



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 09:36 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 wwPDB X-ray Structure Validation Summary 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

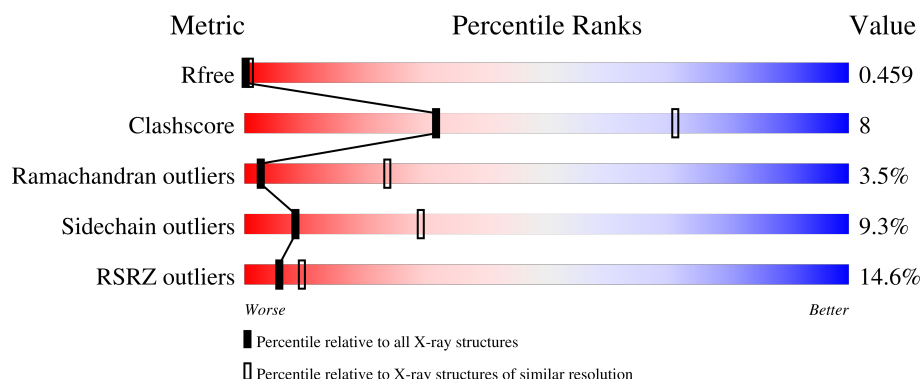
1 Overall quality at a glance

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%

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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			

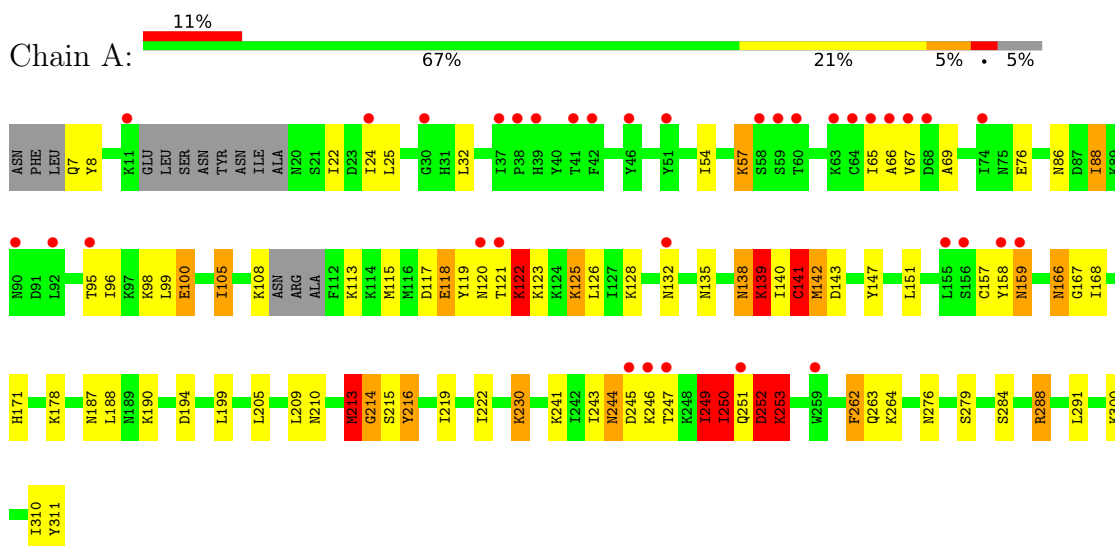
- Molecule 3 is a protein called R5034HV.

