



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 26, 2026 – 05:17 AM EDT

PDB ID : 4U0R / pdb_00004u0r
Title : Plasmodium falciparum reticulocyte-binding protein homologue 5 (PfRH5)
bound to monoclonal antibody 9AD4
Authors : Wright, K.E.; Hjerrild, K.A.; Bartlett, J.; Douglas, A.D.; Jin, J.; Brown, R.E.;
Ashfield, R.; Clemmensen, S.B.; de Jongh, W.A.; Draper, S.J.; Higgins, M.K.
Deposited on : 2014-07-14
Resolution : 2.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

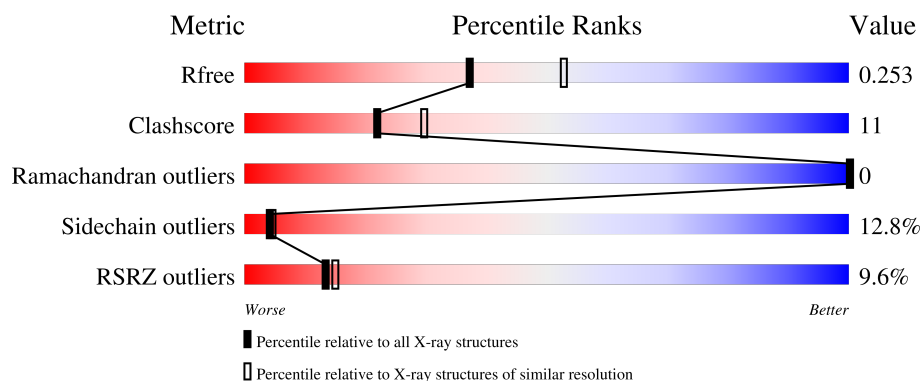
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	526	8% 40% 13% • 45%
2	B	258	6% 64% 16% • • 14%
3	C	238	5% 68% 20% • 9%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6005 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 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	288	Total	C	N	O	S	0	0	0
			2450	1584	410	441	15			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	216	ALA	THR	conflict	UNP B2L3N7

- Molecule 2 is a protein called Monoclonal antibody 9AD4 heavy chain.

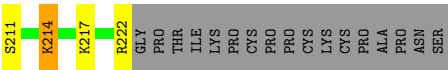
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	221	Total	C	N	O	S	0	0	0
			1668	1060	272	327	9			

- Molecule 3 is a protein called Monoclonal antibody 9AD4 light chain.

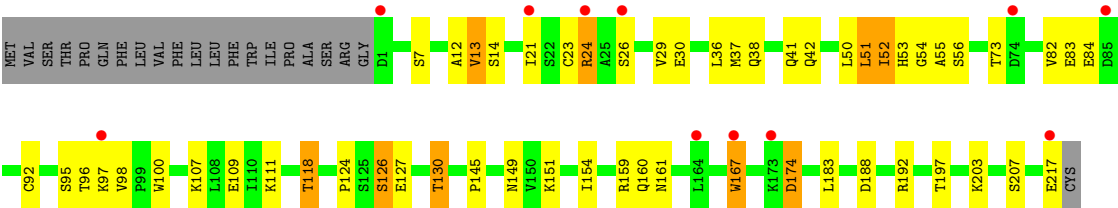
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	217	Total	C	N	O	S	0	0	0
			1677	1046	286	338	7			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	45	Total	O	0	0
			45	45		
4	B	100	Total	O	0	0
			100	100		
4	C	65	Total	O	0	0
			65	65		



• Molecule 3: Monoclonal antibody 9AD4 light chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	39.79Å 86.66Å 324.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.83 – 2.30 40.83 – 2.30	Depositor EDS
% Data completeness (in resolution range)	96.1 (40.83-2.30) 96.1 (40.83-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.75 (at 2.29Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.221 , 0.258 0.236 , 0.253	Depositor DCC
R_{free} test set	2462 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	41.1	Xtriage
Anisotropy	0.603	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 50.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6005	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.70% 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	0.88	0/2502	1.52	15/3354 (0.4%)
2	B	0.84	0/1714	1.30	14/2343 (0.6%)
3	C	0.97	3/1717 (0.2%)	1.20	11/2332 (0.5%)
All	All	0.89	3/5933 (0.1%)	1.37	40/8029 (0.5%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	50	LEU	C-N	-14.78	1.16	1.33
3	C	51	LEU	C-N	-12.03	1.16	1.33
3	C	52	ILE	CG1-CD1	-5.18	1.31	1.51

