



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 21, 2021 – 12:10 PM EST

PDB ID : 6WTU
Title : Plasmodium vivax reticulocyte binding protein 2b (PvRBP2b) bound to human monoclonal antibody 273264
Authors : Chan, L.J.; Dietrich, M.H.; Tham, W.H.
Deposited on : 2020-05-04
Resolution : 2.55 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	:	2.16
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)	:	2.16

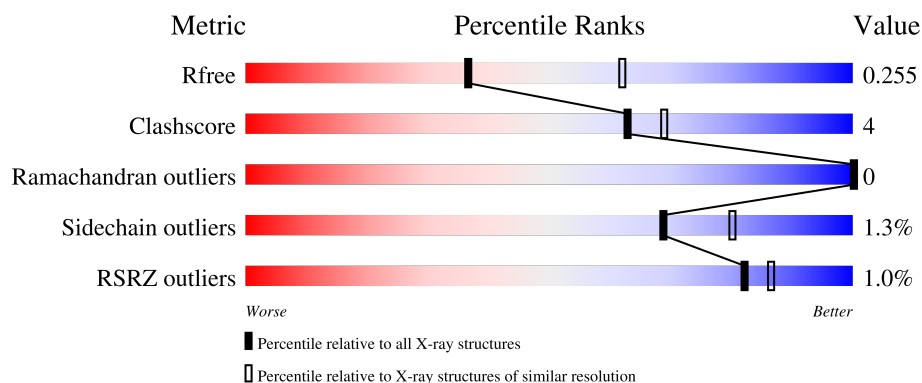
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

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	307	<div> <div>%</div> <div> <div></div> <div>84%</div> <div>14%</div> <div>.</div> </div> </div>
1	D	307	<div> <div></div> <div>90%</div> <div>7%</div> <div>...</div> </div>
1	G	307	<div> <div></div> <div>87%</div> <div>9%</div> <div>.</div> </div>
1	J	307	<div> <div></div> <div>87%</div> <div>9%</div> <div>.</div> </div>
2	B	238	<div> <div></div> <div>83%</div> <div>9%</div> <div>8%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	E	238	<div><div><div></div><div></div><div></div></div><div><div>%</div><div>81%</div><div>11%</div><div>8%</div></div></div>
2	H	238	<div><div><div></div><div></div><div></div></div><div><div>2%</div><div>79%</div><div>12%</div><div>8%</div></div></div>
2	K	238	<div><div><div></div><div></div><div></div></div><div><div>2%</div><div>74%</div><div>18%</div><div>9%</div></div></div>
3	C	219	<div><div><div></div><div></div><div></div></div><div><div></div><div>85%</div><div>10%</div><div>5%</div></div></div>
3	F	219	<div><div><div></div><div></div><div></div></div><div><div></div><div>89%</div><div>6%</div><div>5%</div></div></div>
3	I	219	<div><div><div></div><div></div><div></div></div><div><div>%</div><div>84%</div><div>11%</div><div>5%</div></div></div>
3	L	219	<div><div><div></div><div></div><div></div></div><div><div>4%</div><div>84%</div><div>11%</div><div>5%</div></div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 22520 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 2b.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	301	Total	C	N	O	S	0	0	0
			2433	1562	407	455	9			
1	G	297	Total	C	N	O	S	0	0	0
			2408	1547	403	449	9			
1	J	295	Total	C	N	O	S	0	0	0
			2363	1520	392	442	9			
1	D	299	Total	C	N	O	S	0	0	0
			2426	1559	406	452	9			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	164	GLY	-	expression tag	UNP A5K736
A	165	ALA	-	expression tag	UNP A5K736
A	166	MET	-	expression tag	UNP A5K736
A	167	GLY	-	expression tag	UNP A5K736
A	168	SER	-	expression tag	UNP A5K736
G	164	GLY	-	expression tag	UNP A5K736
G	165	ALA	-	expression tag	UNP A5K736
G	166	MET	-	expression tag	UNP A5K736
G	167	GLY	-	expression tag	UNP A5K736
G	168	SER	-	expression tag	UNP A5K736
J	164	GLY	-	expression tag	UNP A5K736
J	165	ALA	-	expression tag	UNP A5K736
J	166	MET	-	expression tag	UNP A5K736
J	167	GLY	-	expression tag	UNP A5K736
J	168	SER	-	expression tag	UNP A5K736
D	164	GLY	-	expression tag	UNP A5K736
D	165	ALA	-	expression tag	UNP A5K736
D	166	MET	-	expression tag	UNP A5K736
D	167	GLY	-	expression tag	UNP A5K736
D	168	SER	-	expression tag	UNP A5K736

- Molecule 2 is a protein called 273264 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	K	217	Total	C	N	O	S	0	0	0
			1565	986	261	311	7			
2	B	219	Total	C	N	O	S	0	0	0
			1618	1021	272	318	7			
2	E	218	Total	C	N	O	S	0	0	0
			1602	1011	267	317	7			
2	H	218	Total	C	N	O	S	0	0	0
			1580	999	261	313	7			