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			

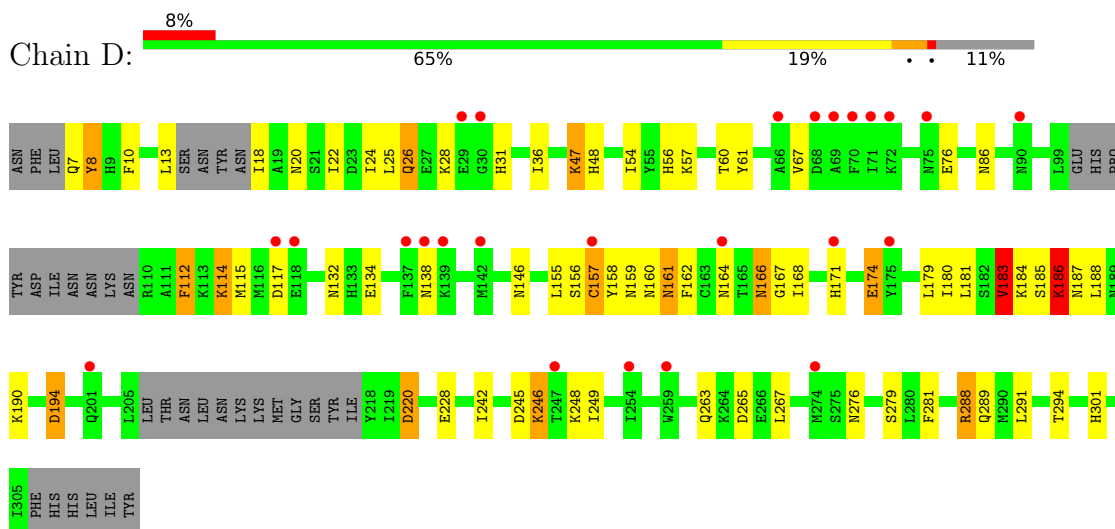
3 Residue-property plots [i](#)

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.

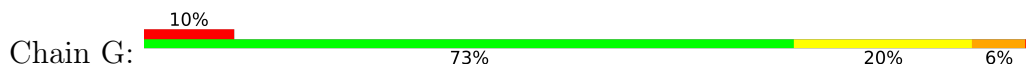
- Molecule 1: Reticulocyte-binding protein-like protein 5