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	503	MET	N-CA-C	10.18	124.33	112.93
3	C	51	LEU	O-C-N	-8.78	111.66	121.76
1	A	501	LEU	N-CA-CB	-8.64	98.51	110.95
2	B	84	SER	N-CA-C	8.37	124.31	113.18
3	C	50	LEU	CA-C-N	7.94	131.89	122.44
3	C	50	LEU	C-N-CA	7.94	131.89	122.44
3	C	145	PRO	CA-C-N	7.23	130.28	120.38
3	C	145	PRO	C-N-CA	7.23	130.28	120.38
3	C	118	THR	CB-CA-C	7.16	122.24	110.78
2	B	68	PHE	CA-CB-CG	6.83	120.63	113.80
1	A	503	MET	N-CA-CB	-6.62	101.43	110.56
1	A	446	ILE	N-CA-C	6.41	122.68	109.34
1	A	502	GLN	N-CA-C	6.40	124.44	110.80
3	C	174	ASP	CA-CB-CG	6.28	118.88	112.60
2	B	193	THR	CB-CA-C	6.22	119.61	109.90
1	A	364	ILE	N-CA-C	6.18	116.91	111.90
2	B	48	VAL	N-CA-C	6.17	116.90	111.90
2	B	191	THR	CB-CA-C	6.09	120.27	110.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	33	GLY	N-CA-C	-6.07	104.31	112.14
2	B	146	THR	CB-CA-C	5.96	120.61	109.71
2	B	65	THR	CB-CA-C	5.67	118.35	109.84
1	A	207	ASP	CA-CB-CG	5.62	118.22	112.60
3	C	126	SER	CA-C-N	5.48	127.57	120.44
3	C	126	SER	C-N-CA	5.48	127.57	120.44
3	C	51	LEU	CA-C-N	5.41	130.46	122.94
3	C	51	LEU	C-N-CA	5.41	130.46	122.94
1	A	176	ILE	N-CA-CB	5.40	114.14	110.52
2	B	64	VAL	CB-CA-C	5.34	115.65	110.63
1	A	403	SER	CA-C-N	5.29	127.63	120.38
1	A	403	SER	C-N-CA	5.29	127.63	120.38
2	B	193	THR	CA-C-N	5.28	128.74	120.82
2	B	193	THR	C-N-CA	5.28	128.74	120.82
2	B	93	MET	N-CA-C	-5.21	100.67	108.96
1	A	365	HIS	N-CA-C	5.21	117.36	111.11
1	A	303	MET	CA-C-N	5.07	127.49	120.29
1	A	303	MET	C-N-CA	5.07	127.49	120.29
1	A	451	GLN	N-CA-C	-5.05	102.80	110.28
2	B	52	SER	CA-C-N	5.03	128.36	120.82
2	B	52	SER	C-N-CA	5.03	128.36	120.82
1	A	500	VAL	CB-CA-C	5.01	120.32	112.16

There are no chirality outliers.

There are no planarity outliers.

