



Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 04:30 pm BST

PDB ID : 4U1G
Title : Plasmodium falciparum reticulocyte-binding protein homologue 5 (PfRH5)
bound to monoclonal antibody QA1
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 : 2014-07-15
Resolution : 3.10 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 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	:	2.11
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)	:	2.11

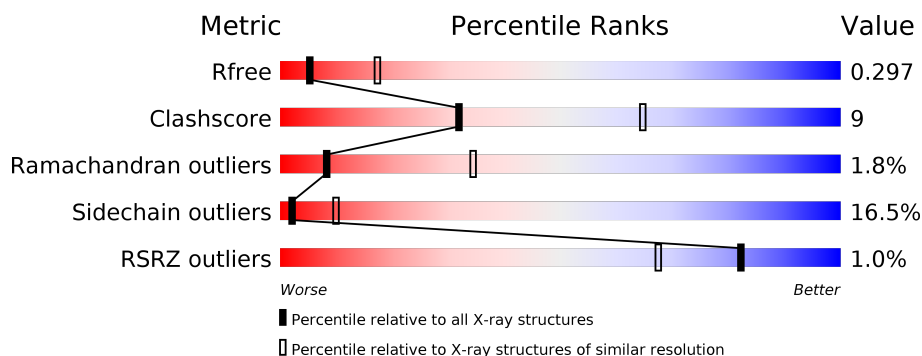
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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 on 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	<div> <div>36%</div> <div>16%</div> <div>•</div> <div>45%</div> </div>
1	D	526	<div> <div>38%</div> <div>14%</div> <div>•</div> <div>45%</div> </div>
2	B	258	<div> <div>57%</div> <div>21%</div> <div>5%</div> <div>17%</div> </div>
2	E	258	<div> <div>55%</div> <div>23%</div> <div>•</div> <div>17%</div> </div>
3	C	238	<div> <div>63%</div> <div>24%</div> <div>•</div> <div>10%</div> </div>
3	F	238	<div> <div>60%</div> <div>28%</div> <div>•</div> <div>10%</div> </div>

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 11478 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
			2446	1579	411	441	15			
1	D	289	Total	C	N	O	S	0	0	0
			2458	1588	412	443	15			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	216	ALA	THR	engineered mutation	UNP B2L3N7
D	216	ALA	THR	engineered mutation	UNP B2L3N7

- Molecule 2 is a protein called QA1 monoclonal antibody heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	213	Total	C	N	O	S	0	0	0
			1611	1020	262	320	9			
2	E	213	Total	C	N	O	S	0	0	0
			1611	1020	262	320	9			

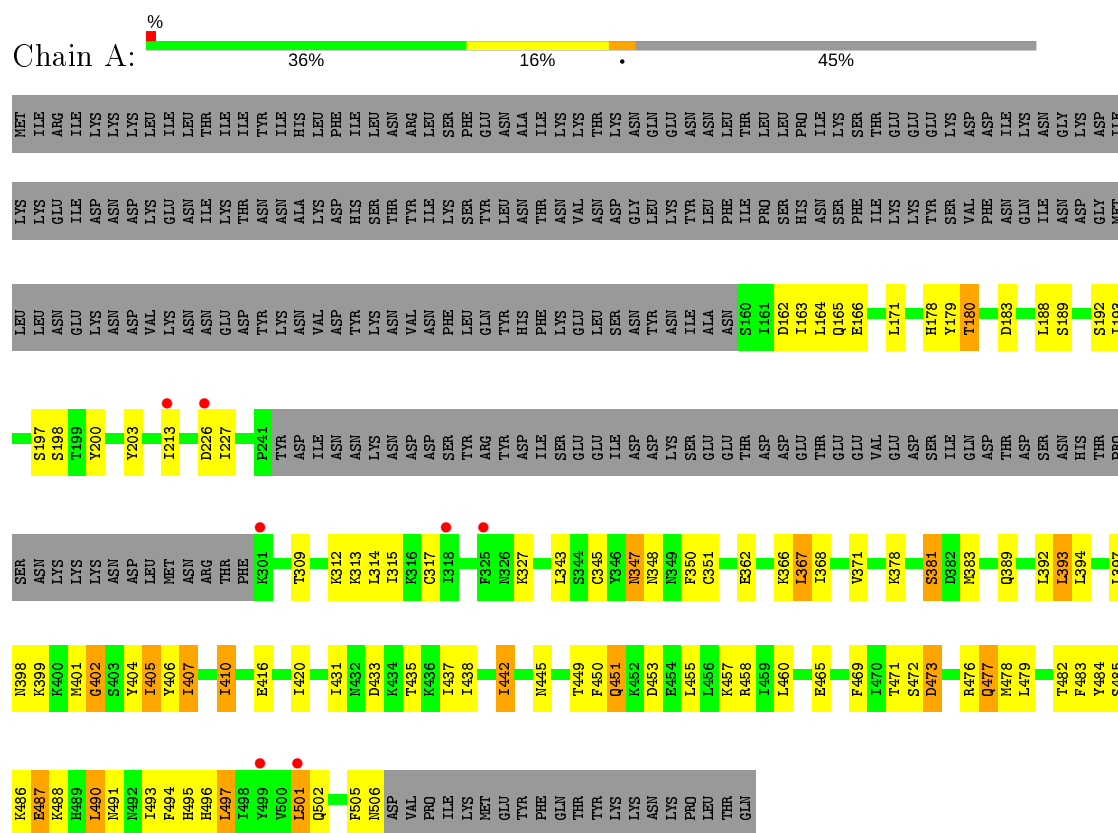
- Molecule 3 is a protein called QA1 monoclonal antibody light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	215	Total	C	N	O	S	0	0	0
			1676	1049	283	339	5			
3	F	215	Total	C	N	O	S	0	0	0
			1676	1049	283	339	5			