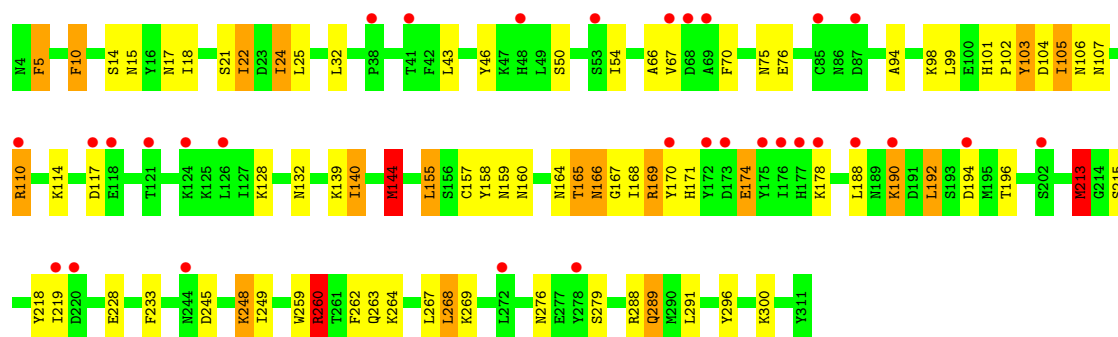


- Molecule 1: Reticulocyte-binding protein-like protein 5

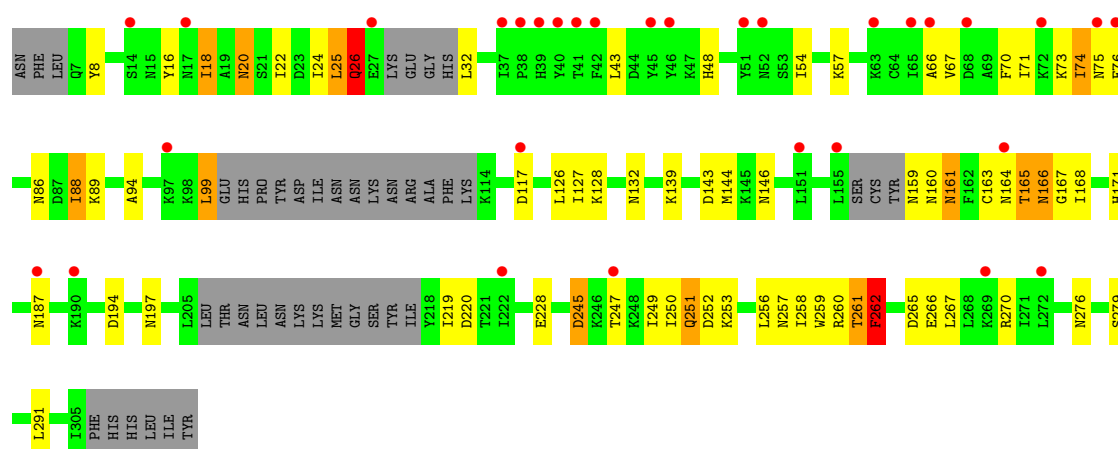


- Molecule 1: Reticulocyte-binding protein-like protein 5

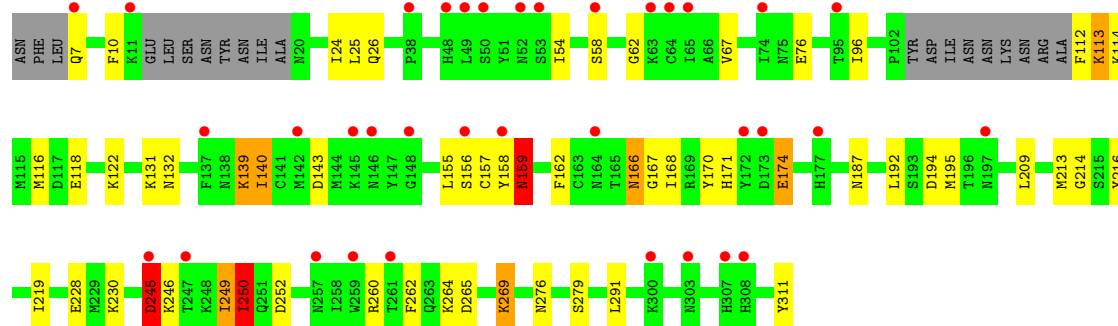
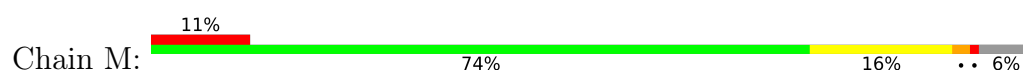