- Molecule 3 is a protein called 273264 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	207	Total	C	N	O	S	0	0	0
			1492	936	248	303	5			
3	I	209	Total	C	N	O	S	0	0	0
			1527	955	253	314	5			
3	C	209	Total	C	N	O	S	0	0	0
			1551	972	261	313	5			
3	F	209	Total	C	N	O	S	0	0	0
			1563	978	264	316	5			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	57	Total	O	0	0
			57	57		
4	K	12	Total	O	0	0
			12	12		
4	L	7	Total	O	0	0
			7	7		
4	B	47	Total	O	0	0
			47	47		
4	E	36	Total	O	0	0
			36	36		
4	I	11	Total	O	0	0
			11	11		
4	H	37	Total	O	0	0
			37	37		
4	G	49	Total	O	0	0
			49	49		
4	C	25	Total	O	0	0
			25	25		

Continued on next page...

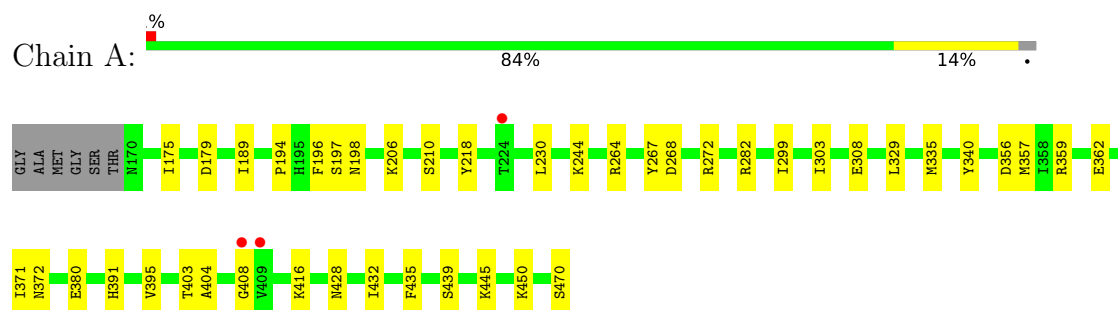
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	F	36	Total 36	O 36	0	0
4	J	28	Total 28	O 28	0	0
4	D	47	Total 47	O 47	0	0

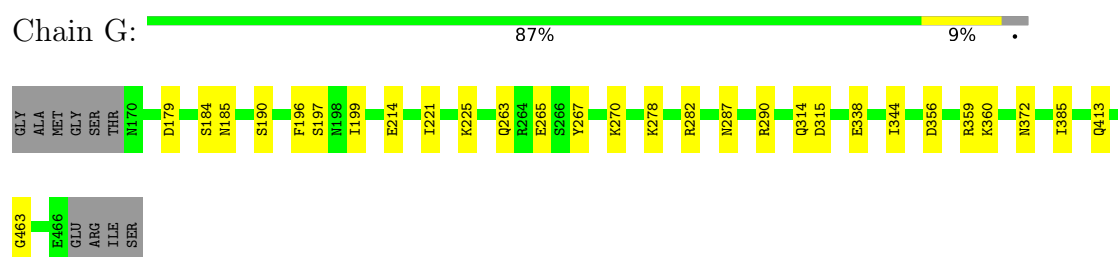
3 Residue-property plots [i](#)

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.

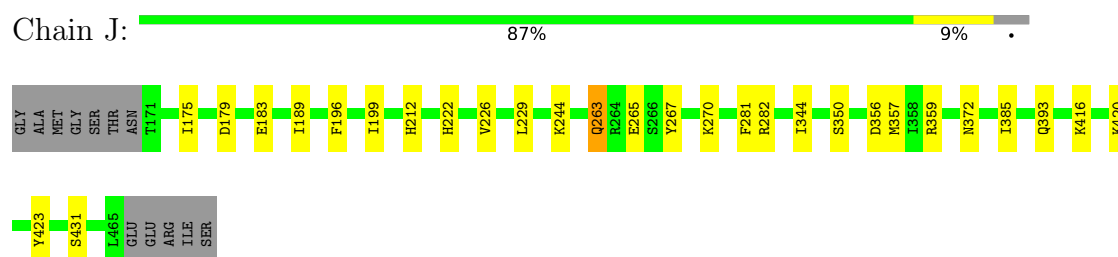
- Molecule 1: reticulocyte binding protein 2b



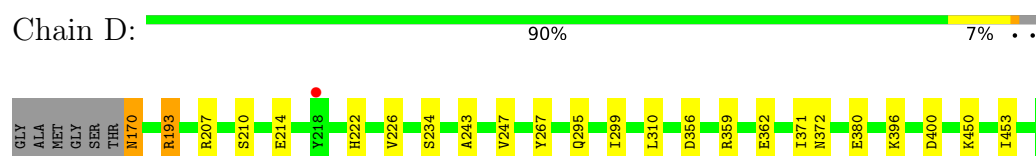
- Molecule 1: reticulocyte binding protein 2b