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	2450	0	2481	62	0
2	B	1668	0	1612	35	0
3	C	1677	0	1605	26	0
4	A	45	0	0	15	0
4	B	100	0	0	14	0
4	C	65	0	0	5	0
All	All	6005	0	5698	119	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (119) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:LEU:CD2	1:A:300:PHE:HE2	1.45	1.29
1:A:238:LEU:CD2	1:A:300:PHE:CE2	2.17	1.27
1:A:496:HIS:O	1:A:501:LEU:HD13	1.32	1.23
2:B:21:SER:HB2	4:B:309:HOH:O	1.35	1.22
1:A:501:LEU:HD12	1:A:501:LEU:N	1.59	1.16
1:A:496:HIS:O	1:A:501:LEU:CD1	1.95	1.14
1:A:238:LEU:HD21	1:A:300:PHE:CE2	1.79	1.13
1:A:500:VAL:C	1:A:501:LEU:HD12	1.75	1.11
1:A:238:LEU:HD23	1:A:300:PHE:HE2	1.15	1.10
1:A:300:PHE:CE2	1:A:409:THR:HG22	1.87	1.09
3:C:217:GLU:HG2	4:C:352:HOH:O	1.62	0.98
2:B:97:THR:HG21	2:B:109:PHE:HB3	1.45	0.98
1:A:501:LEU:N	1:A:501:LEU:CD1	2.30	0.91
3:C:23:CYS:HG	3:C:92:CYS:HG	1.15	0.89
1:A:451:GLN:HE22	1:A:453:ASP:HB3	1.44	0.83
1:A:478:MET:O	1:A:482:THR:HG23	1.78	0.82
1:A:238:LEU:HD23	1:A:300:PHE:CE2	2.02	0.82
3:C:188:ASP:OD2	3:C:192:ARG:NH1	2.12	0.81
2:B:128:PRO:HB3	2:B:154:TYR:HB3	1.66	0.77
2:B:39:GLN:HE22	3:C:42:GLN:HE22	1.33	0.76
1:A:500:VAL:CA	1:A:501:LEU:HD12	2.17	0.75
1:A:476:ARG:NH2	4:A:623:HOH:O	1.86	0.75
1:A:503:MET:O	1:A:504:LYS:C	2.30	0.74
2:B:97:THR:CG2	2:B:109:PHE:HB3	2.17	0.73
1:A:345:CYS:HG	1:A:351:CYS:HG	0.73	0.72
3:C:154:ILE:HD11	3:C:183:LEU:HD21	1.72	0.71
1:A:366:LYS:HE3	4:A:636:HOH:O	1.91	0.70
1:A:164:LEU:HD22	1:A:478:MET:HB3	1.74	0.70
1:A:238:LEU:HD21	1:A:300:PHE:CZ	2.26	0.69
2:B:13:GLN:NE2	4:B:301:HOH:O	2.26	0.68
2:B:65:THR:HG21	4:B:397:HOH:O	1.92	0.68
2:B:64:VAL:HG13	2:B:68:PHE:HB2	1.80	0.63
2:B:156:PRO:O	2:B:208:HIS:HE1	1.82	0.62
2:B:7:SER:HB2	4:B:309:HOH:O	1.99	0.61
1:A:381:SER:HB3	4:A:640:HOH:O	2.00	0.61
2:B:193:THR:HG23	4:B:315:HOH:O	2.00	0.61
2:B:222:ARG:NH2	3:C:124:PRO:O	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:PHE:CD2	1:A:409:THR:HG22	2.36	0.60