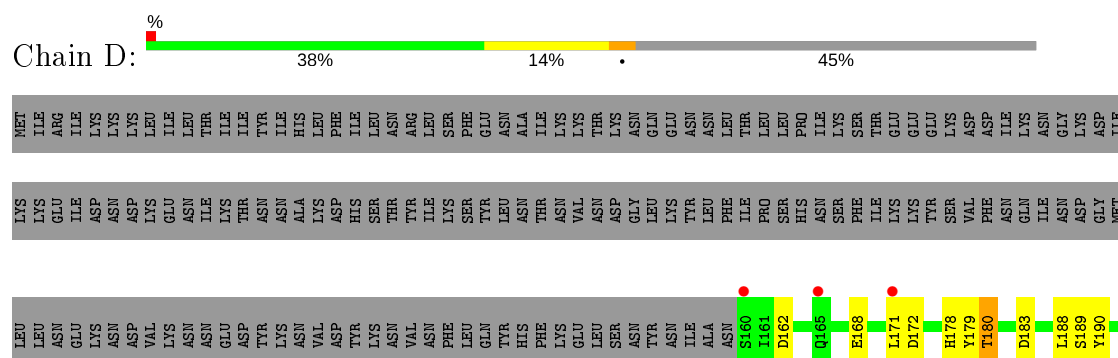
3 Residue-property plots [i](#)

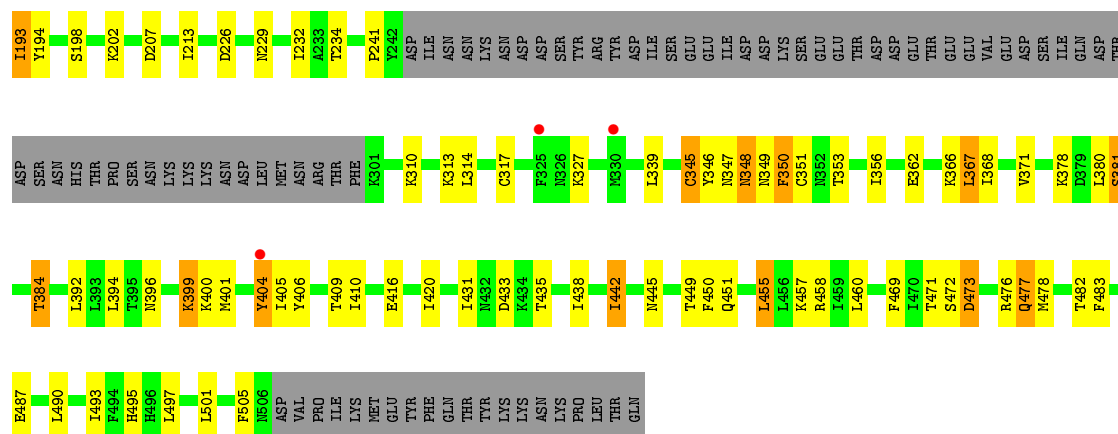
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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 5



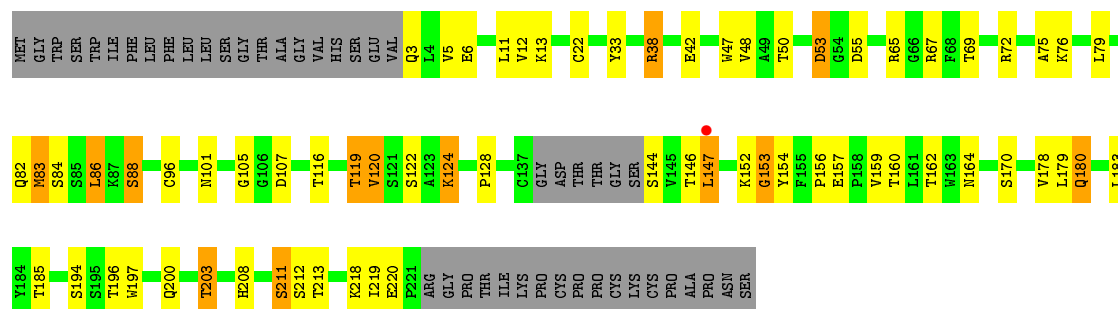
• Molecule 1: Reticulocyte binding protein 5