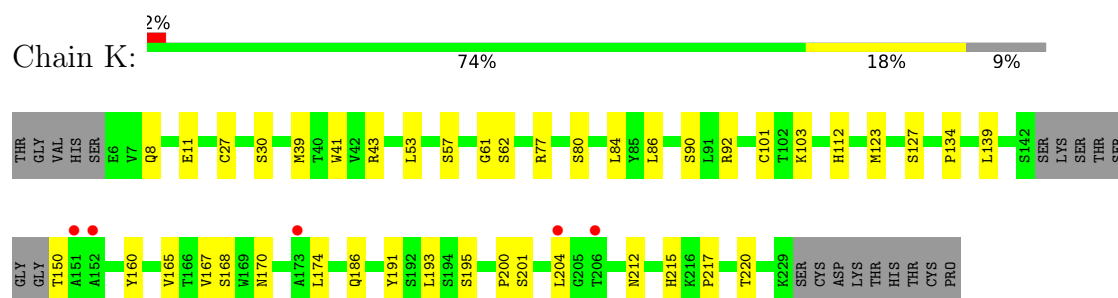
- Molecule 1: reticulocyte binding protein 2b



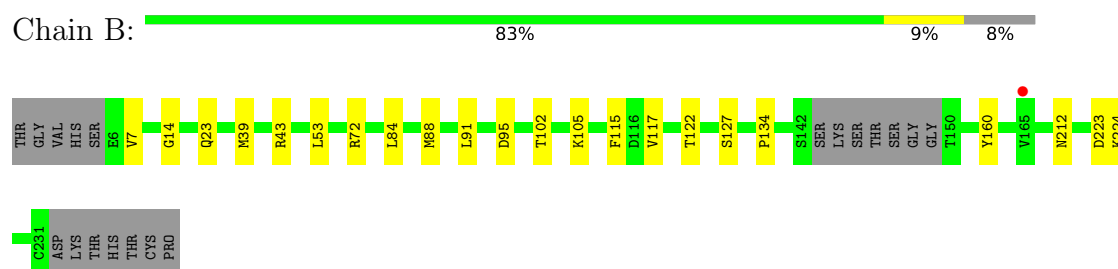
- Molecule 1: reticulocyte binding protein 2b