• Molecule 1: Reticulocyte-binding protein-like protein 5

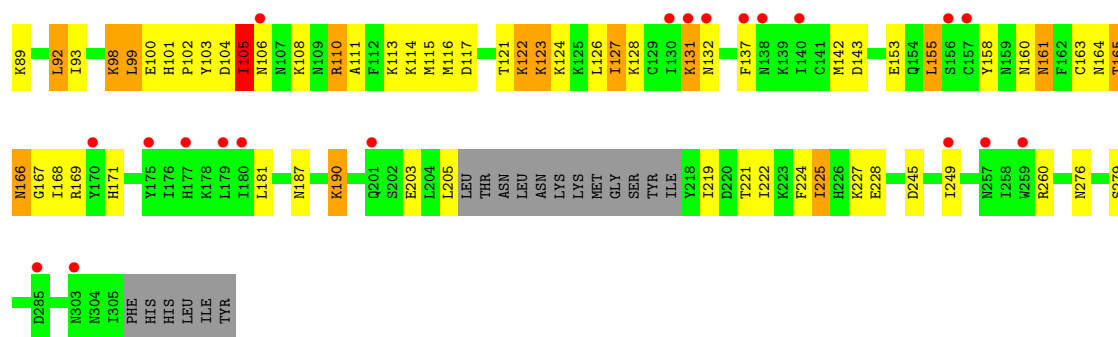


• Molecule 1: Reticulocyte-binding protein-like protein 5

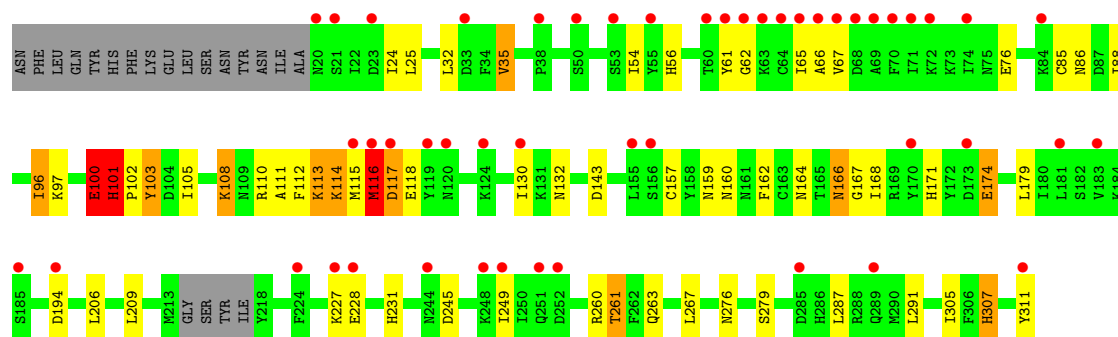


• Molecule 1: Reticulocyte-binding protein-like protein 5

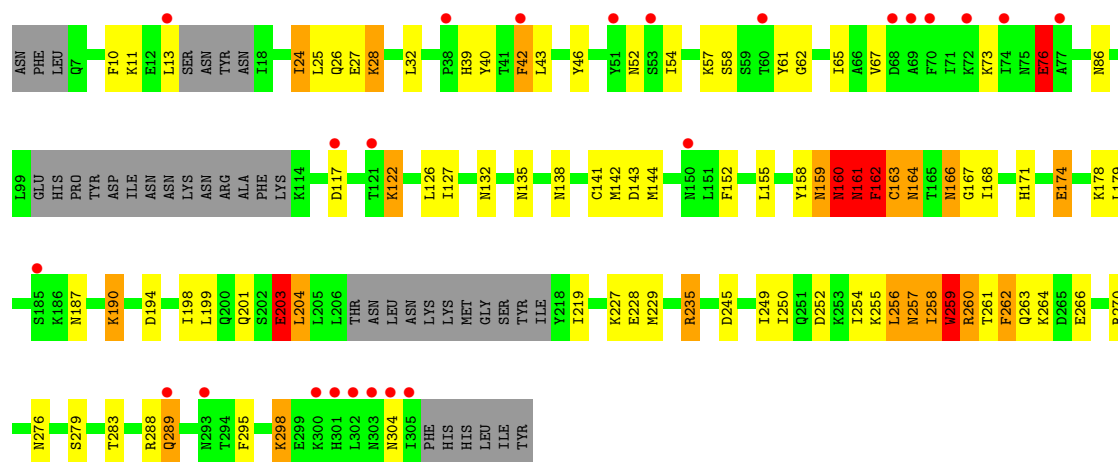




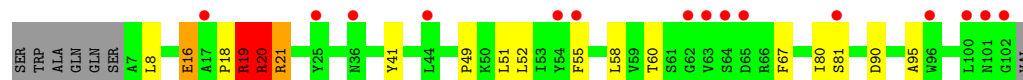
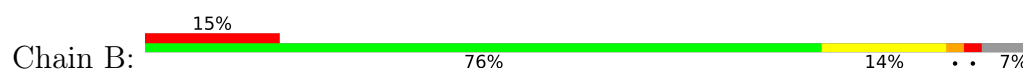
• Molecule 1: Reticulocyte-binding protein-like protein 5