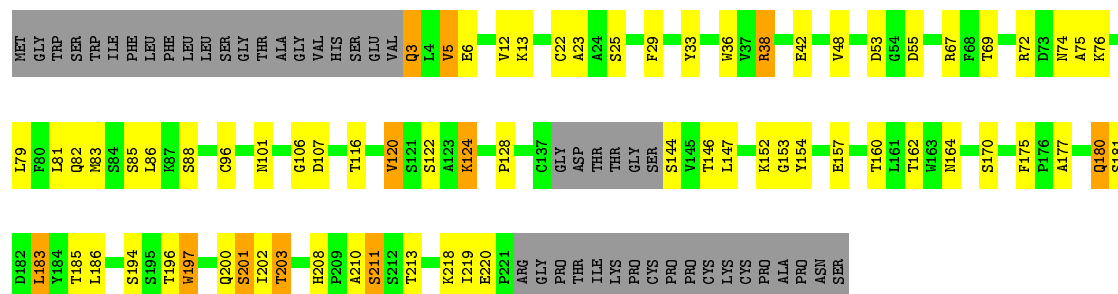
• Molecule 2: QA1 monoclonal antibody heavy chain

Chain B: 57% 21% 5% 17%



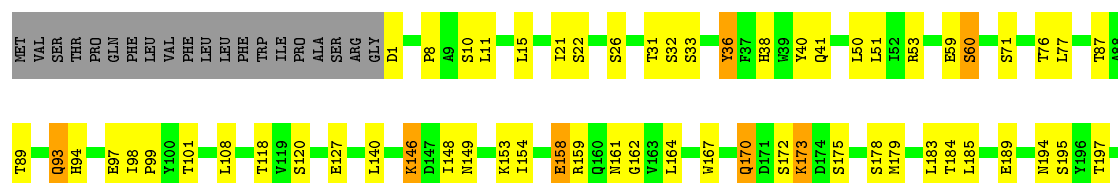
• Molecule 2: QA1 monoclonal antibody heavy chain

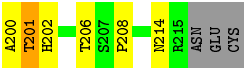
Chain E: 55% 23% 17%



• Molecule 3: QA1 monoclonal antibody light chain

Chain C: 63% 24% 10%





● Molecule 3: QA1 monoclonal antibody light chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2 ₁	Depositor
Cell constants a, b, c, α , β , γ	65.12Å 137.30Å 228.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.57 – 3.10 46.57 – 3.10	Depositor EDS
% Data completeness (in resolution range)	95.1 (46.57-3.10) 95.1 (46.57-3.10)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.16 (at 3.12Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.236 , 0.281 0.253 , 0.297	Depositor DCC
R_{free} test set	1793 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	90.1	Xtriage
Anisotropy	0.677	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 84.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	11478	wwPDB-VP
Average B, all atoms (Å ²)	102.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.66% 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 [i](#)

5.1 Standard geometry [i](#)

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	0/2497	0.74	0/3347
1	D	0.51	0/2510	0.75	0/3365
2	B	0.54	0/1651	0.88	1/2248 (0.0%)
2	E	0.57	0/1651	0.89	0/2248
3	C	0.53	0/1719	0.81	0/2340
3	F	0.52	0/1719	0.78	0/2340
All	All	0.53	0/11747	0.80	1/15888 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	159	VAL	N-CA-CB	6.12	124.97	111.50

There are no chirality outliers.

There are no planarity outliers.

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	2446	0	2474	53	0
1	D	2458	0	2483	43	0
2	B	1611	0	1559	40	0
2	E	1611	0	1559	33	0
3	C	1676	0	1597	28	0
3	F	1676	0	1597	25	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	11478	0	11269	203	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 9.

