



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 10, 2023 – 02:39 PM EDT

PDB ID : 6WTV
Title : Plasmodium vivax reticulocyte binding protein 2b (PvRBP2b) bound to human monoclonal antibody 258259
Authors : Chan, L.J.; Dietrich, M.H.; Tham, W.H.
Deposited on : 2020-05-04
Resolution : 3.05 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.35.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35.1

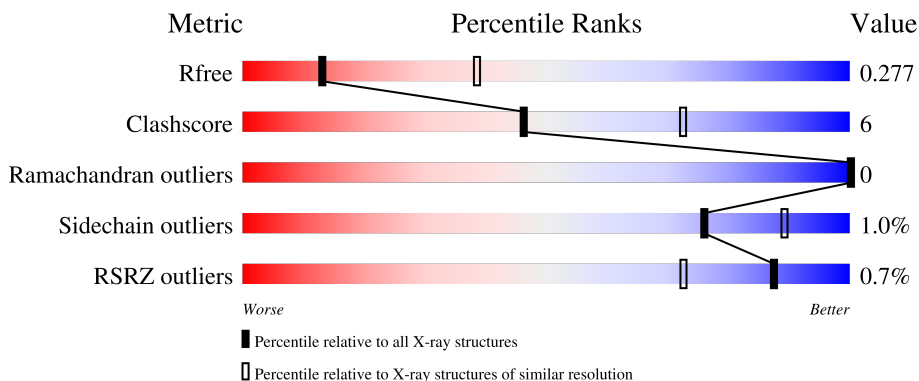
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.05 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	1754 (3.10-3.02)
Clashscore	141614	1864 (3.10-3.02)
Ramachandran outliers	138981	1794 (3.10-3.02)
Sidechain outliers	138945	1793 (3.10-3.02)
RSRZ outliers	127900	1713 (3.10-3.02)

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	85% 12% ..
1	D	307	87% 11% ..
1	G	307	86% 10% .
1	J	307	78% 18% .
2	C	219	79% 16% 5%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	F	219	 78% 16% 6%
2	I	219	 2% 70% 16% 14%
2	L	219	 5% 75% 8% 17%
3	B	238	 73% 17% 10%
3	E	238	 71% 18% 10%
3	H	238	 % 68% 16% 16%
3	K	238	 66% 17% 17%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 20978 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
			Total	C	N	O	S			
1	A	299	2343	1508	393	433	9	0	0	0
1	G	295	2331	1497	385	440	9	0	0	0
1	J	296	2335	1504	388	434	9	0	0	0
1	D	303	2338	1504	389	436	9	0	0	0

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 258259 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	209	Total	C	N	O	S	0	0	0
			1520	958	254	303	5			
2	I	188	Total	C	N	O	S	0	0	0
			1313	816	220	272	5			
2	L	181	Total	C	N	O	S	0	0	0
			1264	800	208	251	5			
2	F	206	Total	C	N	O	S	0	0	0
			1517	954	256	302	5			


- Molecule 3 is a protein called 258259 Fab heavy chain.

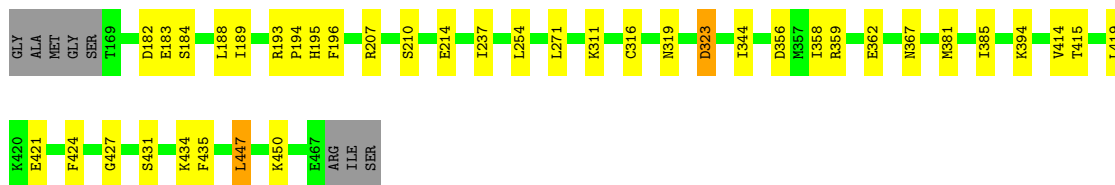
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	B	215	Total	C	N	O	S	0	0	0
			1576	1000	261	307	8			
3	H	201	Total	C	N	O	S	0	0	0
			1450	918	239	285	8			
3	K	197	Total	C	N	O	S	0	0	0
			1433	905	236	284	8			
3	E	214	Total	C	N	O	S	0	0	0
			1558	989	260	301	8			

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.

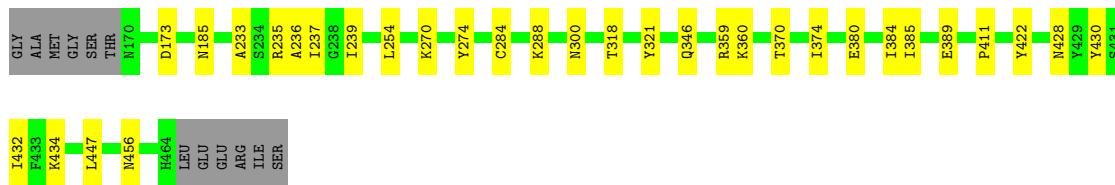
- Molecule 1: reticulocyte binding protein 2b

