (93%)	91 (98%)	2 (2%)	52 71
3	L	94/100 (94%)	83 (88%)	11 (12%)	5 24
3	P	96/100 (96%)	87 (91%)	9 (9%)	8 31
3	R	95/100 (95%)	92 (97%)	3 (3%)	39 62
3	V	95/100 (95%)	92 (97%)	3 (3%)	39 62
3	X	95/100 (95%)	88 (93%)	7 (7%)	13 41
All	All	3582/3864 (93%)	3240 (90%)	342 (10%)	8 31

All (342) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	LYS

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Mol	Chain	Res	Type
1	A	64	CYS
1	A	98	LYS
1	A	99	LEU
1	A	100	GLU
1	A	113	LYS
1	A	115	MET
1	A	122	LYS
1	A	125	LYS
1	A	128	LYS
1	A	132	ASN
1	A	139	LYS
1	A	159	ASN
1	A	169	ARG
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	230	LYS
1	A	244	ASN
1	A	249	ILE
1	A	250	ILE
1	A	251	GLN
1	A	252	ASP
1	A	262	PHE
1	A	276	ASN
1	A	279	SER
1	A	288	ARG
1	A	300	LYS
1	A	307	HIS
1	A	311	TYR
2	B	16	GLU
2	B	19	ARG
2	B	20	ARG
2	B	21	ARG
2	B	49	PRO
2	B	51	LEU
2	B	52	LEU
2	B	60	THR
2	B	90	ASP
3	C	105	VAL

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Mol	Chain	Res	Type
1	D	20	ASN
1	D	26	GLN
1	D	28	LYS
1	D	39	HIS
1	D	47	LYS
1	D	50	SER
1	D	64	CYS
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	276	ASN
1	D	279	SER
1	D	288	ARG
2	E	35	ASN
2	E	49	PRO
2	E	51	LEU
2	E	52	LEU
2	E	60	THR
2	E	98	ASP
3	F	19	ARG
3	F	27	PHE
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	39	HIS
1	G	50	SER
1	G	64	CYS
1	G	110	ARG
1	G	132	ASN

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Mol	Chain	Res	Type
1	G	140	ILE
1	G	144	MET
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	197	ASN
1	G	213	MET
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	G	307	HIS
1	H	20	ASN
1	H	24	ILE
1	H	25	LEU
1	H	27	GLU
1	H	39	HIS
1	H	50	SER
1	H	57	LYS
1	H	64	CYS
1	H	74	ILE
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	203	GLU

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Mol	Chain	Res	Type
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	19	ARG
2	I	20	ARG
2	I	21	ARG
2	I	35	ASN
2	I	49	PRO
2	I	51	LEU
2	I	52	LEU
2	I	60	THR
3	J	27	PHE
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
3	L	17	SER
3	L	27	PHE
3	L	32	TYR
3	L	56	SER
3	L	76	LYS
3	L	77	LYS
3	L	91	THR
3	L	98	ARG
3	L	117	THR
3	L	119	SER
1	M	40	TYR
1	M	50	SER
1	M	64	CYS
1	M	86	ASN
1	M	132	ASN
1	M	140	ILE

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Mol	Chain	Res	Type
1	M	159	ASN
1	M	171	HIS
1	M	174	GLU
1	M	194	ASP
1	M	197	ASN
1	M	209	LEU
1	M	213	MET
1	M	245	ASP
1	M	250	ILE
1	M	269	LYS
1	M	276	ASN
1	M	279	SER
1	M	307	HIS
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	39	HIS
1	N	50	SER
1	N	64	CYS
1	N	72	LYS
1	N	73	LYS
1	N	84	LYS
1	N	92	LEU
1	N	99	LEU
1	N	105	ILE
1	N	107	ASN
1	N	110	ARG
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	132	ASN
1	N	155	LEU
1	N	159	ASN
1	N	161	ASN

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Mol	Chain	Res	Type
1	N	166	ASN
1	N	171	HIS
1	N	181	LEU
1	N	190	LYS
1	N	197	ASN
1	N	203	GLU
1	N	205	LEU
1	N	225	ILE
1	N	276	ASN
1	N	279	SER
2	O	16	GLU
2	O	20	ARG
2	O	26	CYS
2	O	51	LEU
2	O	52	LEU
2	O	60	THR
2	O	101	ASN
3	P	27	PHE
3	P	29	PHE
3	P	43	LYS
3	P	98	ARG
3	P	99	ASP
3	P	100	ASN
3	P	105	VAL
3	P	108	ASP
3	P	109	VAL
2	Q	20	ARG
2	Q	51	LEU
2	Q	52	LEU
2	Q	60	THR
2	Q	90	ASP
2	Q	99	ARG
3	R	29	PHE
3	R	98	ARG
3	R	100	ASN
1	S	35	VAL
1	S	39	HIS
1	S	50	SER
1	S	64	CYS
1	S	96	ILE
1	S	100	GLU
1	S	101	HIS