All (203) 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:B:75:ALA:HB1	2:E:75:ALA:HB1	1.51	0.92
1:D:179:TYR:HD2	1:D:471:THR:HG22	1.35	0.91
1:A:179:TYR:HD2	1:A:471:THR:HG22	1.34	0.90
2:B:11:LEU:HD11	2:B:156:PRO:HG3	1.53	0.90
2:B:153:GLY:HA2	2:B:183:LEU:HB3	1.60	0.81
1:A:192:SER:HA	1:A:343:LEU:HD12	1.61	0.80
3:C:38:HIS:ND1	3:C:53:ARG:O	2.13	0.79
1:D:347:ASN:HB3	1:D:350:PHE:HB2	1.65	0.78
2:B:152:LYS:HA	2:B:185:THR:HG22	1.65	0.77
2:B:11:LEU:HD11	2:B:156:PRO:CG	2.17	0.75
1:A:402:GLY:HA2	1:A:407:ILE:HD13	1.68	0.74
2:E:128:PRO:HB3	2:E:154:TYR:HB3	1.69	0.73
1:D:190:TYR:OH	1:D:207:ASP:OD1	2.06	0.73
2:E:208:HIS:ND1	2:E:211:SER:HB2	2.03	0.72
2:B:11:LEU:CD1	2:B:156:PRO:HG3	2.22	0.70
2:B:128:PRO:HB3	2:B:154:TYR:HB3	1.75	0.69
2:B:11:LEU:HD23	2:B:119:THR:HG23	1.74	0.68
2:E:153:GLY:HA2	2:E:183:LEU:HB3	1.73	0.68
2:E:208:HIS:CE1	2:E:210:ALA:HB3	2.29	0.67
1:A:405:ILE:HG12	1:A:497:LEU:HD23	1.75	0.67
1:A:179:TYR:CD2	1:A:471:THR:HG22	2.23	0.67
1:D:179:TYR:CD2	1:D:471:THR:HG22	2.24	0.66
2:B:153:GLY:CA	2:B:183:LEU:HB3	2.24	0.66
1:A:345:CYS:HB2	1:A:348:ASN:HD22	1.61	0.66
2:E:180:GLN:OE1	2:E:180:GLN:HA	1.95	0.65
2:E:22:CYS:HB3	2:E:79:LEU:HB3	1.79	0.64
2:B:180:GLN:HE22	2:B:185:THR:CG2	2.11	0.64
1:D:193:ILE:HD13	1:D:339:LEU:HD13	1.79	0.64
1:D:351:CYS:HB2	1:D:450:PHE:O	1.98	0.63
1:D:241:PRO:HG3	1:D:409:THR:HG21	1.80	0.63
1:A:348:ASN:HB2	3:C:36:TYR:OH	1.99	0.63
3:F:148:ILE:HG22	3:F:167:TRP:CH2	2.34	0.63
1:A:484:TYR:HD1	1:A:487:GLU:HG2	1.63	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:501:LEU:HB3	1:D:501:LEU:HD22	1.81	0.62
2:E:6:GLU:HB3	2:E:116:THR:HG22	1.81	0.62
1:A:394:LEU:HD21	1:A:410:ILE:HB	1.83	0.61
1:A:478:MET:O	1:A:482:THR:HG23	2.00	0.61
2:E:144:SER:N	2:E:194:SER:HG	1.99	0.60
3:F:194:ASN:O	3:F:214:ASN:HA	2.02	0.60
2:B:144:SER:N	2:B:194:SER:HG	1.99	0.60
2:E:197:TRP:HH2	2:E:219:ILE:O	1.85	0.60
1:D:349:ASN:ND2	3:F:34:TYR:OH	2.35	0.60
1:A:345:CYS:HB2	1:A:348:ASN:ND2	2.17	0.59
2:B:180:GLN:HB3	3:C:164:LEU:HD11	1.84	0.59
2:E:69:THR:HB	2:E:82:GLN:HB3	1.84	0.59
2:E:211:SER:HB3	2:E:213:THR:HG23	1.85	0.58
3:C:31:THR:O	3:C:33:SER:N	2.36	0.58
3:C:31:THR:HG22	3:C:33:SER:H	1.69	0.58
1:A:476:ARG:HH11	1:A:477:GLN:HG2	1.69	0.57
1:D:478:MET:O	1:D:482:THR:HG23	2.04	0.57
3:F:21:ILE:HD13	3:F:77:LEU:HD23	1.87	0.57
2:B:208:HIS:ND1	2:B:211:SER:HB2	2.20	0.56
2:E:83:MET:HB3	2:E:86:LEU:HD21	1.87	0.56
2:E:124:LYS:HE2	2:E:124:LYS:H	1.71	0.56
2:B:124:LYS:HE2	2:B:124:LYS:H	1.70	0.56
2:E:88:SER:HA	2:E:120:VAL:HB	1.87	0.56
2:B:38:ARG:HG2	2:B:48:VAL:HG23	1.88	0.56
1:D:180:THR:HA	1:D:471:THR:HG21	1.88	0.56
2:E:5:VAL:HG23	2:E:23:ALA:HB3	1.88	0.56
1:A:431:ILE:HD11	1:A:473:ASP:HA	1.88	0.55
1:D:371:VAL:HG11	1:D:435:THR:HG21	1.89	0.55
3:C:21:ILE:HD13	3:C:77:LEU:HD23	1.88	0.55
1:D:431:ILE:HD11	1:D:473:ASP:HA	1.89	0.55
1:A:393:LEU:O	1:A:397:LEU:HB2	2.07	0.55
1:A:451:GLN:OE1	1:A:453:ASP:HB2	2.06	0.55
2:B:6:GLU:HB3	2:B:116:THR:HG22	1.88	0.54
1:A:505:PHE:CE2	1:D:501:LEU:HD23	2.42	0.54
3:C:31:THR:C	3:C:33:SER:H	2.10	0.54
2:B:42:GLU:CD	2:B:42:GLU:H	2.11	0.54
2:B:105:GLY:HA2	3:C:36:TYR:OH	2.08	0.53