1:A:500:VAL:C	1:A:501:LEU:CD1	2.66	0.60
2:B:72:ARG:HD3	2:B:74:ASN:OD1	2.02	0.60
2:B:124:LYS:HD3	4:B:301:HOH:O	2.02	0.60
1:A:238:LEU:CD2	1:A:300:PHE:CZ	2.82	0.59
1:A:300:PHE:HE1	1:A:412:PHE:HB2	1.66	0.59
2:B:145:VAL:HG22	2:B:194:SER:HA	1.84	0.59
1:A:498:ILE:O	1:A:502:GLN:HA	2.02	0.59
3:C:54:GLY:O	3:C:55:ALA:HB3	2.02	0.59
2:B:39:GLN:NE2	3:C:42:GLN:HE22	1.99	0.59
1:A:487:GLU:CG	4:A:603:HOH:O	2.51	0.58
1:A:501:LEU:HD12	1:A:501:LEU:H	1.63	0.58
1:A:211:LYS:HD3	4:A:643:HOH:O	2.03	0.58
1:A:427:HIS:ND1	1:A:472:SER:HB2	2.19	0.57
1:A:491:ASN:O	4:A:601:HOH:O	2.17	0.57
1:A:366:LYS:HG3	4:A:636:HOH:O	2.05	0.57
1:A:429:LYS:HG3	4:A:639:HOH:O	2.06	0.56
3:C:83:GLU:OE2	4:C:360:HOH:O	2.18	0.56
3:C:36:LEU:HD12	3:C:96:THR:HA	1.89	0.55
1:A:341:GLU:HG2	2:B:53:ASN:HB2	1.89	0.54
3:C:26:SER:HB3	4:C:326:HOH:O	2.08	0.54
3:C:217:GLU:CG	4:C:352:HOH:O	2.35	0.54
2:B:124:LYS:CE	4:B:301:HOH:O	2.57	0.53
1:A:393:LEU:O	1:A:397:LEU:HB2	2.08	0.53
3:C:127:GLU:HB2	4:C:321:HOH:O	2.09	0.53
1:A:501:LEU:C	1:A:502:GLN:NE2	2.66	0.53
1:A:186:LYS:HG3	1:A:210:ILE:HD13	1.91	0.53
3:C:41:GLN:HB2	3:C:51:LEU:HD11	1.91	0.53
1:A:300:PHE:CE2	1:A:409:THR:CG2	2.78	0.52
2:B:207:ALA:HB2	2:B:214:LYS:HD3	1.90	0.52
1:A:361:ASP:O	4:A:636:HOH:O	2.19	0.52
1:A:300:PHE:CE1	1:A:412:PHE:HB2	2.45	0.51
2:B:191:THR:HG23	4:B:347:HOH:O	2.10	0.51
2:B:62:ASP:CB	4:B:397:HOH:O	2.59	0.50
2:B:208:HIS:HD2	2:B:211:SER:OG	1.95	0.49
2:B:62:ASP:HB3	4:B:397:HOH:O	2.11	0.49
1:A:419:HIS:HB3	1:A:423:ARG:NH2	2.27	0.49
1:A:381:SER:CB	4:A:640:HOH:O	2.60	0.49
3:C:154:ILE:HD12	3:C:159:ARG:HG3	1.95	0.49
1:A:362:GLU:O	1:A:362:GLU:HG3	2.11	0.49
1:A:186:LYS:CE	4:A:638:HOH:O	2.62	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:38:GLN:OE1	3:C:53:HIS:O	2.32	0.48
3:C:95:SER:HA	3:C:100:TRP:CD1	2.49	0.48
3:C:54:GLY:C	3:C:56:SER:H	2.22	0.48
1:A:500:VAL:CB	1:A:501:LEU:HD12	2.43	0.48
1:A:504:LYS:HB2	1:A:504:LYS:HE3	1.75	0.46