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Mol	Chain	Res	Type
1	S	104	ASP
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	158	TYR
1	S	171	HIS
1	S	174	GLU
1	S	179	LEU
1	S	194	ASP
1	S	197	ASN
1	S	209	LEU
1	S	227	LYS
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	24	ILE
1	T	25	LEU
1	T	26	GLN
1	T	39	HIS
1	T	42	PHE
1	T	50	SER
1	T	57	LYS
1	T	64	CYS
1	T	122	LYS
1	T	127	ILE
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

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Mol	Chain	Res	Type
1	T	179	LEU
1	T	190	LYS
1	T	194	ASP
1	T	197	ASN
1	T	199	LEU
1	T	203	GLU
1	T	219	ILE
1	T	220	ASP
1	T	227	LYS
1	T	228	GLU
1	T	229	MET
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	35	ASN
2	U	49	PRO
2	U	51	LEU
2	U	52	LEU
2	U	60	THR
2	U	101	ASN
3	V	98	ARG
3	V	105	VAL
3	V	109	VAL
2	W	12	PRO
2	W	16	GLU
2	W	20	ARG
2	W	26	CYS
2	W	27	SER
2	W	35	ASN
2	W	52	LEU
2	W	60	THR
2	W	86	GLU
2	W	93	CYS
3	X	56	SER
3	X	77	LYS

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Mol	Chain	Res	Type
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 (64) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	GLN
1	A	20	ASN
1	A	26	GLN
1	A	120	ASN
1	A	135	ASN
1	A	257	ASN
1	A	289	GLN
3	C	82	GLN
1	D	7	GLN
1	D	20	ASN
1	D	26	GLN
1	D	56	HIS
1	D	146	ASN
1	D	263	GLN
2	E	35	ASN
3	F	82	GLN
1	G	4	ASN
1	G	106	ASN
1	G	159	ASN
1	G	234	ASN
1	G	257	ASN
1	H	7	GLN
1	H	9	HIS
1	H	56	HIS
1	H	146	ASN
1	H	234	ASN
1	H	257	ASN
2	I	10	GLN
2	I	35	ASN
2	I	36	ASN
2	I	43	GLN
3	J	39	GLN
1	M	26	GLN

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Mol	Chain	Res	Type
1	M	146	ASN
1	M	234	ASN
1	M	257	ASN
1	N	7	GLN
1	N	56	HIS
1	N	146	ASN
1	N	159	ASN
1	N	160	ASN
1	N	177	HIS
1	N	234	ASN
1	N	257	ASN
2	O	32	ASN
3	P	82	GLN
3	P	100	ASN
3	P	112	GLN
3	R	82	GLN
1	S	26	GLN
1	S	56	HIS
1	S	146	ASN
1	S	159	ASN
1	S	234	ASN
1	S	257	ASN
1	S	308	HIS
1	T	52	ASN
1	T	138	ASN
1	T	146	ASN
1	T	234	ASN
1	T	304	ASN
3	V	82	GLN
2	W	10	GLN
3	X	13	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 monosaccharides 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, 95^{th} 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%)	0.56	38 (12%)	3	4	25, 112, 211, 269	0
1	D	273/308 (88%)	0.56	44 (16%)	1	2	32, 133, 218, 269	0
1	G	308/308 (100%)	0.66	48 (15%)	2	2	42, 143, 257, 359	0
1	H	266/308 (86%)	0.57	40 (15%)	2	3	20, 167, 290, 353	0
1	M	288/308 (93%)	0.43	35 (12%)	4	5	19, 108, 205, 282	0
1	N	283/308 (91%)	0.40	31 (10%)	5	5	22, 149, 253, 398	0
1	S	288/308 (93%)	0.39	37 (12%)	3	4	51, 141, 262, 391	0
1	T	270/308 (87%)	0.20	25 (9%)	8	8	36, 135, 255, 338	0
2	B	96/103 (93%)	0.55	12 (12%)	3	5	88, 199, 275, 316	0
2	E	97/103 (94%)	-0.03	1 (1%)	82	74	89, 195, 327, 365	0
2	I	97/103 (94%)	0.75	18 (18%)	1	1	118, 244, 386, 435	0
2	K	97/103 (94%)	1.08	24 (24%)	0	0	103, 248, 405, 484	0
2	O	96/103 (93%)	0.97	20 (20%)	1	1	106, 180, 281, 301	0
2	Q	93/103 (90%)	2.65	45 (48%)	0	0	84, 204, 294, 326	0
2	U	94/103 (91%)	1.75	31 (32%)	0	0	123, 225, 378, 400	0
2	W	97/103 (94%)	1.02	24 (24%)	0	0	131, 232, 436, 496	0
3	C	120/125 (96%)	1.19	25 (20%)	1	1	52, 168, 317, 438	0
3	F	120/125 (96%)	1.69	43 (35%)	0	0	38, 136, 259, 328	0
3	J	120/125 (96%)	0.94	22 (18%)	1	2	41, 176, 295, 361	0
3	L	120/125 (96%)	1.50	33 (27%)	0	0	62, 194, 310, 475	0
3	P	120/125 (96%)	1.58	36 (30%)	0	0	30, 162, 283, 322	0
3	R	120/125 (96%)	1.13	31 (25%)	0	0	68, 163, 328, 366	0
3	V	120/125 (96%)	1.43	28 (23%)	0	0	63, 181, 321, 443	0
3	X	120/125 (96%)	1.52	25 (20%)	1	1	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%)	0.81	716 (17%) 1 2	19, 159, 304, 496	0