1:D:476:ARG:HH11	1:D:477:GLN:HG2	1.73	0.53
1:A:180:THR:HA	1:A:471:THR:HG21	1.91	0.53
2:E:38:ARG:HG2	2:E:48:VAL:HG23	1.90	0.53
1:A:371:VAL:HG11	1:A:435:THR:HG21	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:97:GLU:HB3	3:C:99:PRO:HD2	1.90	0.53
3:F:148:ILE:HG22	3:F:167:TRP:CZ3	2.43	0.53
1:A:165:GLN:HE22	1:A:486:LYS:NZ	2.07	0.52
1:A:165:GLN:HE22	1:A:486:LYS:HZ1	1.56	0.52
2:B:11:LEU:HD23	2:B:119:THR:CG2	2.39	0.52
3:F:31:THR:HG23	3:F:33:SER:H	1.74	0.52
3:F:52:ILE:HG22	3:F:54:TYR:O	2.09	0.52
1:A:197:SER:HB2	2:B:53:ASP:OD1	2.09	0.52
1:D:347:ASN:C	1:D:349:ASN:H	2.13	0.52
2:B:88:SER:HA	2:B:120:VAL:HB	1.90	0.52
2:E:42:GLU:H	2:E:42:GLU:CD	2.12	0.52
2:B:180:GLN:NE2	2:B:185:THR:HG23	2.26	0.51
2:E:38:ARG:HG2	2:E:48:VAL:CG2	2.40	0.51
2:B:38:ARG:HG2	2:B:48:VAL:CG2	2.40	0.51
2:B:180:GLN:HE22	2:B:185:THR:HG23	1.76	0.51
1:D:396:ASN:O	1:D:399:LYS:HB3	2.11	0.51
1:D:350:PHE:CZ	3:F:98:ILE:HD12	2.46	0.51
2:B:11:LEU:HD21	2:B:156:PRO:HB3	1.93	0.51
3:F:97:GLU:HB3	3:F:99:PRO:HD2	1.91	0.51
2:E:180:GLN:HG2	3:F:164:LEU:HD11	1.93	0.51
2:B:83:MET:HB3	2:B:86:LEU:HD23	1.92	0.50
1:A:491:ASN:HA	1:A:494:PHE:HB2	1.94	0.50
3:C:194:ASN:OD1	3:C:214:ASN:HB3	2.11	0.50
1:A:165:GLN:NE2	1:A:486:LYS:NZ	2.59	0.50
2:E:6:GLU:HB3	2:E:116:THR:CG2	2.42	0.50
2:E:177:ALA:HB2	2:E:186:LEU:HD23	1.94	0.50
1:D:345:CYS:HB2	1:D:348:ASN:HD22	1.77	0.49
3:C:40:TYR:HE2	3:C:93:GLN:HG2	1.77	0.49
1:A:457:LYS:HA	1:A:460:LEU:HD12	1.95	0.49
2:B:211:SER:HB3	2:B:213:THR:HG23	1.94	0.49
3:F:40:TYR:HE2	3:F:93:GLN:HG2	1.78	0.48
3:F:167:TRP:CD1	3:F:167:TRP:N	2.81	0.48
1:D:190:TYR:HD1	1:D:194:TYR:CE2	2.30	0.48
2:B:152:LYS:HD3	2:B:185:THR:HG21	1.95	0.48
2:B:178:VAL:CG2	3:C:164:LEU:HD13	2.44	0.48
2:E:175:PHE:CD2	3:F:168:THR:HG23	2.50	0.47
1:D:193:ILE:HD11	1:D:202:LYS:HD3	1.95	0.47
1:D:457:LYS:HA	1:D:460:LEU:HD12	1.96	0.47
3:C:167:TRP:CD1	3:C:167:TRP:N	2.82	0.47
3:C:148:ILE:HG13	3:C:202:HIS:HB2	1.96	0.47
2:B:6:GLU:HB3	2:B:116:THR:CG2	2.44	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:351:CYS:O	1:D:449:THR:HA	2.15	0.47
1:A:165:GLN:NE2	1:A:486:LYS:HZ2	2.12	0.47
1:D:346:TYR:O	2:E:106:GLY:HA2	2.15	0.46
3:F:38:HIS:ND1	3:F:53:ARG:O	2.49	0.46
1:A:438:ILE:O	1:A:442:ILE:HG13	2.15	0.46
1:A:166:GLU:N	1:A:482:THR:HG22	2.31	0.46
1:A:420:ILE:HG21	1:A:483:PHE:HB2	1.98	0.46
1:A:163:ILE:C	1:A:164:LEU:HG	2.36	0.46
1:D:229:ASN:HA	1:D:232:ILE:HD12	1.98	0.46
1:D:380:LEU:O	1:D:384:THR:OG1	2.34	0.46
3:C:154:ILE:HD11	3:C:183:LEU:HD21	1.98	0.46
2:B:69:THR:HB	2:B:82:GLN:HB3	1.97	0.46
1:D:405:ILE:HG13	1:D:406:TYR:CE2	2.51	0.46
3:F:8:PRO:HG3	3:F:11:LEU:HD13	1.98	0.46
2:E:197:TRP:HZ3	2:E:202:ILE:H	1.64	0.45
1:A:506:ASN:HD21	1:D:399:LYS:HD2	1.80	0.45
1:D:420:ILE:HG21	1:D:483:PHE:HB2	1.99	0.45
2:E:152:LYS:HE2	2:E:185:THR:HG21	1.99	0.45
3:C:50:LEU:HD21	3:C:53:ARG:HD2	1.98	0.45
1:A:351:CYS:O	1:A:449:THR:HA	2.16	0.45
3:F:59:GLU:HB2	3:F:62:VAL:CG2	2.46	0.45
1:D:438:ILE:O	1:D:442:ILE:HG13	2.16	0.45
3:C:31:THR:C	3:C:33:SER:N	2.70	0.45
1:D:180:THR:CA	1:D:471:THR:HG21	2.47	0.45
1:A:378:LYS:HA	1:A:381:SER:HB2	1.99	0.45
3:C:170:GLN:HE21	3:C:175:SER:HB3	1.80	0.45
