Full wwPDB X-ray Structure Validation Report ⓘ

Oct 9, 2023 – 01:57 PM EDT

PDB ID	:	6WOZ
Title	:	Plasmodium vivax reticulocyte binding protein 2b (PvRBP2b) bound to human monoclonal antibody 251249
Authors	:	Chan, L.J.; Dietrich, M.H.; Tham, W.H.
Deposited on	:	2020-04-26
Resolution	:	2.90 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:

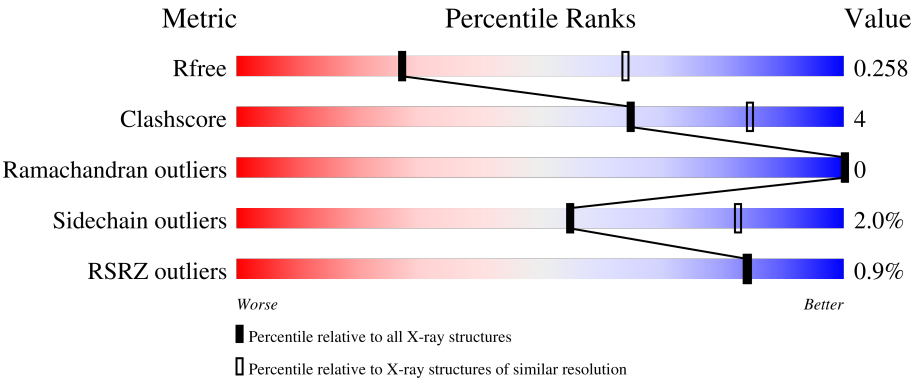
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 <=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% 11% ·
1	D	307	% 84% 12% ·
1	G	307	% 86% 11% ·
1	J	307	% 85% 11% ·
2	B	241	85% 9% 6%

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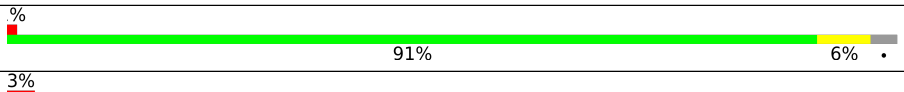
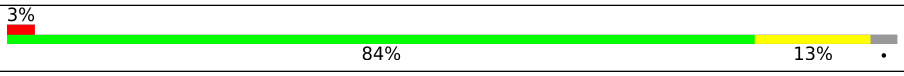
Mol	Chain	Length	Quality of chain
2	E	241	
2	H	241	
2	K	241	
3	C	219	
3	F	219	
3	I	219	
3	L	219	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 22580 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	J	297	Total	C	N	O	S	0	0	0
			2354	1514	392	439	9			
1	D	296	Total	C	N	O	S	0	0	0
			2390	1536	403	442	9			
1	A	296	Total	C	N	O	S	0	0	0
			2396	1541	400	446	9			
1	G	298	Total	C	N	O	S	0	0	0
			2407	1547	402	449	9			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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
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

- Molecule 2 is a protein called 251249 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	229	Total	C	N	O	S	0	0	0
			1674	1068	271	329	6			
2	B	227	Total	C	N	O	S	0	0	0
			1669	1065	269	329	6			
2	H	227	Total	C	N	O	S	0	0	0
			1668	1064	271	327	6			
2	K	226	Total	C	N	O	S	0	0	0
			1658	1057	267	328	6			

- Molecule 3 is a protein called 251249 Fab light chain.