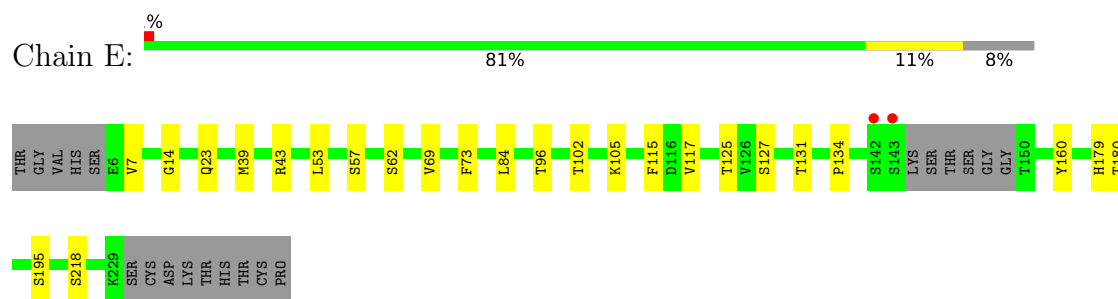
- Molecule 2: 273264 Fab heavy chain



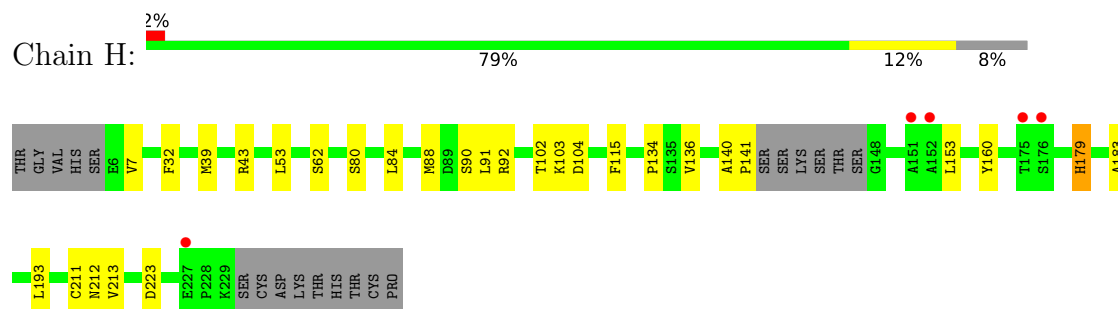
- Molecule 2: 273264 Fab heavy chain



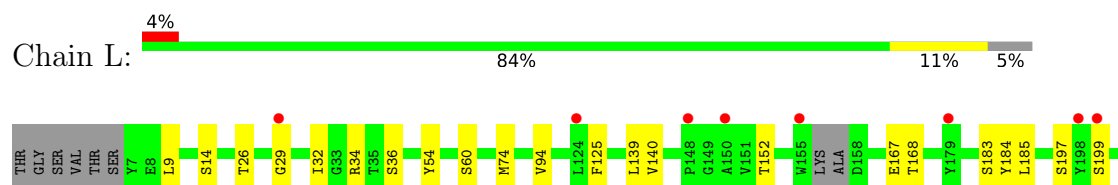
- Molecule 2: 273264 Fab heavy chain

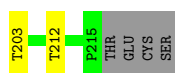


- Molecule 2: 273264 Fab heavy chain

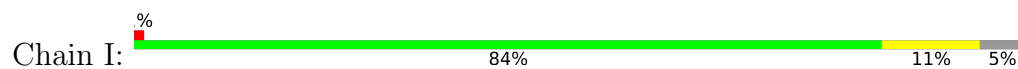


- Molecule 3: 273264 Fab light chain

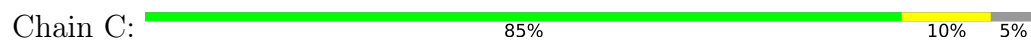




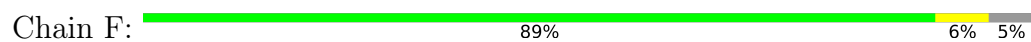
- Molecule 3: 273264 Fab light chain



- Molecule 3: 273264 Fab light chain



- Molecule 3: 273264 Fab light chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	93.99Å 99.51Å 103.49Å 114.72° 104.98° 89.81°	Depositor
Resolution (Å)	49.03 – 2.55 49.03 – 2.55	Depositor EDS
% Data completeness (in resolution range)	98.4 (49.03-2.55) 98.4 (49.03-2.55)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.64 (at 2.54Å)	Xtriage
Refinement program	PHENIX 1.15_3459	Depositor
R, R_{free}	0.208 , 0.255 0.208 , 0.255	Depositor DCC
R_{free} test set	5241 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	49.2	Xtriage
Anisotropy	0.380	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 43.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	22520	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.21% 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	0.24	0/2480	0.36	0/3347
1	D	0.24	0/2474	0.36	0/3337
1	G	0.25	0/2455	0.35	0/3311
1	J	0.24	0/2410	0.36	0/3255
2	B	0.27	0/1656	0.46	0/2257
2	E	0.26	0/1640	0.48	0/2237
2	H	0.28	0/1618	0.48	0/2210
2	K	0.28	0/1602	0.49	0/2190
3	C	0.24	0/1592	0.43	0/2183
3	F	0.25	0/1604	0.45	0/2198
3	I	0.25	0/1568	0.44	0/2158
3	L	0.25	0/1531	0.46	0/2106
All	All	0.25	0/22630	0.42	0/30789

There are no bond length outliers.

There are no bond angle outliers.

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	2433	0	2326	20	0
1	D	2426	0	2327	16	0
1	G	2408	0	2325	17	0
1	J	2363	0	2241	15	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1618	0	1548	12	0
2	E	1602	0	1528	15	0
2	H	1580	0	1481	18	0
2	K	1565	0	1444	27	0
3	C	1551	0	1450	12	0
3	F	1563	0	1468	11	0
3	I	1527	0	1393	16	0
3	L	1492	0	1343	18	0
4	A	57	0	0	0	0
4	B	47	0	0	0	0
4	C	25	0	0	0	0
4	D	47	0	0	1	0
4	E	36	0	0	0	0
4	F	36	0	0	0	0
4	G	49	0	0	2	0
4	H	37	0	0	0	0
4	I	11	0	0	1	0
4	J	28	0	0	0	0
4	K	12	0	0	1	0
4	L	7	0	0	0	0
All	All	22520	0	20874	183	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 4.