3:C:41:GLN:HB2	3:C:51:LEU:HD12	1.98	0.45
1:A:312:LYS:HA	1:A:315:ILE:HD12	1.99	0.44
1:A:347:ASN:HB3	1:A:350:PHE:H	1.82	0.44
1:D:234:THR:HG21	1:D:310:LYS:HG3	1.98	0.44
3:F:193:HIS:O	3:F:215:ARG:NH1	2.48	0.44
1:A:180:THR:CA	1:A:471:THR:HG21	2.47	0.44
1:A:383:MET:HG2	1:A:483:PHE:CE2	2.52	0.44
1:A:479:LEU:HA	1:A:482:THR:OG1	2.18	0.44
3:C:146:LYS:O	3:C:167:TRP:HZ3	2.00	0.44
1:D:401:MET:HE1	1:D:501:LEU:HD21	1.99	0.44
2:B:75:ALA:HB1	2:E:75:ALA:CB	2.35	0.44
3:F:185:LEU:HD22	3:F:189:GLU:HB3	2.00	0.43
2:B:178:VAL:HG21	3:C:164:LEU:HD13	1.99	0.43
1:A:165:GLN:C	1:A:482:THR:HG22	2.39	0.43
3:F:41:GLN:HB2	3:F:51:LEU:HD12	1.99	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:LEU:HD21	1:A:460:LEU:HD23	2.00	0.43
1:A:347:ASN:OD1	1:A:350:PHE:HB2	2.19	0.43
2:B:47:TRP:HZ2	2:B:50:THR:HG1	1.61	0.43
1:D:505:PHE:O	1:D:505:PHE:CG	2.71	0.43
2:E:208:HIS:NE2	2:E:210:ALA:HB3	2.33	0.43
3:F:201:THR:HG22	3:F:208:PRO:HB3	2.01	0.43
1:A:502:GLN:O	1:D:399:LYS:NZ	2.51	0.43
1:D:410:ILE:HD11	1:D:493:ILE:HG22	2.00	0.43
2:B:22:CYS:HB3	2:B:79:LEU:HB3	2.01	0.42
3:F:94:HIS:CE1	3:F:101:THR:H	2.37	0.42
3:F:111:LYS:HA	3:F:144:TYR:OH	2.19	0.42
1:A:485:SER:HA	1:A:488:LYS:HE3	2.01	0.42
1:A:484:TYR:CD1	1:A:487:GLU:HG2	2.51	0.42
2:B:203:THR:HB	2:B:218:LYS:HA	2.01	0.42
1:D:378:LYS:HA	1:D:381:SER:HB2	2.00	0.42
1:A:505:PHE:HE2	1:D:501:LEU:HD23	1.83	0.42
2:B:76:LYS:HD3	2:E:76:LYS:HA	2.01	0.42
3:F:37:PHE:CZ	3:F:92:CYS:HB2	2.55	0.42
3:F:54:TYR:O	3:F:56:SER:N	2.52	0.42
1:A:437:ILE:HG21	1:A:465:GLU:HG2	2.02	0.42
1:D:188:LEU:HD21	1:D:460:LEU:HD23	2.00	0.42
1:A:404:TYR:C	1:A:406:TYR:H	2.22	0.42
2:E:3:GLN:N	2:E:25:SER:O	2.53	0.42
3:C:94:HIS:CE1	3:C:101:THR:H	2.37	0.42
1:A:367:LEU:HB3	1:A:469:PHE:CE2	2.55	0.41
2:B:11:LEU:CG	2:B:156:PRO:HG3	2.50	0.41
2:B:180:GLN:HB3	2:B:180:GLN:HE21	1.73	0.41
3:C:185:LEU:HD22	3:C:189:GLU:HB3	2.01	0.41
1:D:351:CYS:HB3	1:D:455:LEU:HG	2.02	0.41
3:C:201:THR:HG22	3:C:208:PRO:HB3	2.01	0.41
2:E:29:PHE:CD2	2:E:74:ASN:HA	2.55	0.41
1:A:397:LEU:O	1:A:401:MET:HB3	2.20	0.41
1:A:490:LEU:HA	1:A:490:LEU:HD23	1.89	0.41
1:D:405:ILE:HG13	1:D:406:TYR:CD2	2.56	0.41
3:C:53:ARG:HD3	3:C:59:GLU:OE1	2.21	0.41
3:C:8:PRO:HG3	3:C:11:LEU:HD13	2.03	0.41
3:C:140:LEU:HD21	3:C:200:ALA:CB	2.51	0.41
1:A:227:ILE:HD12	1:A:227:ILE:H	1.87	0.40
1:A:367:LEU:HB3	1:A:469:PHE:HE2	1.86	0.40
1:D:367:LEU:HB3	1:D:469:PHE:CE2	2.56	0.40
2:E:36:TRP:CE2	2:E:81:LEU:HB2	2.56	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:147:LEU:HD12	2:B:219:ILE:HD12	2.03	0.40
1:D:353:THR:HG22	1:D:356:ILE:HD12	2.01	0.40
3:F:153:LYS:HA	3:F:158:GLU:HA	2.03	0.40
1:A:351:CYS:HB2	1:A:450:PHE:O	2.21	0.40
3:C:153:LYS:HA	3:C:158:GLU:HA	2.03	0.40
2:E:203:THR:HB	2:E:218:LYS:HA	2.03	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%)	261 (92%)	19 (7%)	4 (1%)	11	40
1	D	285/526 (54%)	261 (92%)	22 (8%)	2 (1%)	22	57
2	B	209/258 (81%)	186 (89%)	20 (10%)	3 (1%)	11	40
2	E	209/258 (81%)	182 (87%)	23 (11%)	4 (2%)	8	33
3	C	213/238 (90%)	190 (89%)	15 (7%)	8 (4%)	3	19
3	F	213/238 (90%)	187 (88%)	21 (10%)	5 (2%)	6	28
All	All	1413/2044 (69%)	1267 (90%)	120 (8%)	26 (2%)	8	34