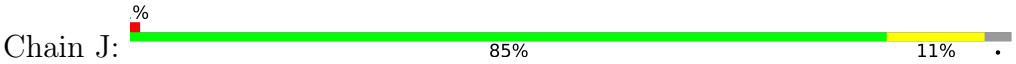
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	213	Total	C	N	O	S	0	0	0
			1593	995	271	323	4			
3	C	213	Total	C	N	O	S	0	0	0
			1603	1006	269	324	4			
3	I	213	Total	C	N	O	S	0	0	0
			1586	994	268	320	4			
3	L	213	Total	C	N	O	S	0	0	0
			1582	991	263	324	4			

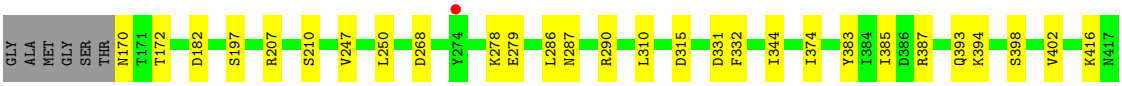
3 Residue-property plots (i)

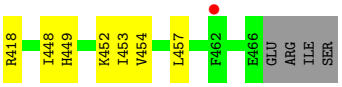
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

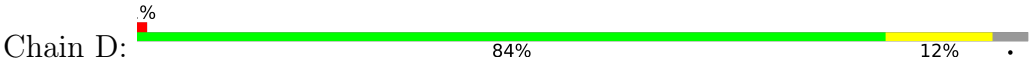


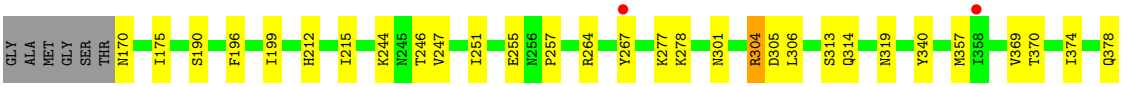




• Molecule 1: reticulocyte binding protein 2b

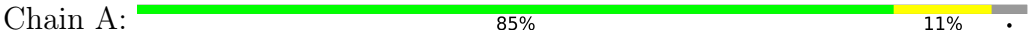
Chain D:

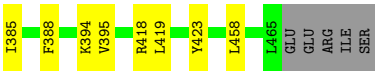




• Molecule 1: reticulocyte binding protein 2b

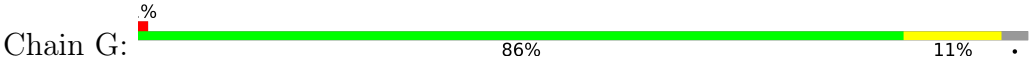
Chain A:





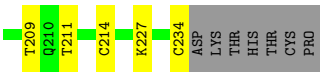
• Molecule 1: reticulocyte binding protein 2b

Chain G:



• Molecule 2: 251249 Fab heavy chain

Chain E:

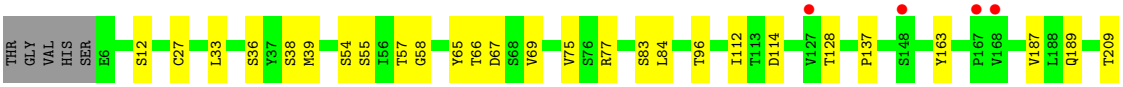


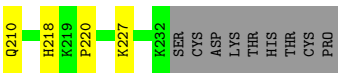
• Molecule 2: 251249 Fab heavy chain

Chain B:

• Molecule 2: 251249 Fab heavy chain

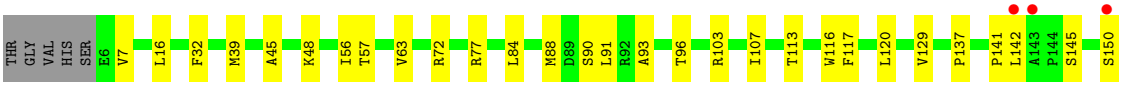
Chain H:

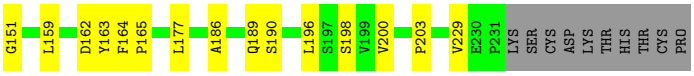




• Molecule 2: 251249 Fab heavy chain

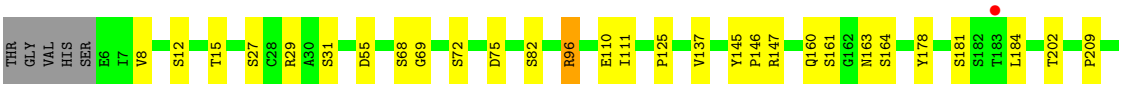
Chain K:





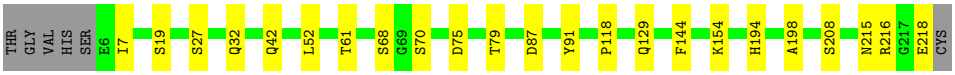
• Molecule 3: 251249 Fab light chain

Chain F:



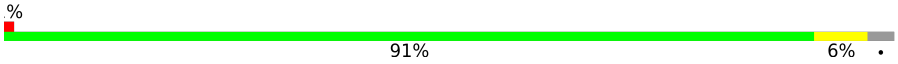
• Molecule 3: 251249 Fab light chain

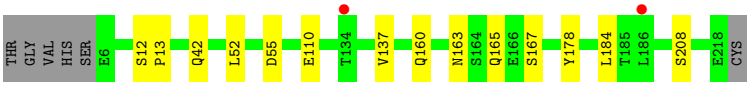
Chain C:



• Molecule 3: 251249 Fab light chain

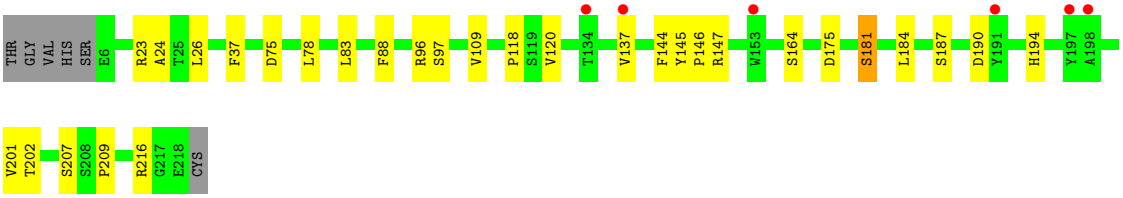
Chain I:





• Molecule 3: 251249 Fab light chain

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	99.57Å 163.55Å 121.76Å 90.00° 99.19° 90.00°	Depositor
Resolution (Å)	49.15 – 2.90 49.14 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.15-2.90) 99.9 (49.14-2.90)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.41 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.15_3459	Depositor
R, R_{free}	0.211 , 0.258 0.211 , 0.258	Depositor DCC
R_{free} test set	4253 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	64.4	Xtriage
Anisotropy	0.165	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 33.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	22580	wwPDB-VP
Average B, all atoms (Å^2)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 33.40 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 8.0486e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.25	0/2443	0.35	0/3294
1	D	0.24	0/2438	0.36	0/3291
1	G	0.25	0/2456	0.36	0/3319
1	J	0.24	0/2402	0.35	0/3248
2	B	0.26	0/1711	0.46	0/2341
2	E	0.26	0/1716	0.45	0/2350
2	H	0.26	0/1710	0.46	0/2341
2	K	0.26	0/1700	0.45	0/2329
3	C	0.26	0/1638	0.45	0/2232
3	F	0.25	0/1628	0.45	0/2221
3	I	0.25	0/1621	0.46	0/2213
3	L	0.25	0/1617	0.44	0/2209
All	All	0.25	0/23080	0.42	0/31388