All (183) 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:H:88:MET:HB3	2:H:91:LEU:HD21	1.54	0.85
2:H:136:VAL:HG21	2:H:213:VAL:HG21	1.58	0.85
2:E:102:THR:HG21	2:E:115:PHE:HB3	1.71	0.73
3:L:32:ILE:H	3:L:32:ILE:HD12	1.53	0.72
1:D:193:ARG:HH12	1:D:234:SER:HB2	1.55	0.70
2:H:134:PRO:HB3	2:H:160:TYR:HB3	1.73	0.70
2:K:134:PRO:HB3	2:K:160:TYR:HB3	1.73	0.70
1:A:404:ALA:O	1:A:408:GLY:N	2.26	0.69
2:B:72:ARG:NH2	2:B:95:ASP:OD2	2.26	0.68
1:A:356:ASP:HA	1:A:359:ARG:HD2	1.77	0.65
3:C:31:ASN:HB3	3:C:34:ARG:HD2	1.78	0.65
3:L:29:GLY:N	3:L:32:ILE:HD11	2.12	0.64
3:I:34:ARG:NH1	3:I:97:SER:OG	2.31	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:143:ILE:HG12	3:I:202:VAL:HG21	1.79	0.64
2:K:215:HIS:HB3	2:K:220:THR:HB	1.80	0.63
1:D:222:HIS:HA	1:D:226:VAL:HG22	1.81	0.63
2:B:134:PRO:HB3	2:B:160:TYR:HB3	1.81	0.63
2:K:27:CYS:HB3	2:K:84:LEU:HB3	1.81	0.62
1:A:329:LEU:HD22	1:A:403:THR:HG22	1.82	0.62
3:I:174:GLN:OE1	2:H:179:HIS:NE2	2.32	0.62
3:L:36:SER:HB3	3:L:54:TYR:HA	1.81	0.62
2:B:14:GLY:H	2:B:122:THR:HG21	1.64	0.61
1:G:314:GLN:NE2	4:G:501:HOH:O	2.32	0.61
3:I:24:ARG:NH1	4:I:301:HOH:O	2.34	0.61
2:H:212:ASN:ND2	2:H:223:ASP:OD1	2.35	0.60
2:H:141:PRO:HG3	2:H:153:LEU:HB3	1.84	0.60
2:H:183:ALA:HB2	2:H:193:LEU:HD23	1.85	0.58
1:J:344:ILE:HD11	1:J:385:ILE:HG23	1.86	0.58
3:L:199:SER:OG	3:L:212:THR:HA	2.03	0.58
2:K:186:GLN:HG2	3:L:167:GLU:HG3	1.85	0.58
1:J:175:ILE:HD11	1:J:244:LYS:HG3	1.85	0.57
1:G:344:ILE:HD11	1:G:385:ILE:HG23	1.87	0.57
3:I:100:ASP:OD2	3:C:34:ARG:NH1	2.34	0.57
1:D:214:GLU:HG3	1:D:310:LEU:HA	1.86	0.56
2:E:53:LEU:HD22	2:E:69:VAL:HG21	1.86	0.56
1:D:193:ARG:HH12	1:D:234:SER:CB	2.19	0.56
1:D:193:ARG:NH1	4:D:502:HOH:O	2.35	0.56
1:J:356:ASP:HA	1:J:359:ARG:HD2	1.86	0.56
2:H:43:ARG:HD3	2:H:53:LEU:HD11	1.87	0.55
2:K:80:SER:OG	1:J:183:GLU:O	2.25	0.55
3:L:168:THR:HG22	3:L:183:SER:HB2	1.89	0.55
3:C:139:LEU:HD12	3:C:185:LEU:HD23	1.88	0.54
1:J:212:HIS:HE2	1:J:423:TYR:HH	1.56	0.54
3:I:34:ARG:HD2	3:I:35:THR:HG23	1.90	0.54
1:J:263:GLN:HG3	1:J:265:GLU:H	1.72	0.54
3:L:152:THR:HB	3:L:203:THR:HB	1.91	0.53
2:E:134:PRO:HB3	2:E:160:TYR:HB3	1.91	0.53
1:A:268:ASP:OD2	1:A:272:ARG:NH2	2.42	0.53
3:I:36:SER:HB3	3:I:54:TYR:HA	1.89	0.53
2:H:183:ALA:HA	2:H:193:LEU:HB3	1.91	0.53
1:D:207:ARG:O	1:D:210:SER:OG	2.21	0.52
3:C:115:GLN:HB2	3:C:147:TYR:CE1	2.44	0.52
2:K:43:ARG:HD3	2:K:53:LEU:HD11	1.91	0.52
1:D:362:GLU:HG3	1:D:371:ILE:HG21	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:9:LEU:HD11	3:C:94:VAL:HG22	1.93	0.51
3:F:203:THR:HG23	3:F:208:THR:HG22	1.91	0.51
3:I:138:THR:HG22	3:I:186:SER:HB2	1.93	0.51
1:J:416:LYS:O	1:J:420:LYS:HG3	2.11	0.51
1:G:315:ASP:HB3	1:G:413:GLN:OE1	2.11	0.51
3:C:27:CYS:HB3	3:C:75:ALA:HB3	1.92	0.51
3:I:188:THR:HG23	3:I:191:GLN:H	1.76	0.51
3:F:115:GLN:HB2	3:F:147:TYR:CZ	2.46	0.50
3:L:9:LEU:HD11	3:L:94:VAL:HG22	1.93	0.50
2:B:212:ASN:ND2	2:B:223:ASP:OD1	2.41	0.50
1:A:175:ILE:HD11	1:A:244:LYS:HG2	1.94	0.50
2:K:134:PRO:HD2	2:K:220:THR:HG21	1.94	0.50
1:D:226:VAL:HG12	1:D:299:ILE:HD13	1.93	0.50
1:D:356:ASP:HA	1:D:359:ARG:HD2	1.94	0.50
2:E:43:ARG:HB3	2:E:53:LEU:HD11	1.93	0.49