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	200	TYR
3	C	172	SER
2	E	55	ASP
2	E	197	TRP
3	F	55	ALA
1	A	399	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	402	GLY
1	A	405	ILE
2	B	55	ASP
2	B	153	GLY
3	C	32	SER
3	C	162	GLY
2	E	181	SER
3	F	58	LEU
2	B	197	TRP
3	C	170	GLN
3	F	170	GLN
3	C	60	SER
3	C	161	ASN
1	D	348	ASN
2	E	201	SER
3	F	172	SER
3	C	173	LYS
3	F	161	ASN
3	C	36	TYR
1	D	404	TYR

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	279/511 (55%)	234 (84%)	45 (16%)	2	10
1	D	280/511 (55%)	237 (85%)	43 (15%)	2	11
2	B	182/219 (83%)	146 (80%)	36 (20%)	1	5
2	E	182/219 (83%)	151 (83%)	31 (17%)	2	9
3	C	190/211 (90%)	162 (85%)	28 (15%)	3	13
3	F	190/211 (90%)	158 (83%)	32 (17%)	2	9
All	All	1303/1882 (69%)	1088 (84%)	215 (16%)	2	10

All (215) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	162	ASP
1	A	171	LEU
1	A	178	HIS
1	A	180	THR
1	A	183	ASP
1	A	189	SER
1	A	193	ILE
1	A	198	SER
1	A	203	TYR
1	A	213	ILE
1	A	226	ASP
1	A	309	THR
1	A	313	LYS
1	A	314	LEU
1	A	317	CYS
1	A	327	LYS
1	A	347	ASN
1	A	362	GLU
1	A	366	LYS
1	A	367	LEU
1	A	368	ILE
1	A	381	SER
1	A	389	GLN
1	A	392	LEU
1	A	393	LEU
1	A	398	ASN
1	A	407	ILE
1	A	410	ILE
1	A	416	GLU
1	A	433	ASP
1	A	442	ILE
1	A	445	ASN
1	A	451	GLN
1	A	455	LEU
1	A	458	ARG
1	A	472	SER
1	A	473	ASP
1	A	477	GLN
1	A	487	GLU
1	A	490	LEU
1	A	493	ILE
1	A	495	HIS
1	A	496	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	497	LEU
1	A	501	LEU
2	B	3	GLN
2	B	5	VAL
2	B	12	VAL
2	B	13	LYS
2	B	33	TYR
2	B	38	ARG
2	B	53	ASP
2	B	65	ARG
2	B	67	ARG
2	B	72	ARG
2	B	83	MET
2	B	84	SER
2	B	86	LEU
2	B	88	SER
2	B	96	CYS
2	B	101	ASN
2	B	107	ASP
2	B	119	THR
2	B	120	VAL
2	B	122	SER
2	B	124	LYS
2	B	146	THR
2	B	147	LEU
2	B	157	GLU
2	B	160	THR
2	B	162	THR
2	B	164	ASN
2	B	170	SER
2	B	179	LEU
2	B	180	GLN
2	B	196	THR
2	B	200	GLN
2	B	203	THR
2	B	211	SER
2	B	212	SER
2	B	220	GLU
3	C	1	ASP
3	C	10	SER
3	C	15	LEU
3	C	22	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	26	SER
3	C	60	SER
3	C	71	SER
3	C	76	THR
3	C	87	THR
3	C	89	THR
3	C	93	GLN
3	C	98	ILE
3	C	108	LEU
3	C	118	THR
3	C	120	SER
3	C	127	GLU
3	C	146	LYS
3	C	149	ASN
3	C	158	GLU
3	C	159	ARG
3	C	173	LYS
3	C	178	SER
3	C	179	MET
3	C	184	THR
3	C	195	SER
3	C	197	THR
3	C	201	THR
3	C	206	THR
1	D	162	ASP
1	D	168	GLU
1	D	171	LEU
1	D	172	ASP
1	D	178	HIS
1	D	180	THR
1	D	183	ASP
1	D	189	SER
1	D	193	ILE
1	D	198	SER
1	D	213	ILE
1	D	226	ASP
1	D	313	LYS
1	D	314	LEU
1	D	317	CYS
1	D	327	LYS
1	D	345	CYS
1	D	350	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	362	GLU
1	D	366	LYS
1	D	367	LEU
1	D	368	ILE
1	D	381	SER
1	D	384	THR
1	D	392	LEU
1	D	394	LEU
1	D	399	LYS
1	D	400	LYS
1	D	404	TYR
1	D	416	GLU
1	D	433	ASP
1	D	442	ILE
1	D	445	ASN
1	D	451	GLN
1	D	455	LEU
1	D	458	ARG
1	D	472	SER
1	D	473	ASP
1	D	477	GLN
1	D	487	GLU
1	D	490	LEU
1	D	495	HIS
1	D	497	LEU
2	E	3	GLN
2	E	5	VAL
2	E	12	VAL
2	E	13	LYS
2	E	33	TYR
2	E	38	ARG
2	E	53	ASP
2	E	67	ARG
2	E	72	ARG
2	E	85	SER
2	E	96	CYS
2	E	101	ASN
2	E	107	ASP
2	E	120	VAL
2	E	122	SER
2	E	124	LYS
2	E	146	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	E	147	LEU
2	E	157	GLU
2	E	160	THR
2	E	162	THR
2	E	164	ASN
2	E	170	SER
2	E	180	GLN
2	E	183	LEU
2	E	196	THR
2	E	200	GLN
2	E	201	SER
2	E	203	THR
2	E	211	SER
2	E	220	GLU
3	F	1	ASP
3	F	10	SER
3	F	15	LEU
3	F	22	SER
3	F	26	SER
3	F	33	SER
3	F	58	LEU
3	F	60	SER
3	F	69	SER
3	F	71	SER
3	F	76	THR
3	F	87	THR
3	F	89	THR
3	F	93	GLN
3	F	98	ILE
3	F	108	LEU
3	F	118	THR
3	F	120	SER
3	F	127	GLU
3	F	141	ASN
3	F	146	LYS
3	F	149	ASN
3	F	158	GLU
3	F	159	ARG
3	F	169	ASP
3	F	174	ASP
3	F	179	MET
3	F	181	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	F	184	THR
3	F	197	THR
3	F	201	THR
3	F	206	THR