Chain A: 




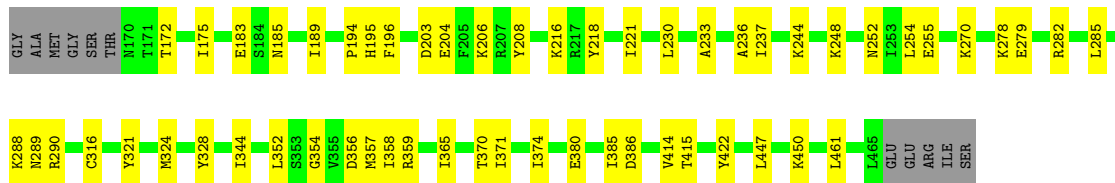
- Molecule 1: reticulocyte binding protein 2b

Chain G: 




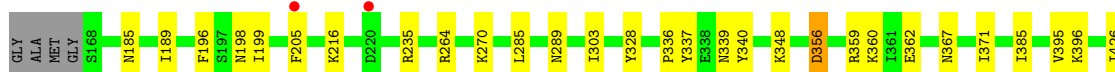
- Molecule 1: reticulocyte binding protein 2b

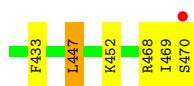
Chain J: 



- Molecule 1: reticulocyte binding protein 2b

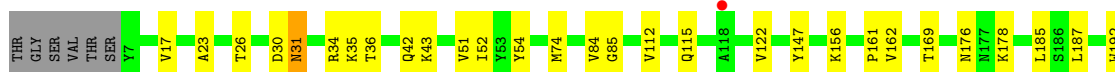
Chain D: 