1:A:300:PHE:CD2	1:A:409:THR:CG2	2.97	0.46
1:A:304:MET:HE3	1:A:308:ASN:HD21	1.81	0.46
3:C:126:SER:O	3:C:130:THR:HG23	2.16	0.46
1:A:186:LYS:NZ	4:A:638:HOH:O	2.25	0.45
1:A:345:CYS:HG	1:A:351:CYS:CB	2.25	0.45
2:B:62:ASP:HA	4:B:397:HOH:O	2.16	0.45
1:A:501:LEU:CD1	1:A:501:LEU:H	2.23	0.45
3:C:167:TRP:CD1	3:C:167:TRP:N	2.84	0.45
2:B:12:VAL:CG2	2:B:18:ARG:HG3	2.47	0.44
1:A:419:HIS:HB2	4:A:628:HOH:O	2.18	0.44
2:B:124:LYS:HE2	4:B:301:HOH:O	2.17	0.44
1:A:477:GLN:HG2	4:A:611:HOH:O	2.18	0.44
3:C:149:ASN:HD21	3:C:151:LYS:HE3	1.83	0.44
2:B:65:THR:CG2	4:B:397:HOH:O	2.56	0.44
2:B:191:THR:CG2	4:B:347:HOH:O	2.66	0.43
1:A:500:VAL:HB	1:A:501:LEU:CD1	2.48	0.43
2:B:83:MET:HB3	2:B:86:LEU:HD21	2.00	0.43
2:B:146:THR:HB	2:B:191:THR:HG22	2.01	0.43
2:B:32:TYR:O	2:B:72:ARG:NH2	2.49	0.43
2:B:128:PRO:CB	2:B:154:TYR:HB3	2.43	0.43
1:A:497:LEU:O	1:A:503:MET:HG3	2.19	0.42
1:A:195:HIS:CB	1:A:343:LEU:HD11	2.49	0.42
1:A:419:HIS:HB3	1:A:423:ARG:HH22	1.83	0.42
3:C:24:ARG:HA	3:C:73:THR:O	2.20	0.42
2:B:180:GLN:O	2:B:180:GLN:HG2	2.19	0.42
2:B:146:THR:HB	2:B:191:THR:HB	2.02	0.42
1:A:415:LYS:HE3	1:A:415:LYS:HB3	1.39	0.41
3:C:12:ALA:HB1	3:C:111:LYS:HG3	2.03	0.41
1:A:419:HIS:CB	4:A:628:HOH:O	2.68	0.41
3:C:13:VAL:HG11	3:C:82:VAL:HG21	2.03	0.41
1:A:451:GLN:NE2	1:A:453:ASP:HB3	2.25	0.41
2:B:19:LYS:HG3	2:B:82:GLU:HG2	2.03	0.41
3:C:29:VAL:HG21	3:C:37:MET:HE2	2.01	0.41
3:C:188:ASP:CG	3:C:192:ARG:HH12	2.15	0.41
1:A:240:HIS:HE2	1:A:489:HIS:HE2	1.69	0.41
1:A:300:PHE:CE1	1:A:412:PHE:CB	3.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	284/526 (54%)	274 (96%)	10 (4%)	0	100	100
2	B	219/258 (85%)	212 (97%)	7 (3%)	0	100	100
3	C	215/238 (90%)	208 (97%)	7 (3%)	0	100	100
All	All	718/1022 (70%)	694 (97%)	24 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	279/511 (55%)	244 (88%)	35 (12%)	4	5
2	B	185/216 (86%)	157 (85%)	28 (15%)	3	3
3	C	190/209 (91%)	169 (89%)	21 (11%)	6	7
All	All	654/936 (70%)	570 (87%)	84 (13%)	4	4