All (716) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	X	111	GLY	26.2
2	U	95	ALA	18.9
3	X	110	TRP	18.5
3	C	65	ARG	17.7
3	L	2	VAL	17.3
3	V	120	SER	17.1
3	C	64	VAL	16.9
3	C	63	SER	15.9
3	X	2	VAL	15.6
1	S	20	ASN	15.5
3	X	112	GLN	15.3
3	X	1	GLU	14.6
3	L	1	GLU	14.0
1	S	64	CYS	13.9
3	J	50	ASN	13.5
3	P	18	LEU	12.8
3	C	66	GLY	12.6
1	G	220	ASP	12.5
2	B	36	ASN	11.9
3	V	119	SER	11.5
2	Q	96	TRP	11.3
1	G	219	ILE	11.2
2	Q	101	ASN	11.1
3	F	118	VAL	11.1
3	F	66	GLY	11.0
2	U	94	ALA	10.9
2	U	24	ILE	10.7
3	L	66	GLY	10.6
3	V	99	ASP	10.4
2	K	68	SER	10.2
3	X	3	GLN	10.1
3	J	59	ASP	10.1
3	V	28	THR	9.9
2	Q	95	ALA	9.6
3	P	82	GLN	9.5
3	J	65	ARG	9.4
2	I	100	LEU	9.4

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Mol	Chain	Res	Type	RSRZ
1	A	156	SER	9.4
3	V	57	GLU	9.3
2	K	69	GLY	9.3
2	K	72	SER	9.3
1	S	21	SER	9.1
1	N	137	PHE	9.0
1	M	7	GLN	9.0
1	A	67	VAL	9.0
1	N	65	ILE	8.9
2	Q	36	ASN	8.8
1	N	177	HIS	8.8
3	J	58	LYS	8.8
1	A	58	SER	8.6
2	U	29	SER	8.6
1	H	45	TYR	8.6
3	L	92	ALA	8.5
3	L	84	ASN	8.5
1	A	38	PRO	8.5
1	S	65	ILE	8.4
2	Q	87	ASP	8.3
2	U	102	GLY	8.3
1	M	53	SER	8.3
3	F	120	SER	8.3
1	M	307	HIS	8.2
2	Q	44	LEU	8.2
2	U	25	TYR	8.2
2	I	103	VAL	8.2
3	P	21	SER	8.1
1	H	38	PRO	8.1
1	G	176	ILE	8.1
3	F	62	ASN	8.0
3	L	18	LEU	7.9
3	P	17	SER	7.9
2	W	96	TRP	7.9
3	L	65	ARG	7.8
1	M	52	ASN	7.7
3	P	83	MET	7.7
3	L	41	PRO	7.6
1	S	120	ASN	7.6
2	W	88	GLU	7.5
1	S	63	LYS	7.5
3	F	81	LEU	7.5