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

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	2396	0	2314	18	0
1	D	2390	0	2282	22	0
1	G	2407	0	2295	19	0
1	J	2354	0	2203	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1669	0	1575	14	0
2	E	1674	0	1567	20	0
2	H	1668	0	1577	20	0
2	K	1658	0	1558	24	0
3	C	1603	0	1513	9	0
3	F	1593	0	1488	13	0
3	I	1586	0	1481	7	0
3	L	1582	0	1463	14	0
All	All	22580	0	21316	181	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 (181) 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:K:96:THR:HG22	2:K:129:VAL:H	1.38	0.87
3:F:125:PRO:HD3	3:F:137:VAL:HG22	1.64	0.79
3:F:164:SER:HB2	3:F:184:LEU:HA	1.70	0.73
2:B:137:PRO:HB3	2:B:163:TYR:HB3	1.73	0.71
2:H:96:THR:HG23	2:H:128:THR:HA	1.75	0.69
3:F:55:ASP:OD1	3:F:96:ARG:NH1	2.27	0.68
3:F:160:GLN:HB3	3:F:163:ASN:HD21	1.58	0.68
2:H:189:GLN:HA	3:I:165:GLN:HE22	1.60	0.67
1:A:175:ILE:HD11	1:A:244:LYS:HG3	1.77	0.66
3:I:42:GLN:HB2	3:I:52:LEU:HD11	1.78	0.65
2:H:114:ASP:OD1	1:G:301:ASN:ND2	2.29	0.65
3:F:96:ARG:NH2	1:D:305:ASP:OD1	2.30	0.64
2:B:96:THR:HG23	2:B:128:THR:HA	1.79	0.64
3:C:42:GLN:HB2	3:C:52:LEU:HD11	1.78	0.63
1:G:365:ILE:HG21	1:G:461:LEU:HD11	1.81	0.63
1:G:385:ILE:HG12	1:G:447:LEU:HD11	1.80	0.63
3:C:215:ASN:HB2	3:C:218:GLU:HG3	1.81	0.62
1:D:170:ASN:OD1	1:D:456:ASN:ND2	2.32	0.62
2:E:96:THR:HG23	2:E:128:THR:HA	1.82	0.62
2:H:54:SER:OG	2:H:75:VAL:HG21	1.98	0.62
2:B:114:ASP:HB2	1:A:297:LYS:HD3	1.82	0.61
1:J:182:ASP:HB3	1:J:286:LEU:HD11	1.83	0.60
1:D:247:VAL:HG12	1:D:277:LYS:HB3	1.83	0.60
1:A:316:CYS:HB3	1:A:419:LEU:HD12	1.84	0.59
2:B:161:LYS:HA	2:B:195:SER:HB2	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:394:LYS:HG2	1:G:432:ILE:HG21	1.86	0.58
3:L:120:VAL:HG21	3:L:201:VAL:HG21	1.85	0.58
2:B:39:MET:HB3	2:B:84:LEU:HD22	1.86	0.57
1:A:218:TYR:O	1:A:222:HIS:N	2.32	0.57
2:K:186:ALA:HB2	2:K:196:LEU:HD23	1.85	0.57
3:L:26:LEU:HD13	3:L:78:LEU:HD23	1.87	0.57
1:D:196:PHE:HB2	1:D:199:ILE:HD12	1.86	0.56
3:C:154:LYS:HB2	3:C:198:ALA:HB3	1.87	0.56
1:J:207:ARG:O	1:J:210:SER:OG	2.23	0.55
3:C:194:HIS:O	3:C:216:ARG:NH2	2.38	0.55
2:B:102:ALA:HB1	2:B:118:PHE:HB3	1.89	0.55
2:B:139:VAL:HG21	2:B:216:VAL:HG11	1.89	0.55
2:K:16:LEU:HD22	2:K:165:PRO:HG3	1.90	0.54
3:L:194:HIS:O	3:L:216:ARG:NE	2.33	0.54
1:G:462:PHE:HA	1:G:465:LEU:HD11	1.89	0.54