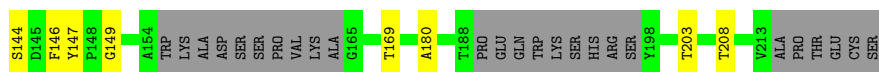
- Molecule 2: 258259 Fab light chain

Chain C: 79% 16% 5%



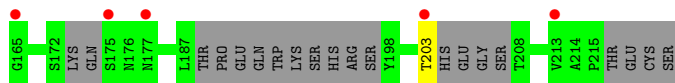
- Molecule 2: 258259 Fab light chain

Chain I: 2% 70% 16% 14%



- Molecule 2: 258259 Fab light chain

Chain L: 5% 75% 8% 17%



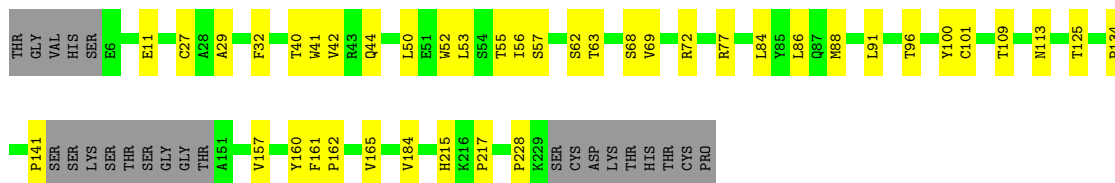
- Molecule 2: 258259 Fab light chain

Chain F: 78% 16% 6%

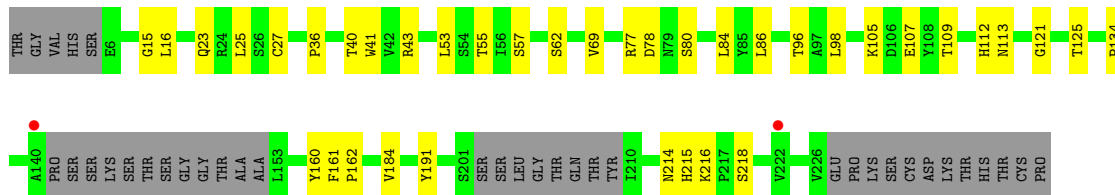


- Molecule 3: 258259 Fab heavy chain

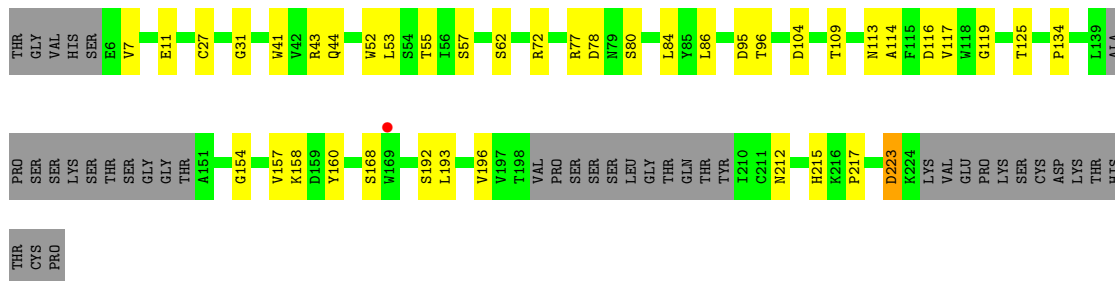
Chain B: 73% 17% 10%



• Molecule 3: 258259 Fab heavy chain



• Molecule 3: 258259 Fab heavy chain



• Molecule 3: 258259 Fab heavy chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	93.80Å 98.65Å 103.09Å 114.15° 105.00° 89.69°	Depositor
Resolution (Å)	45.01 – 3.05 49.17 – 3.05	Depositor EDS
% Data completeness (in resolution range)	98.1 (45.01-3.05) 98.1 (49.17-3.05)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.76 (at 3.07Å)	Xtrriage
Refinement program	PHENIX 1.15_3459	Depositor
R, R_{free}	0.235 , 0.277 0.235 , 0.277	Depositor DCC
R_{free} test set	3026 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	45.0	Xtrriage
Anisotropy	0.329	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 33.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	20978	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.90% 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	0.23	0/2390	0.34	0/3235
1	D	0.24	0/2383	0.34	0/3229
1	G	0.23	0/2379	0.34	0/3223
1	J	0.23	0/2382	0.34	0/3220
2	C	0.24	0/1560	0.43	0/2146
2	F	0.25	0/1556	0.44	0/2137
2	I	0.24	0/1341	0.44	0/1843
2	L	0.24	0/1291	0.44	0/1775
3	B	0.25	0/1615	0.45	0/2206
3	E	0.25	0/1596	0.45	0/2180
3	H	0.25	0/1485	0.45	0/2030
3	K	0.25	0/1467	0.46	0/2002
All	All	0.24	0/21445	0.40	0/29226

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	2343	0	2174	22	0
1	D	2338	0	2131	21	0
1	G	2331	0	2159	18	0
1	J	2335	0	2187	33	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	1520	0	1391	20	0
2	F	1517	0	1404	25	0
2	I	1313	0	1138	21	0
2	L	1264	0	1115	11	0
3	B	1576	0	1490	23	0
3	E	1558	0	1453	29	0
3	H	1450	0	1315	28	0
3	K	1433	0	1312	25	0
All	All	20978	0	19269	253	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 6.