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Mol	Chain	Res	Type	RSRZ
1	A	41	THR	7.4
2	Q	103	VAL	7.4
3	C	112	GLN	7.3
3	L	83	MET	7.3
2	W	86	GLU	7.3
3	F	65	ARG	7.3
3	F	88	ALA	7.3
3	V	52	GLN	7.3
3	J	49	ALA	7.3
3	V	107	PHE	7.2
2	Q	42	GLN	7.2
2	O	54	TYR	7.2
2	I	101	ASN	7.1
1	N	77	ALA	7.1
3	R	64	VAL	7.1
3	V	98	ARG	7.1
3	P	114	ALA	7.0
2	O	15	SER	7.0
1	D	139	LYS	6.9
3	L	116	VAL	6.9
3	L	118	VAL	6.9
1	A	68	ASP	6.9
1	A	39	HIS	6.9
2	Q	34	GLY	6.9
2	W	87	ASP	6.8
2	W	74	THR	6.8
3	X	107	PHE	6.8
3	J	112	GLN	6.8
1	H	41	THR	6.8
3	R	28	THR	6.8
1	H	39	HIS	6.8
3	P	101	PRO	6.6
1	H	42	PHE	6.6
1	M	64	CYS	6.6
1	A	42	PHE	6.6
1	N	66	ALA	6.5
2	Q	84	GLN	6.5
1	T	115	MET	6.5
3	F	83	MET	6.5
3	V	117	THR	6.5
1	A	66	ALA	6.5
2	Q	43	GLN	6.5

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Mol	Chain	Res	Type	RSRZ
2	O	55	PHE	6.4
2	K	79	ALA	6.4
3	J	60	TYR	6.4
3	V	54	ASP	6.4
3	V	55	GLY	6.4
3	J	62	ASN	6.4
3	V	106	ALA	6.3
2	W	46	GLY	6.3
3	P	22	CYS	6.3
3	C	62	ASN	6.3
1	T	303	ASN	6.2
3	P	5	VAL	6.2
3	J	51	ILE	6.2
3	R	65	ARG	6.1
3	X	77	LYS	6.1
1	A	37	ILE	6.1
1	T	293	ASN	6.1
3	P	23	ALA	6.1
2	Q	37	ALA	6.1
3	C	67	ARG	6.1
3	J	61	LEU	6.1
3	P	45	LEU	6.1
3	V	56	SER	6.0
3	X	63	SER	6.0
3	J	25	SER	6.0
3	X	21	SER	5.9
1	D	74	ILE	5.9
3	R	120	SER	5.9
2	Q	7	ALA	5.9
3	L	19	ARG	5.9
1	H	155	LEU	5.8
2	Q	52	LEU	5.8
3	F	82	GLN	5.8
1	G	225	ILE	5.8
1	A	59	SER	5.7
2	U	99	ARG	5.7
3	L	42	GLY	5.7
1	M	258	ILE	5.7
2	I	33	ILE	5.7
1	H	46	TYR	5.7
3	F	99	ASP	5.6
2	K	57	ASP	5.6

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Mol	Chain	Res	Type	RSRZ
2	O	56	ASP	5.6
1	H	153	GLU	5.6
2	Q	71	LYS	5.6
2	Q	25	TYR	5.5
2	U	40	TRP	5.5
3	J	47	TRP	5.5
3	J	26	GLY	5.5
2	Q	85	SER	5.5
1	N	72	LYS	5.5
3	F	63	SER	5.5
2	I	96	TRP	5.4
1	D	65	ILE	5.4
3	V	97	ALA	5.4
2	I	87	ASP	5.4
3	R	102	ALA	5.4
3	R	70	ILE	5.3
2	K	11	PRO	5.3
3	F	14	PRO	5.3
1	H	164	ASN	5.3
3	J	48	VAL	5.3
2	W	63	VAL	5.3
3	L	91	THR	5.3
3	P	115	MET	5.3
1	D	138	ASN	5.3
2	Q	51	LEU	5.3
2	W	64	SER	5.3
1	G	63	LYS	5.2
1	S	68	ASP	5.2
1	G	68	ASP	5.2
1	H	40	TYR	5.2
3	J	70	ILE	5.2
3	P	108	ASP	5.1
2	Q	35	ASN	5.1
2	W	48	SER	5.1
3	F	89	GLU	5.1
2	I	7	ALA	5.1
3	V	105	VAL	5.1
1	G	251	GLN	5.0
1	H	265	ASP	5.0
1	N	69	ALA	5.0
1	G	117	ASP	5.0
3	V	29	PHE	5.0