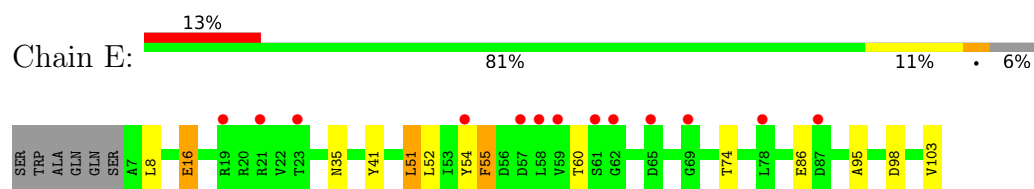
• Molecule 1: Reticulocyte-binding protein-like protein 5



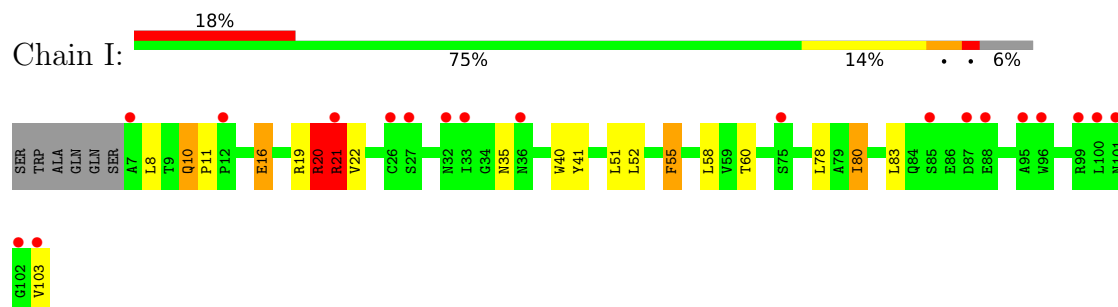
• Molecule 2: Immunoglobulin lambda variable 1-36



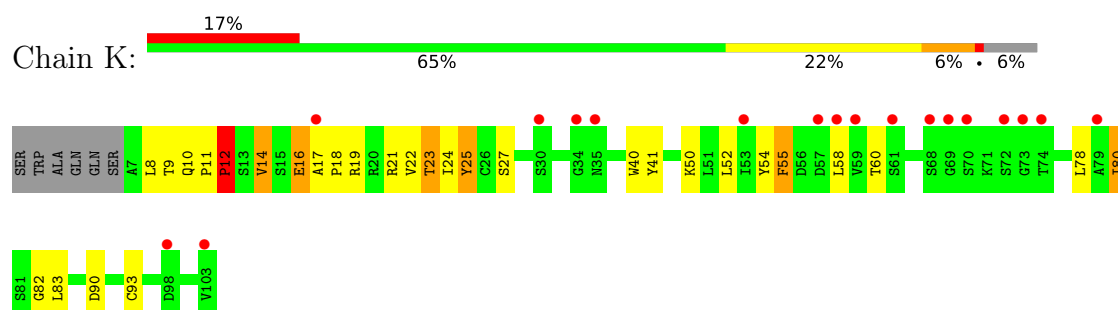
- Molecule 2: Immunoglobulin lambda variable 1-36



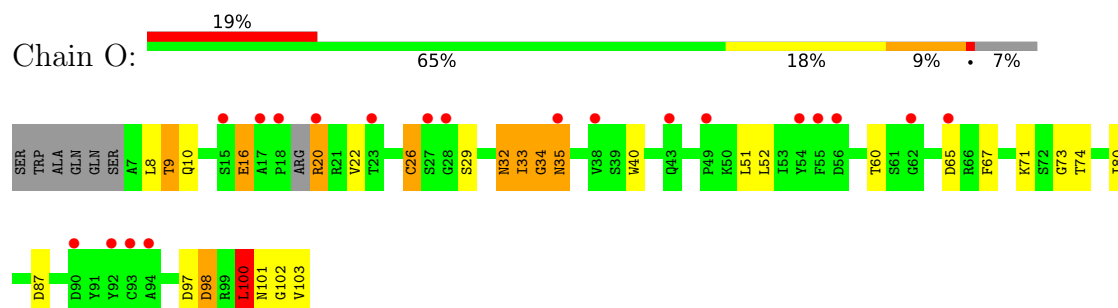
- Molecule 2: Immunoglobulin lambda variable 1-36