Some 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	365	HIS
1	A	477	GLN
2	B	173	HIS
2	B	180	GLN
3	C	80	HIS
3	C	94	HIS
3	C	128	GLN
3	C	141	ASN
3	C	142	ASN
3	C	161	ASN
1	D	349	ASN
1	D	365	HIS
1	D	477	GLN
3	F	80	HIS
3	F	94	HIS
3	F	141	ASN
3	F	193	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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%)	0.02	7 (2%) 59 37	67, 108, 171, 199	0
1	D	289/526 (54%)	0.12	6 (2%) 63 43	77, 113, 174, 203	0
2	B	213/258 (82%)	-0.14	1 (0%) 91 81	51, 84, 123, 136	0
2	E	213/258 (82%)	-0.17	0 100 100	51, 84, 119, 142	0
3	C	215/238 (90%)	-0.11	0 100 100	57, 90, 122, 141	1 (0%)
3	F	215/238 (90%)	0.06	0 100 100	55, 99, 129, 143	1 (0%)
All	All	1433/2044 (70%)	-0.03	14 (0%) 82 67	51, 97, 153, 203	2 (0%)

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	404	TYR	3.7
1	D	160	SER	3.3
1	D	325	PHE	3.1
1	A	226	ASP	3.1
1	D	171	LEU	2.9
1	D	165	GLN	2.8
1	A	501	LEU	2.8
1	A	318	ILE	2.7
1	A	213	ILE	2.5
2	B	147	LEU	2.4
1	A	325	PHE	2.4
1	A	499	TYR	2.4
1	D	330	MET	2.3
1	A	301	LYS	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 carbohydrates 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.