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Mol	Chain	Res	Type	RSRZ
2	Q	24	ILE	5.0
3	R	50	ASN	5.0
2	I	99	ARG	5.0
3	L	119	SER	5.0
3	C	3	GLN	5.0
3	F	119	SER	4.9
3	X	78	SER	4.9
1	D	137	PHE	4.9
3	C	61	LEU	4.9
2	K	17	ALA	4.9
3	X	106	ALA	4.9
2	O	24	ILE	4.9
2	Q	91	TYR	4.9
2	O	49	PRO	4.9
3	R	101	PRO	4.9
2	Q	49	PRO	4.8
3	P	20	LEU	4.8
1	N	170	TYR	4.8
2	K	98	ASP	4.8
2	W	97	ASP	4.8
2	Q	88	GLU	4.8
2	B	101	ASN	4.8
2	B	73	GLY	4.7
3	X	109	VAL	4.7
1	G	69	ALA	4.7
2	K	9	THR	4.7
3	V	11	LEU	4.7
1	S	23	ASP	4.7
3	L	115	MET	4.6
1	N	171	HIS	4.6
1	N	105	ILE	4.6
3	P	19	ARG	4.6
3	R	37	VAL	4.6
2	W	57	ASP	4.5
2	I	36	ASN	4.5
3	P	90	ASP	4.5
2	W	52	LEU	4.5
3	R	57	GLU	4.5
3	R	107	PHE	4.5
3	C	111	GLY	4.4
3	J	57	GLU	4.4
1	N	138	ASN	4.4

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Mol	Chain	Res	Type	RSRZ
3	L	73	ASP	4.4
1	M	164	ASN	4.4
2	W	98	ASP	4.4
2	I	27	SER	4.4
1	G	175	TYR	4.4
1	G	118	GLU	4.4
1	N	76	GLU	4.4
2	U	78	LEU	4.4
3	X	113	GLY	4.3
3	P	69	THR	4.3
1	D	68	ASP	4.3
1	H	272	LEU	4.3
1	A	30	GLY	4.3
2	B	44	LEU	4.3
2	E	58	LEU	4.3
3	F	80	TYR	4.3
1	G	177	HIS	4.3
2	I	95	ALA	4.3
1	S	38	PRO	4.3
1	D	69	ALA	4.2
1	H	37	ILE	4.2
2	U	69	GLY	4.2
1	G	110	ARG	4.2
3	R	61	LEU	4.2
3	V	100	ASN	4.2
1	H	190	LYS	4.2
3	C	8	GLY	4.2
1	G	121	THR	4.2
3	F	91	THR	4.2
3	P	84	ASN	4.2
3	V	118	VAL	4.2
1	D	70	PHE	4.2
1	A	155	LEU	4.2
1	N	68	ASP	4.2
1	H	53	SER	4.1
2	I	23	THR	4.1
1	D	140	ILE	4.1
1	G	170	TYR	4.1
1	M	27	GLU	4.1
2	W	47	LYS	4.1
1	A	60	THR	4.1
2	Q	102	GLY	4.1

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Mol	Chain	Res	Type	RSRZ
2	U	93	CYS	4.1
2	I	32	ASN	4.1
1	S	53	SER	4.1
3	R	118	VAL	4.1
2	Q	83	LEU	4.1
1	N	74	ILE	4.1
1	G	224	PHE	4.1
1	G	48	HIS	4.1
3	L	77	LYS	4.0
3	F	21	SER	4.0
2	B	55	PHE	4.0
2	W	55	PHE	4.0
1	M	65	ILE	4.0
1	S	117	ASP	4.0
2	K	70	SER	4.0
3	V	104	ALA	4.0
3	J	64	VAL	4.0
2	U	23	THR	4.0
1	A	74	ILE	4.0
1	M	303	ASN	4.0
2	Q	53	ILE	4.0
1	M	173	ASP	4.0
3	R	32	TYR	3.9
1	T	68	ASP	3.9
1	D	66	ALA	3.9
2	B	102	GLY	3.9
1	D	168	ILE	3.9
2	I	24	ILE	3.9
2	U	73	GLY	3.9
2	Q	17	ALA	3.9
2	U	35	ASN	3.9
2	O	80	ILE	3.9
1	N	180	ILE	3.8
3	J	28	THR	3.8
2	K	13	SER	3.8
1	A	24	ILE	3.8
1	G	223	LYS	3.8
1	A	65	ILE	3.8
1	A	8	TYR	3.8
3	R	60	TYR	3.8
1	G	90	ASN	3.8
2	U	101	ASN	3.8