All (84) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	164	LEU
1	A	165	GLN

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Mol	Chain	Res	Type
1	A	188	LEU
1	A	213	ILE
1	A	221	LYS
1	A	222	SER
1	A	224	CYS
1	A	226	ASP
1	A	230	ASP
1	A	238	LEU
1	A	301	LYS
1	A	314	LEU
1	A	316	LYS
1	A	322	GLU
1	A	327	LYS
1	A	330	MET
1	A	347	ASN
1	A	368	ILE
1	A	390	SER
1	A	392	LEU
1	A	394	LEU
1	A	397	LEU
1	A	415	LYS
1	A	416	GLU
1	A	418	LYS
1	A	436	LYS
1	A	455	LEU
1	A	458	ARG
1	A	465	GLU
1	A	475	LEU
1	A	482	THR
1	A	487	GLU
1	A	501	LEU
1	A	502	GLN
1	A	504	LYS
2	B	4	LEU
2	B	18	ARG
2	B	20	LEU
2	B	64	VAL
2	B	65	THR
2	B	82	GLU
2	B	84	SER
2	B	97	THR
2	B	98	ARG

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Mol	Chain	Res	Type
2	B	125	THR
2	B	126	THR
2	B	145	VAL
2	B	146	THR
2	B	152	LYS
2	B	159	VAL
2	B	161	LEU
2	B	168	LEU
2	B	180	GLN
2	B	183	LEU
2	B	186	LEU
2	B	187	SER
2	B	191	THR
2	B	193	THR
2	B	194	SER
2	B	201	SER
2	B	205	ASN
2	B	214	LYS
2	B	217	LYS
3	C	7	SER
3	C	13	VAL
3	C	14	SER
3	C	21	ILE
3	C	24	ARG
3	C	30	GLU
3	C	52	ILE
3	C	84	GLU
3	C	97	LYS
3	C	98	VAL
3	C	107	LYS
3	C	109	GLU
3	C	118	THR
3	C	130	THR
3	C	160	GLN
3	C	161	ASN
3	C	167	TRP
3	C	174	ASP
3	C	197	THR
3	C	203	LYS
3	C	207	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	165	GLN
1	A	195	HIS
1	A	308	ASN
1	A	334	ASN
1	A	347	ASN
1	A	375	ASN
1	A	388	GLN
1	A	439	GLN
1	A	451	GLN
1	A	502	GLN
2	B	39	GLN
2	B	53	ASN
2	B	208	HIS
3	C	17	GLN
3	C	57	ASN
3	C	142	ASN
3	C	149	ASN
3	C	214	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	C	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	50:LEU	C	51:LEU	N	1.16
1	C	51:LEU	C	52:ILE	N	1.16

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	288/526 (54%)	1.08	44 (15%) 5 6	24, 67, 93, 117	0
2	B	221/258 (85%)	0.72	15 (6%) 23 25	2, 40, 61, 72	8 (3%)
3	C	217/238 (91%)	0.39	11 (5%) 33 35	29, 46, 66, 106	0
All	All	726/1022 (71%)	0.77	70 (9%) 13 15	2, 49, 87, 117	8 (1%)

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	138	GLY	26.4
2	B	140	THR	24.3
2	B	142	GLY	18.3
2	B	137	CYS	13.8
2	B	141	THR	8.6
1	A	300	PHE	8.4
2	B	139	ASP	6.8
1	A	301	LYS	5.3
2	B	136	VAL	5.0
1	A	242	TYR	4.7
1	A	446	ILE	4.6
1	A	319	LYS	4.5
3	C	217	GLU	4.2
1	A	453	ASP	3.8
3	C	97	LYS	3.4
1	A	223	LYS	3.3
1	A	404	TYR	3.3
1	A	238	LEU	3.3
1	A	504	LYS	3.3
1	A	374	LYS	3.1
1	A	327	LYS	3.1
2	B	143	SER	3.1
1	A	236	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
3	C	24	ARG	3.0
1	A	302	LYS	2.9
1	A	486	LYS	2.8
1	A	501	LEU	2.8
1	A	303	MET	2.8
1	A	493	ILE	2.7
2	B	53	ASN	2.7
1	A	405	ILE	2.7
1	A	168	GLU	2.6
3	C	26	SER	2.6
3	C	164	LEU	2.6
1	A	396	ASN	2.6
1	A	237	LYS	2.5
1	A	160	SER	2.5
1	A	312	LYS	2.4
1	A	392	LEU	2.4
1	A	415	LYS	2.3
1	A	499	TYR	2.3
2	B	48	VAL	2.3
1	A	316	LYS	2.3
3	C	74	ASP	2.3
1	A	313	LYS	2.3
1	A	200	TYR	2.2
1	A	502	GLN	2.2
2	B	84	SER	2.2
1	A	305	ASP	2.2
1	A	309	THR	2.2
1	A	399	LYS	2.2
1	A	403	SER	2.2
3	C	21	ILE	2.2
1	A	429	LYS	2.2
3	C	167	TRP	2.1
1	A	167	LYS	2.1
3	C	173	LYS	2.1
2	B	180	GLN	2.1
1	A	224	CYS	2.1
1	A	207	ASP	2.1
2	B	182	ASP	2.1
3	C	85	ASP	2.1
2	B	64	VAL	2.1
1	A	340	PHE	2.1
2	B	165	SER	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	503	MET	2.0
1	A	483	PHE	2.0
1	A	409	THR	2.0
1	A	388	GLN	2.0
3	C	1	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.