1:A:299:ILE:O	1:A:303:ILE:HD12	2.13	0.49
2:K:150:THR:HA	2:K:200:PRO:HA	1.93	0.49
2:E:39:MET:HB3	2:E:84:LEU:HD22	1.95	0.49
1:A:308:GLU:O	1:A:416:LYS:NZ	2.43	0.49
2:B:105:LYS:NZ	3:C:54:TYR:OH	2.44	0.49
1:G:221:ILE:HG23	1:G:225:LYS:HD2	1.94	0.49
1:D:193:ARG:NH1	1:D:234:SER:HB2	2.25	0.48
3:C:17:VAL:HG22	3:C:110:LEU:HD11	1.94	0.48
3:L:140:VAL:HG12	3:L:184:TYR:CE2	2.47	0.48
3:I:127:PRO:HD3	3:I:139:LEU:HG	1.95	0.48
3:I:55:ASP:OD2	1:G:360:LYS:NZ	2.42	0.48
2:K:168:SER:HB2	2:K:212:ASN:HB2	1.94	0.48
1:A:267:TYR:CZ	1:A:372:ASN:HB3	2.49	0.48
3:F:115:GLN:HB2	3:F:147:TYR:CE2	2.48	0.48
2:K:39:MET:HB3	2:K:84:LEU:HD22	1.96	0.48
3:F:187:LEU:HD12	3:F:188:THR:O	2.13	0.48
2:K:57:SER:HB3	2:K:62:SER:HB3	1.96	0.48
2:B:39:MET:HB3	2:B:84:LEU:HD22	1.95	0.47
1:J:199:ILE:HD11	1:J:229:LEU:HG	1.96	0.47
2:K:57:SER:O	2:K:77:ARG:NH1	2.46	0.47
1:A:189:ILE:HG12	1:A:196:PHE:HE1	1.79	0.47
1:A:428:ASN:O	1:A:432:ILE:HG12	2.15	0.47
1:G:338:GLU:H	1:G:338:GLU:CD	2.16	0.47
2:K:8:GLN:HB2	2:K:30:SER:OG	2.14	0.47
1:A:380:GLU:OE1	1:A:450:LYS:NZ	2.38	0.47
2:K:90:SER:O	2:K:90:SER:OG	2.31	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:380:GLU:OE2	1:D:450:LYS:NZ	2.39	0.46
1:G:287:ASN:HA	1:G:290:ARG:HG3	1.98	0.46
2:B:102:THR:OG1	2:B:115:PHE:HB3	2.16	0.46
3:I:36:SER:O	3:I:94:VAL:HG23	2.15	0.46
1:D:267:TYR:CZ	1:D:372:ASN:HB3	2.51	0.46
2:K:61:GLY:HA2	1:J:393:GLN:HG3	1.97	0.46
3:L:29:GLY:CA	3:L:32:ILE:HD11	2.46	0.46
1:A:206:LYS:O	1:A:210:SER:OG	2.33	0.45
3:L:26:THR:HB	3:L:74:MET:SD	2.56	0.45
2:H:211:CYS:O	2:H:223:ASP:HA	2.16	0.45
2:K:160:TYR:CE1	2:K:191:TYR:HB2	2.51	0.45
3:L:139:LEU:HB2	3:L:185:LEU:CD2	2.46	0.45
3:L:139:LEU:HB2	3:L:185:LEU:HD21	1.99	0.45
1:J:189:ILE:HG12	1:J:196:PHE:HE1	1.82	0.45
1:D:295:GLN:O	1:D:299:ILE:HG13	2.17	0.45
2:K:92:ARG:HD3	2:H:92:ARG:NH2	2.32	0.44
1:A:194:PRO:HB3	1:A:230:LEU:HD13	2.00	0.44
2:E:69:VAL:HG13	2:E:73:PHE:CG	2.51	0.44
1:G:356:ASP:HA	1:G:359:ARG:HD2	1.99	0.44
2:K:103:LYS:NZ	4:K:303:HOH:O	2.50	0.44
3:L:125:PHE:HB2	3:L:140:VAL:CG2	2.47	0.44
2:E:7:VAL:HG12	2:E:117:VAL:HG11	2.00	0.44
2:K:165:VAL:HB	2:K:193:LEU:HD21	1.99	0.44
2:K:215:HIS:CD2	2:K:217:PRO:HD2	2.53	0.44
1:A:362:GLU:HG3	1:A:371:ILE:HG21	1.98	0.44
3:F:187:LEU:HD11	3:F:192:TRP:HB2	1.99	0.44
1:G:179:ASP:O	1:G:282:ARG:NH1	2.47	0.44
2:K:170:ASN:HB2	2:K:174:LEU:HD13	2.00	0.44
2:B:14:GLY:HA2	2:B:23:GLN:OE1	2.18	0.44
2:E:96:THR:HG23	2:E:125:THR:HA	1.99	0.44
3:I:203:THR:OG1	3:I:208:THR:HG22	2.18	0.44
3:F:143:ILE:HG12	3:F:202:VAL:HG21	1.99	0.44
2:H:80:SER:HB3	1:G:185:ASN:HB2	2.00	0.43
1:G:196:PHE:HB2	1:G:199:ILE:HG13	2.00	0.43
2:K:201:SER:HA	2:K:204:LEU:HG	1.99	0.43
2:H:102:THR:OG1	2:H:115:PHE:HB3	2.18	0.43
2:K:41:TRP:CE2	2:K:86:LEU:HB2	2.53	0.43
3:C:151:VAL:HG12	3:C:204:HIS:HB2	2.00	0.43
2:K:167:VAL:HG11	2:K:195:SER:HB2	2.01	0.43
1:A:179:ASP:O	1:A:282:ARG:NH1	2.48	0.43
3:C:174:GLN:OE1	3:C:180:ALA:HB2	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:243:ALA:O	1:D:247:VAL:HG22	2.19	0.43
2:E:105:LYS:HE2	3:F:53:PHE:CD2	2.54	0.43
1:G:214:GLU:N	1:G:214:GLU:OE1	2.45	0.43
2:H:90:SER:OG	2:H:90:SER:O	2.33	0.43