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Mol	Chain	Res	Type	RSRZ
1	N	106	ASN	3.8
2	U	103	VAL	3.8
3	P	113	GLY	3.8
3	L	117	THR	3.8
1	S	116	MET	3.8
1	M	137	PHE	3.8
3	F	79	LEU	3.7
3	R	97	ALA	3.7
1	T	13	LEU	3.7
1	N	79	ASP	3.7
2	Q	94	ALA	3.7
3	F	15	GLY	3.7
3	J	66	GLY	3.7
1	M	263	GLN	3.7
1	T	289	GLN	3.7
3	L	3	GLN	3.7
3	R	51	ILE	3.7
3	F	1	GLU	3.7
3	F	69	THR	3.7
3	F	67	ARG	3.7
1	D	77	ALA	3.7
1	T	65	ILE	3.6
1	D	247	THR	3.6
2	U	52	LEU	3.6
3	J	52	GLN	3.6
3	L	114	ALA	3.6
1	A	71	ILE	3.6
1	S	62	GLY	3.6
1	H	224	PHE	3.6
3	F	90	ASP	3.6
1	S	170	TYR	3.6
3	L	60	TYR	3.6
2	Q	45	PRO	3.6
1	D	39	HIS	3.6
1	N	156	SER	3.6
1	S	185	SER	3.6
1	T	302	LEU	3.6
2	Q	90	ASP	3.6
2	Q	16	GLU	3.6
3	F	86	LEU	3.6
2	U	53	ILE	3.5
1	G	126	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
1	T	305	ILE	3.5
2	O	65	ASP	3.5
2	O	18	PRO	3.5
1	M	308	HIS	3.5
3	L	12	VAL	3.5
3	R	96	CYS	3.5
3	C	59	ASP	3.5
1	M	300	LYS	3.4
3	F	32	TYR	3.4
3	P	12	VAL	3.4
3	V	27	PHE	3.4
2	O	20	ARG	3.4
1	G	120	ASN	3.4
1	A	64	CYS	3.4
1	N	71	ILE	3.4
3	R	11	LEU	3.4
2	U	70	SER	3.4
3	P	66	GLY	3.4
3	F	18	LEU	3.4
2	U	81	SER	3.4
2	Q	32	ASN	3.4
3	P	102	ALA	3.4
1	M	54	ILE	3.4
1	S	309	LEU	3.4
3	L	120	SER	3.3
1	A	194	ASP	3.3
1	T	301	HIS	3.3
1	D	142	MET	3.3
1	M	177	HIS	3.3
2	I	12	PRO	3.3
2	U	74	THR	3.3
2	U	39	SER	3.3
1	H	52	ASN	3.3
2	O	90	ASP	3.3
3	R	55	GLY	3.3
3	F	56	SER	3.3
1	G	188	LEU	3.3
2	O	67	PHE	3.3
1	H	154	GLN	3.3
1	D	72	LYS	3.2
1	N	78	TYR	3.2
3	V	58	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
2	K	35	ASN	3.2
1	H	72	LYS	3.2
3	P	116	VAL	3.2
3	C	85	SER	3.2
3	F	19	ARG	3.2
1	H	151	LEU	3.2
2	W	44	LEU	3.2
3	X	65	ARG	3.2
1	D	78	TYR	3.2
3	R	119	SER	3.2
2	B	96	TRP	3.2
2	O	93	CYS	3.2
1	N	259	TRP	3.2
2	O	94	ALA	3.2
1	D	157	CYS	3.2
1	S	22	ILE	3.2
1	M	146	ASN	3.1
1	G	137	PHE	3.1
1	H	168	ILE	3.1
1	D	63	LYS	3.1
1	G	254	ILE	3.1
1	M	259	TRP	3.1
1	A	120	ASN	3.1
2	W	73	GLY	3.1
2	Q	100	LEU	3.1
1	G	70	PHE	3.0
1	D	88	ILE	3.0
1	G	85	CYS	3.0
3	F	87	ARG	3.0
1	N	58	SER	3.0
1	S	70	PHE	3.0
1	A	90	ASN	3.0
2	I	102	GLY	3.0
1	T	300	LYS	3.0
1	G	62	GLY	3.0
1	N	157	CYS	3.0
3	R	59	ASP	3.0
2	B	65	ASP	3.0
1	A	46	TYR	3.0
2	B	81	SER	3.0
2	Q	79	ALA	3.0
1	G	244	ASN	3.0