All (253) 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)
3:K:72:ARG:NH2	3:K:95:ASP:OD2	2.21	0.73
1:J:185:ASN:HB2	3:K:80:SER:HB3	1.71	0.72
3:B:27:CYS:HB3	3:B:84:LEU:HB3	1.73	0.71
3:K:109:THR:HG21	3:K:113:ASN:HB2	1.72	0.70
3:B:109:THR:HG21	3:B:113:ASN:HB2	1.73	0.70
3:B:57:SER:HB3	3:B:62:SER:HB3	1.75	0.69
1:J:175:ILE:HD11	1:J:244:LYS:HG3	1.76	0.68
1:D:469:ILE:HG22	1:D:470:SER:H	1.57	0.67
2:F:87:GLU:OE1	2:F:173:LYS:NZ	2.26	0.67
2:L:29:GLY:H	2:L:32:ILE:HD11	1.61	0.66
1:J:218:TYR:HA	1:J:221:ILE:HG22	1.78	0.65
3:E:57:SER:O	3:E:77:ARG:NH1	2.29	0.65
1:J:248:LYS:O	1:J:252:ASN:ND2	2.30	0.65
2:I:7:TYR:N	2:I:96:ASP:OD1	2.31	0.64
3:E:64:TYR:OH	1:D:348:LYS:NZ	2.30	0.64
2:C:43:LYS:NZ	2:C:85:GLY:O	2.31	0.64
2:C:31:ASN:OD1	2:C:34:ARG:NH1	2.30	0.63
3:K:154:GLY:HA3	3:K:196:VAL:HG12	1.81	0.63
1:J:236:ALA:HB1	1:J:288:LYS:HB3	1.80	0.63
2:L:9:LEU:HD11	2:L:94:VAL:HB	1.81	0.62
2:I:65:ARG:NH2	2:I:86:ASP:OD2	2.33	0.62
1:J:356:ASP:HA	1:J:359:ARG:HD2	1.81	0.62
1:J:365:ILE:HD13	1:J:461:LEU:HD11	1.82	0.62
2:F:65:ARG:NH2	2:F:86:ASP:OD2	2.33	0.61
3:K:57:SER:HB2	3:K:62:SER:HB2	1.83	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:380:GLU:OE2	1:J:450:LYS:NZ	2.28	0.61
1:D:385:ILE:HG12	1:D:447:LEU:HD11	1.84	0.60
2:C:122:VAL:HG11	2:C:202:VAL:HG11	1.84	0.60
3:H:109:THR:HG21	3:H:113:ASN:HB2	1.82	0.60
1:A:188:LEU:HD23	1:A:435:PHE:HE2	1.66	0.60
3:E:22:SER:OG	3:E:87:GLN:NE2	2.34	0.60
3:H:40:THR:HG23	3:H:55:THR:HB	1.84	0.60
2:L:26:THR:OG1	2:L:74:MET:SD	2.59	0.59
3:K:212:ASN:ND2	3:K:223:ASP:OD1	2.32	0.59
2:F:26:THR:OG1	2:F:74:MET:SD	2.60	0.59
3:H:98:LEU:HD21	3:H:121:GLY:HA3	1.83	0.59
3:K:27:CYS:HB3	3:K:84:LEU:HB3	1.85	0.59
2:L:29:GLY:N	2:L:32:ILE:HD11	2.18	0.59
2:C:26:THR:OG1	2:C:74:MET:SD	2.62	0.58
2:F:51:VAL:HG12	2:F:52:ILE:HG12	1.86	0.58
3:E:88:MET:HB3	3:E:91:LEU:HD21	1.85	0.58
1:J:208:TYR:HE1	1:J:324:MET:HG3	1.68	0.58
3:E:223:ASP:OD1	3:E:223:ASP:N	2.35	0.58
3:K:52:TRP:HZ2	3:K:55:THR:HG22	1.68	0.58
2:C:169:THR:HG22	3:B:184:VAL:HB	1.86	0.57
1:G:236:ALA:HB1	1:G:288:LYS:HB3	1.87	0.57
2:I:26:THR:OG1	2:I:74:MET:SD	2.62	0.57
3:H:134:PRO:HB3	3:H:160:TYR:HB3	1.86	0.57
3:E:57:SER:HB3	3:E:62:SER:HB3	1.86	0.57
3:K:113:ASN:OD1	3:K:114:ALA:N	2.37	0.56
2:F:55:ASP:OD2	1:D:360:LYS:NZ	2.35	0.56
1:A:183:GLU:OE2	1:A:183:GLU:N	2.27	0.56
2:C:203:THR:HA	2:C:208:THR:HA	1.87	0.56
1:G:185:ASN:HB2	3:H:80:SER:HB3	1.86	0.56
3:K:44:GLN:OE1	2:L:42:GLN:NE2	2.32	0.56
2:F:84:VAL:HA	2:F:112:VAL:HG21	1.87	0.56
3:B:41:TRP:NE1	3:B:86:LEU:HB2	2.20	0.56
2:I:94:VAL:HG12	2:I:95:TRP:H	1.70	0.56
3:K:134:PRO:HB3	3:K:160:TYR:HB3	1.85	0.56
2:F:43:LYS:NZ	2:F:85:GLY:O	2.36	0.56
2:C:201:GLN:HG2	2:C:210:GLU:HB2	1.87	0.56
1:J:183:GLU:OE2	1:J:290:ARG:NH2	2.38	0.56
2:F:87:GLU:HG3	2:F:112:VAL:HG22	1.88	0.56
1:A:182:ASP:OD2	1:A:184:SER:OG	2.24	0.55
1:A:385:ILE:HG12	1:A:447:LEU:HD11	1.88	0.55
1:G:359:ARG:NH2	3:H:113:ASN:OD1	2.39	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:96:THR:HG23	3:E:125:THR:HA	1.88	0.55
3:B:40:THR:HG23	3:B:55:THR:HB	1.89	0.54
1:J:386:ASP:OD1	3:K:57:SER:OG	2.26	0.54