2:K:11:GLU:OE1	2:K:101:CYS:N	2.45	0.43
3:L:29:GLY:H	3:L:32:ILE:HD11	1.80	0.43
2:B:7:VAL:HG12	2:B:117:VAL:HG11	2.01	0.43
3:C:197:SER:OG	3:C:198:TYR:N	2.52	0.42
2:K:139:LEU:HD12	3:L:125:PHE:CB	2.49	0.42
2:E:180:THR:HA	2:E:195:SER:HA	2.01	0.42
2:H:140:ALA:HA	2:H:141:PRO:HD3	1.90	0.42
1:G:267:TYR:CE1	1:G:372:ASN:HB3	2.54	0.42
3:F:31:ASN:OD1	3:F:34:ARG:NE	2.53	0.42
1:G:263:GLN:NE2	1:G:265:GLU:HB2	2.34	0.42
1:J:179:ASP:O	1:J:282:ARG:NH2	2.51	0.42
1:A:206:LYS:HG2	1:A:218:TYR:CZ	2.55	0.42
1:A:391:HIS:O	1:A:395:VAL:HG23	2.19	0.42
3:I:203:THR:HG23	3:I:208:THR:HG22	2.01	0.42
1:A:197:SER:HB3	1:A:435:PHE:CG	2.55	0.42
1:J:267:TYR:CE1	1:J:372:ASN:HB3	2.54	0.42
1:D:396:LYS:NZ	1:D:400:ASP:OD2	2.52	0.42
2:E:131:THR:HG22	2:E:218:SER:HB3	2.01	0.42
3:I:156:LYS:HA	3:I:160:SER:O	2.19	0.42
2:B:43:ARG:NE	2:B:53:LEU:HD21	2.34	0.41
2:E:102:THR:CG2	2:E:115:PHE:HB3	2.43	0.41
2:E:69:VAL:HG13	2:E:73:PHE:HB2	2.02	0.41
2:H:103:LYS:HE3	2:H:104:ASP:O	2.21	0.41
3:F:187:LEU:HD13	3:F:191:GLN:HB2	2.01	0.41
1:A:445:LYS:HE2	1:G:463:GLY:O	2.20	0.41
3:F:203:THR:HA	3:F:208:THR:HA	2.03	0.41
1:G:278:LYS:NZ	4:G:505:HOH:O	2.54	0.41
3:L:140:VAL:HG12	3:L:184:TYR:CD2	2.56	0.41
1:D:170:ASN:HB3	1:D:453:ILE:HG12	2.03	0.41
3:I:157:ALA:HB2	3:I:198:TYR:CE2	2.56	0.41
1:J:270:LYS:HA	1:J:270:LYS:HD3	1.84	0.41
2:B:224:LYS:HA	2:B:224:LYS:HD3	1.88	0.41
2:H:7:VAL:HG13	2:H:32:PHE:CD1	2.56	0.41
1:J:244:LYS:HB2	1:J:281:PHE:CE1	2.56	0.41
2:B:88:MET:HB3	2:B:91:LEU:HD21	2.03	0.40
1:A:264:ARG:NE	3:F:56:ASN:OD1	2.53	0.40
2:E:14:GLY:HA2	2:E:23:GLN:OE1	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:222:HIS:O	1:J:226:VAL:HG22	2.21	0.40
1:G:263:GLN:NE2	1:G:270:LYS:HE3	2.36	0.40
3:C:17:VAL:HG11	3:C:23:ALA:HA	2.03	0.40
2:E:57:SER:HB3	2:E:62:SER:OG	2.21	0.40
2:H:39:MET:HB3	2:H:84:LEU:HD22	2.04	0.40
2:K:139:LEU:HD12	3:L:125:PHE:HB3	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	299/307 (97%)	290 (97%)	9 (3%)	0	100	100
1	D	297/307 (97%)	286 (96%)	11 (4%)	0	100	100
1	G	295/307 (96%)	286 (97%)	9 (3%)	0	100	100
1	J	293/307 (95%)	286 (98%)	7 (2%)	0	100	100
2	B	215/238 (90%)	207 (96%)	8 (4%)	0	100	100
2	E	214/238 (90%)	208 (97%)	6 (3%)	0	100	100
2	H	214/238 (90%)	208 (97%)	6 (3%)	0	100	100
2	K	213/238 (90%)	209 (98%)	4 (2%)	0	100	100
3	C	207/219 (94%)	198 (96%)	9 (4%)	0	100	100
3	F	207/219 (94%)	199 (96%)	8 (4%)	0	100	100
3	I	207/219 (94%)	197 (95%)	10 (5%)	0	100	100
3	L	203/219 (93%)	191 (94%)	12 (6%)	0	100	100
All	All	2864/3056 (94%)	2765 (96%)	99 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	253/286 (88%)	247 (98%)	6 (2%)	49	64
1	D	255/286 (89%)	253 (99%)	2 (1%)	81	88
1	G	255/286 (89%)	252 (99%)	3 (1%)	71	81
1	J	244/286 (85%)	240 (98%)	4 (2%)	62	77
2	B	175/200 (88%)	174 (99%)	1 (1%)	86	92
2	E	174/200 (87%)	172 (99%)	2 (1%)	73	83
2	H	166/200 (83%)	164 (99%)	2 (1%)	71	81
2	K	162/200 (81%)	159 (98%)	3 (2%)	57	72
3	C	168/185 (91%)	166 (99%)	2 (1%)	71	81
3	F	170/185 (92%)	170 (100%)	0	100	100
3	I	163/185 (88%)	162 (99%)	1 (1%)	86	92
3	L	153/185 (83%)	149 (97%)	4 (3%)	46	61
All	All	2338/2684 (87%)	2308 (99%)	30 (1%)	69	80