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Mol	Chain	Res	Type	RSRZ
1	M	11	LYS	3.0
1	M	50	SER	2.9
3	R	34	MET	2.9
1	M	142	MET	2.9
1	N	140	ILE	2.9
2	K	30	SER	2.9
3	R	56	SER	2.9
1	G	168	ILE	2.9
2	U	30	SER	2.9
1	G	67	VAL	2.9
3	R	63	SER	2.9
1	H	24	ILE	2.9
1	H	65	ILE	2.9
2	W	28	GLY	2.9
1	H	34	PHE	2.9
1	T	70	PHE	2.9
2	Q	23	THR	2.9
1	H	35	VAL	2.9
3	C	7	SER	2.9
3	V	4	LEU	2.9
2	Q	78	LEU	2.9
1	M	74	ILE	2.8
3	F	54	ASP	2.8
2	W	59	VAL	2.8
3	F	97	ALA	2.8
1	G	53	SER	2.8
3	F	111	GLY	2.8
1	M	39	HIS	2.8
2	K	73	GLY	2.8
1	G	87	ASP	2.8
1	S	71	ILE	2.8
1	H	76	GLU	2.8
1	S	67	VAL	2.8
3	L	75	ALA	2.8
1	T	18	ILE	2.8
3	C	89	GLU	2.8
2	U	64	SER	2.8
1	A	259	TRP	2.8
1	S	60	THR	2.8
2	O	89	ALA	2.8
3	F	64	VAL	2.8
3	C	1	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
3	J	71	SER	2.7
3	L	68	PHE	2.7
1	H	171	HIS	2.7
3	X	64	VAL	2.7
1	G	146	ASN	2.7
1	G	119	TYR	2.7
2	B	37	ALA	2.7
2	Q	47	LYS	2.7
1	A	40	TYR	2.7
1	M	58	SER	2.7
1	M	148	GLY	2.7
2	Q	73	GLY	2.7
3	L	103	SER	2.7
2	I	26	CYS	2.7
3	X	73	ASP	2.7
2	U	87	ASP	2.6
3	P	109	VAL	2.6
1	S	311	TYR	2.6
1	D	251	GLN	2.6
1	G	253	LYS	2.6
3	P	89	GLU	2.6
1	G	229	MET	2.6
1	H	73	LYS	2.6
3	F	85	SER	2.6
3	R	108	ASP	2.6
1	A	121	THR	2.6
1	H	63	LYS	2.6
1	M	145	LYS	2.6
1	H	27	GLU	2.6
2	K	52	LEU	2.6
3	C	91	THR	2.6
3	C	68	PHE	2.6
1	A	63	LYS	2.6
3	P	7	SER	2.6
1	S	251	GLN	2.6
3	P	39	GLN	2.6
1	S	69	ALA	2.6
1	A	133	HIS	2.6
3	P	95	TYR	2.6
2	U	82	GLY	2.6
3	R	100	ASN	2.6
1	H	11	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	T	54	ILE	2.6
3	P	16	GLY	2.6
2	Q	64	SER	2.6
1	A	144	MET	2.5
1	G	142	MET	2.5
1	N	75	ASN	2.5
3	X	29	PHE	2.5
1	D	199	LEU	2.5
3	F	117	THR	2.5
2	U	43	GLN	2.5
3	J	99	ASP	2.5
1	D	121	THR	2.5
1	G	116	MET	2.5
1	M	95	THR	2.5
2	U	34	GLY	2.5
2	W	89	ALA	2.5
2	U	77	SER	2.5
2	K	71	LYS	2.5
3	X	22	CYS	2.5
1	T	114	LYS	2.5
1	H	50	SER	2.5
3	R	110	TRP	2.5
3	P	100	ASN	2.4
3	X	19	ARG	2.4
1	D	34	PHE	2.4
2	B	64	SER	2.4
2	Q	80	ILE	2.4
1	D	146	ASN	2.4
3	C	118	VAL	2.4
1	H	222	ILE	2.4
1	D	164	ASN	2.4
2	K	12	PRO	2.4
3	F	20	LEU	2.4
1	D	166	ASN	2.4
1	S	176	ILE	2.4
3	X	14	PRO	2.4
1	T	53	SER	2.4
2	W	95	ALA	2.4
3	L	85	SER	2.4
1	G	19	ALA	2.4
3	L	9	GLY	2.4
1	G	247	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	N	67	VAL	2.4
1	S	252	ASP	2.4
2	K	67	PHE	2.4
3	P	86	LEU	2.4
3	V	35	SER	2.4
1	A	54	ILE	2.3