3:H:215:HIS:ND1	3:H:218:SER:OG	2.29	0.54
3:H:15:GLY:N	3:H:23:GLN:OE1	2.40	0.54
1:A:189:ILE:HG12	1:A:196:PHE:HE1	1.73	0.53
1:A:427:GLY:O	1:A:431:SER:OG	2.22	0.53
3:H:16:LEU:HB2	3:H:162:PRO:HG3	1.89	0.53
3:E:131:THR:HG22	3:E:162:PRO:HD3	1.91	0.53
1:G:389:GLU:OE1	3:H:62:SER:OG	2.27	0.53
2:F:122:VAL:HG11	2:F:202:VAL:HG11	1.90	0.53
2:I:40:TYR:HE2	2:I:93:GLN:HB3	1.74	0.53
2:C:17:VAL:HG11	2:C:23:ALA:HB2	1.91	0.52
1:J:344:ILE:HD11	1:J:385:ILE:HG23	1.91	0.52
2:F:187:LEU:HD12	2:F:191:GLN:HB3	1.91	0.52
3:K:104:ASP:OD2	3:K:109:THR:HB	2.10	0.51
1:A:356:ASP:OD2	2:C:35:LYS:HD3	2.11	0.51
3:H:96:THR:HG23	3:H:125:THR:HA	1.92	0.51
2:C:51:VAL:HG12	2:C:52:ILE:HG12	1.91	0.51
1:D:196:PHE:HB2	1:D:199:ILE:HG12	1.93	0.51
1:J:172:THR:OG1	1:J:255:GLU:OE2	2.29	0.51
2:F:40:TYR:HE1	2:F:93:GLN:HB3	1.76	0.51
2:I:100:ASP:OD2	2:F:34:ARG:NH2	2.44	0.51
3:E:45:ALA:HB3	3:E:48:LYS:HB2	1.92	0.51
1:G:456:ASN:HA	1:D:452:LYS:HE2	1.93	0.50
3:B:57:SER:O	3:B:77:ARG:NH1	2.43	0.50
1:A:193:ARG:HG2	1:A:194:PRO:HA	1.93	0.50
1:J:189:ILE:HG12	1:J:196:PHE:HE1	1.75	0.50
3:K:168:SER:HB2	3:K:212:ASN:HB2	1.92	0.50
1:D:189:ILE:HG12	1:D:196:PHE:HE1	1.76	0.50
2:C:156:LYS:HA	2:C:161:PRO:HA	1.92	0.50
1:A:358:ILE:O	1:A:362:GLU:HB2	2.12	0.50
3:K:43:ARG:HD3	3:K:53:LEU:HD21	1.93	0.50
3:E:134:PRO:HB3	3:E:160:TYR:HB3	1.94	0.50
2:C:36:THR:HB	2:C:54:TYR:HA	1.94	0.49
1:G:360:LYS:NZ	2:I:33:GLY:O	2.38	0.49
1:J:279:GLU:OE1	1:J:282:ARG:NH1	2.45	0.49
2:F:115:GLN:HB2	2:F:147:TYR:CE1	2.47	0.49
3:H:184:VAL:HB	2:I:169:THR:HG22	1.95	0.49
3:B:96:THR:HG23	3:B:125:THR:HA	1.95	0.49
3:H:41:TRP:CE2	3:H:86:LEU:HB2	2.47	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:120:PRO:HB3	2:I:146:PHE:HB3	1.94	0.49
3:E:42:VAL:HG13	3:E:100:TYR:HB2	1.94	0.49
1:G:428:ASN:O	1:G:432:ILE:HG12	2.13	0.49
3:E:69:VAL:HB	3:E:73:PHE:CG	2.48	0.49
3:E:215:HIS:CD2	3:E:217:PRO:HD2	2.48	0.49
1:J:203:ASP:HA	1:J:206:LYS:HD3	1.94	0.49
2:C:162:VAL:HG11	2:C:185:LEU:HD11	1.95	0.48
2:L:35:LYS:HG2	2:L:94:VAL:HG13	1.94	0.48
2:C:115:GLN:HB2	2:C:147:TYR:CE1	2.48	0.48
2:F:125:PHE:HB2	2:F:140:VAL:HB	1.96	0.48
3:H:78:ASP:OD1	3:H:80:SER:OG	2.25	0.48
2:L:51:VAL:HG12	2:L:52:ILE:HG12	1.94	0.48
3:E:41:TRP:NE1	3:E:86:LEU:HB2	2.28	0.48
1:J:285:LEU:O	1:J:289:ASN:ND2	2.36	0.48
1:J:385:ILE:HG12	1:J:447:LEU:HD11	1.95	0.48
1:A:359:ARG:O	1:D:264:ARG:NH2	2.36	0.48
2:L:32:ILE:HD12	2:L:32:ILE:H	1.78	0.48
3:H:214:ASN:HB3	3:H:216:LYS:HE3	1.95	0.47
3:E:184:VAL:HB	2:F:169:THR:HG22	1.95	0.47
3:E:186:GLN:HA	2:F:167:GLU:OE2	2.14	0.47
1:A:356:ASP:HA	1:A:359:ARG:HD2	1.96	0.47
3:B:68:SER:O	3:B:72:ARG:NH2	2.43	0.47
3:B:215:HIS:CD2	3:B:217:PRO:HD2	2.49	0.47
1:G:254:LEU:HD21	1:G:270:LYS:HB3	1.95	0.47
1:G:274:TYR:OH	1:G:380:GLU:OE2	2.25	0.47
3:H:36:PRO:HB2	3:H:107:GLU:HB2	1.96	0.47
3:B:42:VAL:HG13	3:B:100:TYR:HB2	1.97	0.47
3:B:88:MET:HE2	3:B:91:LEU:HD21	1.97	0.47
2:L:96:ASP:OD2	2:L:99:ASN:HB2	2.15	0.47
1:G:318:THR:OG1	1:G:411:PRO:O	2.26	0.47
3:H:41:TRP:NE1	3:H:86:LEU:HB2	2.29	0.47
3:E:40:THR:HG23	3:E:55:THR:HB	1.96	0.47
2:I:43:LYS:HG2	2:I:88:ALA:HB2	1.97	0.46