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	198	ASN
1	A	335	MET
1	A	340	TYR
1	A	357	MET
1	A	439	SER
1	A	470	SER
2	K	112	HIS
2	K	123	MET
2	K	127	SER
3	L	14	SER
3	L	34	ARG
3	L	60	SER
3	L	197	SER
2	B	127	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	E	127	SER
2	E	179	HIS
3	I	186	SER
2	H	62	SER
2	H	179	HIS
1	G	184	SER
1	G	190	SER
1	G	197	SER
3	C	16	SER
3	C	194	SER
1	J	263	GLN
1	J	350	SER
1	J	357	MET
1	J	431	SER
1	D	170	ASN
1	D	193	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	319	ASN
3	L	115	GLN
2	B	186	GLN
1	J	241	ASN
1	J	372	ASN

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 monosaccharides 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 ⓘ

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	301/307 (98%)	-0.12	3 (0%) 82 86	38, 50, 74, 87	0
1	D	299/307 (97%)	-0.14	1 (0%) 94 96	37, 50, 68, 81	0
1	G	297/307 (96%)	-0.24	0 100 100	35, 51, 67, 77	0
1	J	295/307 (96%)	-0.17	0 100 100	41, 57, 77, 86	0
2	B	219/238 (92%)	-0.14	1 (0%) 91 94	33, 45, 73, 84	0
2	E	218/238 (91%)	-0.16	2 (0%) 84 88	34, 46, 79, 90	0
2	H	218/238 (91%)	-0.09	5 (2%) 60 67	37, 56, 95, 100	0
2	K	217/238 (91%)	0.00	5 (2%) 60 67	38, 58, 90, 99	0
3	C	209/219 (95%)	-0.23	1 (0%) 91 94	35, 52, 67, 74	0
3	F	209/219 (95%)	-0.25	0 100 100	34, 54, 68, 79	0
3	I	209/219 (95%)	0.06	3 (1%) 75 81	40, 61, 93, 104	0
3	L	207/219 (94%)	0.24	8 (3%) 39 45	44, 69, 98, 109	0
All	All	2898/3056 (94%)	-0.11	29 (1%) 82 86	33, 54, 85, 109	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	K	152	ALA	4.8
2	K	151	ALA	3.6
2	H	151	ALA	3.5
3	L	198	TYR	3.4
1	D	218	TYR	3.0
2	K	204	LEU	2.8
2	K	173	ALA	2.5
3	I	164	ALA	2.5
1	A	409	VAL	2.5
1	A	224	THR	2.4
3	I	137	ALA	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	L	199	SER	2.3
3	L	148	PRO	2.3
2	H	175	THR	2.3
3	I	142	LEU	2.3
2	H	227	GLU	2.3
3	L	124	LEU	2.2
2	E	143	SER	2.2
1	A	408	GLY	2.2
2	H	176	SER	2.2
2	K	206	THR	2.1
3	L	179	TYR	2.1
3	L	155	TRP	2.1
2	H	152	ALA	2.1
3	L	150	ALA	2.1
3	C	129	SER	2.0
2	B	165	VAL	2.0
2	E	142	SER	2.0
3	L	29	GLY	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.