1	S	72	LYS	2.4
1	T	146	ASN	2.3
1	A	153	GLU	2.3
1	N	63	LYS	2.3
1	G	278	TYR	2.3
2	W	67	PHE	2.3
3	P	107	PHE	2.3
2	O	51	LEU	2.3
1	S	248	LYS	2.3
3	F	98	ARG	2.3
1	S	181	LEU	2.3
2	Q	81	SER	2.3
1	D	201	GLN	2.3
1	D	75	ASN	2.3
1	D	274	MET	2.3
1	S	124	LYS	2.3
3	L	10	GLY	2.3
1	G	287	LEU	2.3
1	T	304	ASN	2.3
1	D	53	SER	2.3
2	O	95	ALA	2.3
3	P	68	PHE	2.3
1	N	175	TYR	2.3
1	S	249	ILE	2.3
1	D	244	ASN	2.3
2	K	53	ILE	2.3
1	S	50	SER	2.3
2	U	31	SER	2.3
3	L	86	LEU	2.3
3	L	94	TYR	2.3
3	X	60	TYR	2.3
1	M	260	ARG	2.3
2	Q	66	ARG	2.3
3	P	92	ALA	2.3
1	G	99	LEU	2.3
3	F	116	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
2	Q	40	TRP	2.3
1	H	51	TYR	2.3
2	B	54	TYR	2.3
1	A	148	GLY	2.3
1	M	169	ARG	2.3
3	X	4	LEU	2.3
2	O	43	GLN	2.2
1	D	254	ILE	2.2
3	V	53	GLN	2.2
1	M	38	PRO	2.2
1	D	262	PHE	2.2
1	N	70	PHE	2.2
1	G	307	HIS	2.2
1	D	120	ASN	2.2
1	T	150	ASN	2.2
1	A	142	MET	2.2
3	X	18	LEU	2.2
1	D	175	TYR	2.2
1	D	171	HIS	2.2
3	C	48	VAL	2.2
3	F	13	GLN	2.2
3	F	36	TRP	2.2
3	R	54	ASP	2.2
1	G	97	LYS	2.2
1	T	173	ASP	2.2
2	O	92	TYR	2.2
1	T	50	SER	2.2
1	H	26	GLN	2.2
1	D	257	ASN	2.2
2	O	32	ASN	2.2
1	H	93	ILE	2.2
1	M	309	LEU	2.2
2	K	25	TYR	2.2
1	A	159	ASN	2.2
3	F	3	GLN	2.2
1	T	74	ILE	2.2
3	V	101	PRO	2.2
3	C	54	ASP	2.2
1	D	258	ILE	2.2
1	M	57	LYS	2.2
1	D	50	SER	2.2
3	V	113	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	50	SER	2.1
1	D	272	LEU	2.1
1	D	44	ASP	2.1
1	T	164	ASN	2.1
2	W	62	GLY	2.1
3	X	8	GLY	2.1
1	S	74	ILE	2.1
3	C	51	ILE	2.1
3	R	29	PHE	2.1
1	H	187	ASN	2.1
2	K	15	SER	2.1
3	P	9	GLY	2.1
1	H	66	ALA	2.1
3	F	55	GLY	2.1
3	F	71	SER	2.1
2	K	59	VAL	2.1
2	Q	67	PHE	2.1
2	K	29	SER	2.1
1	M	197	ASN	2.1
3	P	8	GLY	2.1
3	V	26	GLY	2.1
2	W	58	LEU	2.1
3	C	60	TYR	2.1
1	N	57	LYS	2.1
1	S	227	LYS	2.1
1	M	144	MET	2.1
1	A	22	ILE	2.1
1	H	68	ASP	2.1
1	N	36	ILE	2.1
3	C	77	LYS	2.1
1	T	151	LEU	2.1
2	Q	50	LYS	2.1
2	K	58	LEU	2.1
1	H	25	LEU	2.1
1	A	132	ASN	2.1
2	I	37	ALA	2.1
1	D	122	LYS	2.1
1	G	72	LYS	2.1
1	S	66	ALA	2.1
1	D	71	ILE	2.1
3	L	74	ASN	2.1
1	T	38	PRO	2.0

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Mol	Chain	Res	Type	RSRZ
1	S	194	ASP	2.0
1	S	61	TYR	2.0
2	U	96	TRP	2.0
1	G	190	LYS	2.0
3	R	99	ASP	2.0
1	G	272	LEU	2.0
3	C	2	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 monosaccharides 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.