2:I:131:GLU:OE2	2:I:138:THR:OG1	2.22	0.46
3:H:105:LYS:HE2	2:I:53:TYR:CE2	2.49	0.46
1:J:371:ILE:HD13	1:J:374:ILE:HD12	1.97	0.46
3:E:162:PRO:HD2	3:E:217:PRO:HG2	1.97	0.46
2:I:144:SER:HA	2:I:180:ALA:HA	1.98	0.46
2:C:84:VAL:HA	2:C:112:VAL:HG21	1.98	0.46
2:C:115:GLN:HB2	2:C:147:TYR:CZ	2.51	0.46
3:B:56:ILE:HG13	3:B:63:THR:HG22	1.96	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:134:PRO:HB3	3:B:160:TYR:HB3	1.96	0.46
1:J:208:TYR:CE1	1:J:324:MET:HG3	2.48	0.46
2:F:36:THR:HB	2:F:54:TYR:HA	1.96	0.46
1:D:185:ASN:ND2	1:D:185:ASN:O	2.48	0.46
2:C:42:GLN:OE1	3:B:44:GLN:NE2	2.45	0.46
2:F:115:GLN:HB2	2:F:147:TYR:CZ	2.51	0.46
3:H:25:LEU:HD12	3:H:86:LEU:HD23	1.98	0.46
3:H:53:LEU:HG	3:H:69:VAL:HG11	1.98	0.46
3:K:215:HIS:CD2	3:K:217:PRO:HD2	2.51	0.46
1:J:414:VAL:HG12	1:J:415:THR:H	1.80	0.46
2:I:35:LYS:HD3	2:I:94:VAL:HG11	1.97	0.45
1:A:381:MET:HG2	1:A:450:LYS:HB3	1.99	0.45
1:J:370:THR:O	1:J:374:ILE:HG13	2.17	0.45
1:D:270:LYS:HD2	1:D:270:LYS:HA	1.74	0.45
1:D:362:GLU:HG3	1:D:371:ILE:HG21	1.98	0.45
1:A:195:HIS:ND1	1:A:237:ILE:HG13	2.32	0.45
1:A:254:LEU:HD13	1:A:271:LEU:HD23	1.98	0.45
1:A:316:CYS:HB3	1:A:419:LEU:HD22	1.98	0.45
1:J:204:GLU:OE1	1:J:328:TYR:OH	2.28	0.45
3:E:161:PHE:HA	3:E:162:PRO:HA	1.79	0.45
1:J:321:TYR:CD1	1:J:422:TYR:HB3	2.52	0.45
1:G:380:GLU:O	1:G:384:ILE:HD12	2.16	0.45
3:B:53:LEU:HG	3:B:69:VAL:HG11	1.99	0.45
3:E:109:THR:HG21	1:D:359:ARG:HH22	1.82	0.45
3:E:112:HIS:NE2	1:D:356:ASP:OD2	2.50	0.45
1:D:216:LYS:HD2	1:D:216:LYS:HA	1.76	0.44
2:C:192:TRP:HH2	2:C:213:VAL:HG13	1.82	0.44
3:K:41:TRP:NE1	3:K:86:LEU:HB2	2.32	0.44
2:I:9:LEU:HD11	2:I:94:VAL:HG23	1.99	0.44
1:A:414:VAL:HG12	1:A:415:THR:H	1.83	0.44
1:J:278:LYS:HE3	1:J:279:GLU:OE2	2.18	0.44
1:J:354:GLY:O	1:J:358:ILE:HG12	2.17	0.44
3:K:158:LYS:HA	3:K:192:SER:HA	1.99	0.44
1:G:321:TYR:CD1	1:G:422:TYR:HB3	2.53	0.44
1:J:352:LEU:HD12	1:J:352:LEU:HA	1.88	0.44
3:B:52:TRP:HZ2	3:B:55:THR:HG22	1.83	0.44
2:I:29:GLY:N	2:I:32:ILE:HD11	2.33	0.44
2:L:10:THR:N	2:L:28:GLY:O	2.37	0.44
1:G:235:ARG:O	1:G:239:ILE:HG13	2.18	0.44
3:H:105:LYS:HB3	3:H:113:ASN:ND2	2.33	0.44
2:I:146:PHE:HE1	2:I:149:GLY:HA2	1.82	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:57:SER:HB3	3:H:62:SER:HB2	2.00	0.44
3:E:43:ARG:HG2	3:E:53:LEU:HD13	2.00	0.44
3:K:11:GLU:OE2	3:K:119:GLY:HA3	2.18	0.43
1:A:207:ARG:O	1:A:210:SER:OG	2.32	0.43
1:A:214:GLU:OE2	1:A:311:LYS:N	2.48	0.43
3:H:27:CYS:HB3	3:H:84:LEU:HB3	1.99	0.43
3:H:43:ARG:HD3	3:H:53:LEU:HD21	1.99	0.43
3:E:43:ARG:NH1	3:E:95:ASP:HA	2.32	0.43
1:G:385:ILE:HG12	1:G:447:LEU:HD11	2.00	0.43
3:H:215:HIS:CE1	3:H:218:SER:HG	2.29	0.43
3:H:57:SER:O	3:H:77:ARG:NH1	2.52	0.43
2:I:39:TRP:HB2	2:I:52:ILE:HB	2.00	0.43
1:G:173:ASP:OD1	1:G:173:ASP:N	2.49	0.43
2:I:203:THR:HA	2:I:208:THR:HA	2.00	0.43
2:F:39:TRP:CD2	2:F:77:LEU:HB2	2.53	0.43
3:E:105:LYS:HE2	2:F:53:TYR:CE2	2.54	0.43
1:J:195:HIS:ND1	1:J:237:ILE:HG13	2.33	0.43
1:J:216:LYS:HB2	1:J:216:LYS:HE3	1.83	0.43
3:K:116:ASP:OD1	3:K:117:VAL:N	2.52	0.42
3:E:169:TRP:HB3	3:E:174:LEU:HD23	2.01	0.42
2:F:54:TYR:HB2	2:F:57:ASP:OD2	2.19	0.42