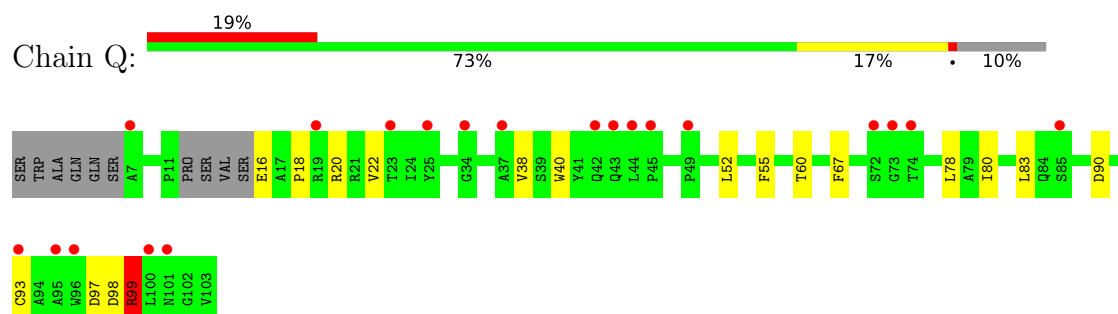
- Molecule 2: Immunoglobulin lambda variable 1-36



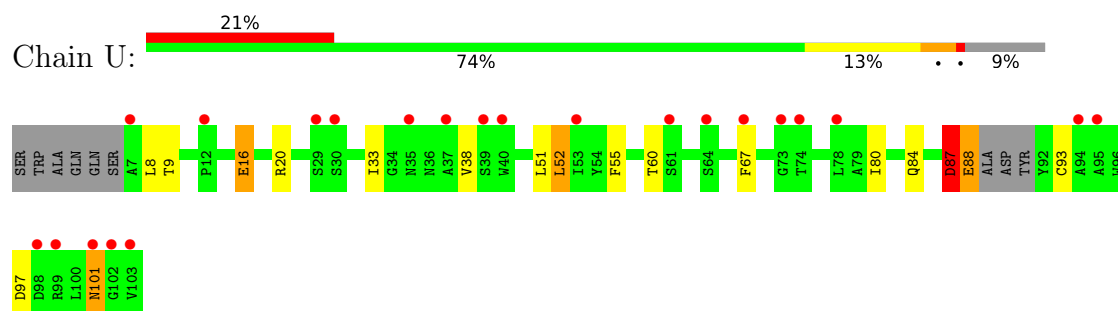
- Molecule 2: Immunoglobulin lambda variable 1-36



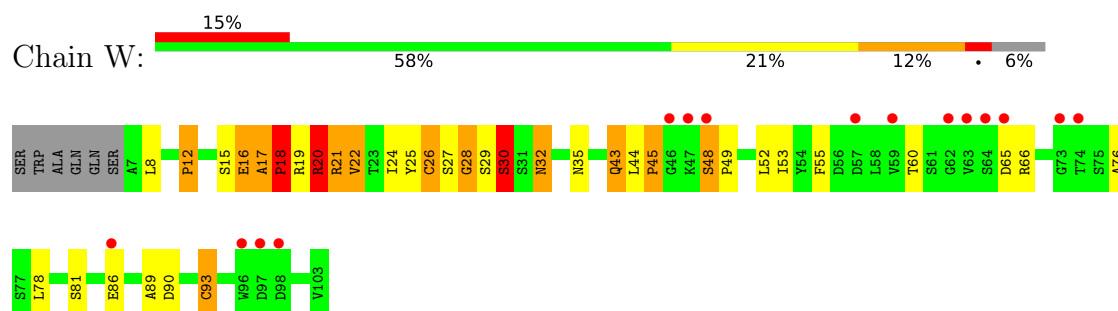
- Molecule 2: Immunoglobulin lambda variable 1-36