3:B:157:VAL:HG11	3:B:165:VAL:HG11	2.00	0.42
3:E:165:VAL:HG12	3:E:215:HIS:CD2	2.53	0.42
1:D:336:PRO:HB2	1:D:339:ASN:HB2	2.01	0.42
1:J:194:PRO:HB3	1:J:230:LEU:HD12	2.01	0.42
3:K:57:SER:O	3:K:77:ARG:NH1	2.52	0.42
3:E:113:ASN:OD1	2:F:54:TYR:OH	2.32	0.42
1:D:337:TYR:OH	1:D:396:LYS:HD2	2.19	0.42
3:B:44:GLN:HB2	3:B:50:LEU:HD23	2.01	0.42
1:A:434:LYS:HE2	1:A:434:LYS:HB3	1.92	0.42
3:H:161:PHE:HA	3:H:162:PRO:HA	1.84	0.42
3:K:96:THR:HG23	3:K:125:THR:HA	2.02	0.42
2:I:115:GLN:HB2	2:I:147:TYR:CE1	2.55	0.42
1:D:395:VAL:HG13	1:D:433:PHE:HD1	1.84	0.42
3:B:29:ALA:HB1	3:B:32:PHE:HE1	1.85	0.41
1:D:367:ASN:O	1:D:469:ILE:HG12	2.20	0.41
3:H:160:TYR:O	3:H:191:TYR:N	2.46	0.41
3:E:106:ASP:HB2	3:E:113:ASN:HD21	1.85	0.41
3:B:141:PRO:HG3	3:B:228:PRO:HG3	2.02	0.41
1:G:370:THR:O	1:G:374:ILE:HG13	2.20	0.41
1:J:233:ALA:O	1:J:237:ILE:HG12	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:176:ASN:HB2	2:C:178:LYS:HG2	2.03	0.41
1:G:233:ALA:O	1:G:237:ILE:HG12	2.21	0.41
1:D:205:PHE:CD1	1:D:303:ILE:HG23	2.56	0.41
1:G:430:TYR:CE2	1:G:434:LYS:HD2	2.55	0.41
3:K:78:ASP:OD1	3:K:80:SER:OG	2.29	0.41
1:A:344:ILE:HD11	1:A:385:ILE:HG23	2.03	0.41
3:B:161:PHE:HA	3:B:162:PRO:HA	1.79	0.41
3:E:23:GLN:NE2	3:E:124:VAL:HG13	2.36	0.41
1:A:319:ASN:O	1:A:323:ASP:HB2	2.21	0.41
1:J:254:LEU:HD21	1:J:270:LYS:HB3	2.02	0.41
1:A:421:GLU:HA	1:A:424:PHE:HB2	2.03	0.40
3:K:7:VAL:HA	3:K:31:GLY:HA3	2.03	0.40
2:L:152:THR:OG1	2:L:203:THR:OG1	2.28	0.40
2:F:37:VAL:HG22	2:F:94:VAL:HG22	2.01	0.40
2:F:39:TRP:CE2	2:F:77:LEU:HB2	2.56	0.40
3:B:11:GLU:HG2	3:B:101:CYS:SG	2.61	0.40
1:J:183:GLU:CD	1:J:290:ARG:HH22	2.24	0.40
2:F:131:GLU:OE2	2:F:138:THR:OG1	2.30	0.40
1:D:328:TYR:HE2	1:D:426:ILE:HB	1.86	0.40
3:K:157:VAL:O	3:K:193:LEU:N	2.48	0.40
2:C:185:LEU:HD22	2:C:187:LEU:HD22	2.04	0.40
2:I:93:GLN:HB2	2:I:104:PHE:CD1	2.57	0.40
1:D:285:LEU:O	1:D:289:ASN:ND2	2.31	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	297/307 (97%)	290 (98%)	7 (2%)	0	100	100
1	D	301/307 (98%)	282 (94%)	19 (6%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	293/307 (95%)	285 (97%)	8 (3%)	0	100	100
1	J	294/307 (96%)	285 (97%)	9 (3%)	0	100	100
2	C	207/219 (94%)	192 (93%)	15 (7%)	0	100	100
2	F	202/219 (92%)	194 (96%)	8 (4%)	0	100	100
2	I	182/219 (83%)	171 (94%)	11 (6%)	0	100	100
2	L	169/219 (77%)	160 (95%)	9 (5%)	0	100	100
3	B	211/238 (89%)	204 (97%)	7 (3%)	0	100	100
3	E	210/238 (88%)	199 (95%)	11 (5%)	0	100	100
3	H	195/238 (82%)	187 (96%)	8 (4%)	0	100	100
3	K	191/238 (80%)	185 (97%)	6 (3%)	0	100	100
All	All	2752/3056 (90%)	2634 (96%)	118 (4%)	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	232/286 (81%)	228 (98%)	4 (2%)	60	82
1	D	226/286 (79%)	220 (97%)	6 (3%)	44	71
1	G	237/286 (83%)	234 (99%)	3 (1%)	69	86
1	J	235/286 (82%)	233 (99%)	2 (1%)	78	90
2	C	156/185 (84%)	154 (99%)	2 (1%)	69	86
2	F	159/185 (86%)	159 (100%)	0	100	100
2	I	127/185 (69%)	126 (99%)	1 (1%)	81	91
2	L	120/185 (65%)	119 (99%)	1 (1%)	81	91
3	B	167/200 (84%)	167 (100%)	0	100	100
3	E	160/200 (80%)	159 (99%)	1 (1%)	86	93
3	H	147/200 (74%)	146 (99%)	1 (1%)	84	92

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	K	148/200 (74%)	147 (99%)	1 (1%)	84	92
All	All	2114/2684 (79%)	2092 (99%)	22 (1%)	76	89

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	323	ASP
1	A	367	ASN
1	A	394	LYS
1	A	447	LEU
2	C	30	ASP
2	C	31	ASN
1	G	284	CYS
1	G	300	ASN
1	G	346	GLN
3	H	112	HIS
2	I	46	GLN
1	J	316	CYS
1	J	357	MET
3	K	223	ASP
2	L	89	ASP
3	E	98	LEU
1	D	198	ASN
1	D	235	ARG
1	D	340	TYR
1	D	356	ASP
1	D	447	LEU
1	D	468	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	397	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	299/307 (97%)	-0.41	0 100 100	21, 34, 56, 70	0
1	D	303/307 (98%)	-0.32	3 (0%) 82 63	19, 39, 66, 75	0
1	G	295/307 (96%)	-0.35	0 100 100	20, 38, 54, 64	0
1	J	296/307 (96%)	-0.34	0 100 100	24, 39, 57, 73	0
2	C	209/219 (95%)	-0.33	1 (0%) 91 79	25, 42, 61, 80	0
2	F	206/219 (94%)	-0.43	0 100 100	20, 37, 55, 67	0
2	I	188/219 (85%)	-0.06	4 (2%) 63 39	24, 48, 78, 83	0
2	L	181/219 (82%)	0.12	10 (5%) 25 10	25, 51, 78, 90	0
3	B	215/238 (90%)	-0.25	0 100 100	19, 32, 71, 82	0
3	E	214/238 (89%)	-0.24	0 100 100	19, 30, 72, 94	0
3	H	201/238 (84%)	-0.23	2 (0%) 82 63	21, 36, 69, 82	0
3	K	197/238 (82%)	-0.31	1 (0%) 91 79	23, 37, 73, 84	0
All	All	2804/3056 (91%)	-0.28	21 (0%) 87 72	19, 38, 70, 94	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	177	ASN	3.6
2	I	120	PRO	3.5
3	H	140	ALA	3.4
1	D	470	SER	3.1
2	L	127	PRO	3.1
3	K	169	TRP	2.9
2	L	165	GLY	2.8
2	L	126	PRO	2.8
1	D	220	ASP	2.6
1	D	205	PHE	2.6
2	L	120	PRO	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	L	203	THR	2.3
2	I	126	PRO	2.3
2	L	175	SER	2.2
3	H	222	VAL	2.1
2	I	124	LEU	2.1
2	L	213	VAL	2.1
2	L	114	GLY	2.1
2	I	129	SER	2.1
2	C	118	ALA	2.0
2	L	124	LEU	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.