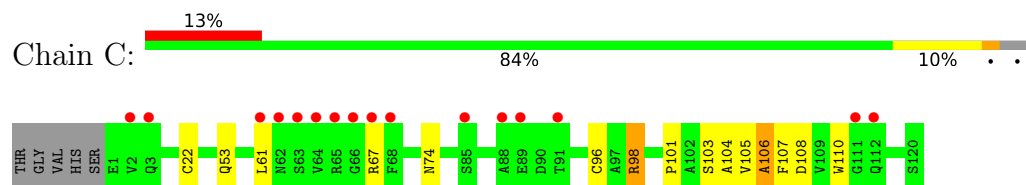
- Molecule 2: Immunoglobulin lambda variable 1-36



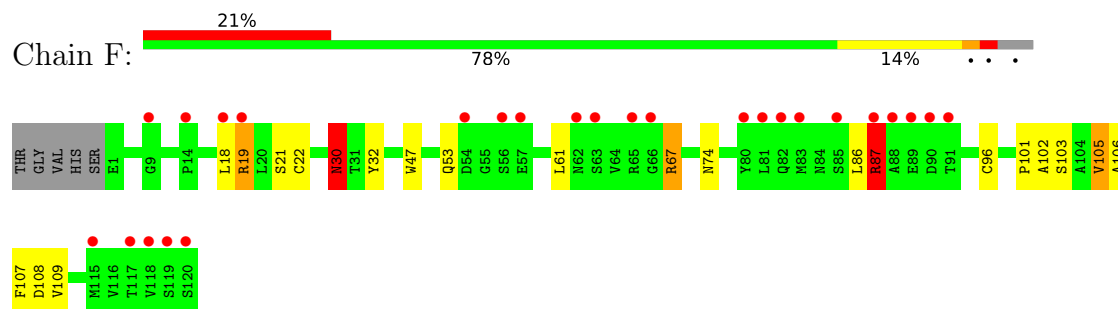
- Molecule 2: Immunoglobulin lambda variable 1-36



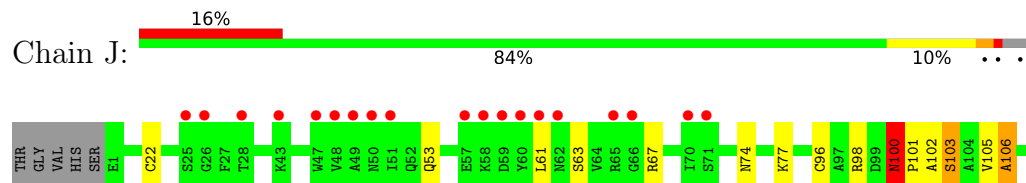
- Molecule 3: R5034HV



- 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

Continued on next page...

Continued from previous page...

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

The worst 5 of 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

There are no chirality outliers.

5 of 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

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
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.

The worst 5 of 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

Continued on next page...

Continued from previous page...

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

The worst 5 of 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

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%)	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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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

5 of 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

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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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

5 of 333 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	P	100	ASN
1	T	164	ASN
2	Q	99	ARG
1	S	209	LEU
1	T	262	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 90 such sidechains are listed below:

Mol	Chain	Res	Type
1	N	201	GLN
1	S	177	HIS
2	O	32	ASN
3	R	82	GLN
1	S	234	ASN

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

Continued on next page...

Continued from previous page...

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%)

The worst 5 of 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

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.