3:F:202:THR:HG22	3:F:209:PRO:HB3	1.90	0.53
1:G:465:LEU:HD12	1:G:465:LEU:H	1.74	0.53
1:J:170:ASN:HA	1:J:453:ILE:HG12	1.89	0.53
2:H:39:MET:HB3	2:H:84:LEU:HD22	1.89	0.53
1:J:453:ILE:O	1:J:457:LEU:HG	2.08	0.53
2:H:218:HIS:CD2	2:H:220:PRO:HD2	2.44	0.53
1:J:247:VAL:HA	1:J:250:LEU:HB2	1.89	0.53
1:J:344:ILE:HD11	1:J:385:ILE:HG23	1.91	0.53
2:K:177:LEU:HD21	2:K:200:VAL:HG21	1.90	0.52
2:H:54:SER:OG	2:H:55:SER:N	2.40	0.52
1:D:374:ILE:O	1:D:378:GLN:HG3	2.10	0.52
1:J:393:GLN:HE22	2:E:211:THR:H	1.58	0.51
3:F:29:ARG:NH1	3:F:75:ASP:OD2	2.44	0.51
2:E:72:ARG:NH1	2:E:90:SER:O	2.43	0.51
2:E:38:SER:HB3	2:E:57:THR:HA	1.93	0.51
1:D:257:PRO:HB3	1:D:369:VAL:HG12	1.93	0.51
1:J:332:PHE:HE2	1:J:402:VAL:HG11	1.76	0.50
1:J:394:LYS:HD2	2:E:209:THR:HB	1.93	0.50
3:C:87:ASP:O	3:C:91:TYR:OH	2.26	0.50
1:A:394:LYS:HD2	2:H:209:THR:HB	1.92	0.50
1:J:310:LEU:O	1:J:416:LYS:NZ	2.44	0.50
2:K:39:MET:HB3	2:K:84:LEU:HD22	1.93	0.50
3:F:68:SER:OG	3:F:69:GLY:N	2.45	0.50
3:F:12:SER:O	3:F:27:SER:HB3	2.11	0.50
2:H:65:TYR:CE2	2:H:75:VAL:HG23	2.47	0.50
2:K:186:ALA:HA	2:K:196:LEU:HB3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:140:PHE:CE2	3:C:129:GLN:HG3	2.47	0.49
1:D:264:ARG:HA	1:D:264:ARG:HE	1.76	0.49
2:H:137:PRO:HB3	2:H:163:TYR:HB3	1.95	0.49
1:D:190:SER:HB2	1:D:435:PHE:CZ	2.47	0.49
2:K:137:PRO:HB3	2:K:163:TYR:HB3	1.94	0.49
1:D:251:ILE:O	1:D:255:GLU:HG2	2.12	0.48
2:E:37:TYR:HH	2:E:108:PHE:HE1	1.61	0.48
1:A:335:MET:CE	1:A:395:VAL:HG11	2.44	0.48
2:H:187:VAL:HG21	3:I:165:GLN:HB2	1.95	0.48
1:G:313:SER:O	1:G:416:LYS:N	2.40	0.48
2:E:114:ASP:OD1	1:D:301:ASN:ND2	2.44	0.47
2:H:33:LEU:HD22	2:H:36:SER:OG	2.13	0.47
2:B:45:ALA:HB3	2:B:48:LYS:HB2	1.97	0.47
1:D:246:THR:HG21	1:D:277:LYS:HD2	1.97	0.46
2:K:103:ARG:HB3	2:K:120:LEU:HB3	1.96	0.46
2:K:117:PHE:CZ	3:L:96:ARG:HG2	2.50	0.46
3:L:137:VAL:HG13	3:L:184:LEU:HB3	1.97	0.46
2:B:152:GLY:HA2	1:D:393:GLN:HB3	1.97	0.46
3:C:68:SER:HB2	3:C:79:THR:HB	1.96	0.46
1:D:175:ILE:HD11	1:D:244:LYS:HG3	1.97	0.46
2:K:88:MET:HB3	2:K:91:LEU:HD21	1.98	0.45
3:I:160:GLN:HG3	3:I:163:ASN:HD21	1.81	0.45
3:L:88:PHE:HA	3:L:109:VAL:HG23	1.97	0.45
1:J:172:THR:HA	1:J:449:HIS:HE2	1.80	0.45
3:L:145:TYR:CD1	3:L:146:PRO:HA	2.51	0.45
1:A:247:VAL:HG12	1:A:277:LYS:HB3	1.99	0.45
2:K:203:PRO:HG3	1:G:397:HIS:NE2	2.31	0.45
1:G:188:LEU:HD23	1:G:435:PHE:HE2	1.81	0.45
3:I:137:VAL:HG13	3:I:184:LEU:HB3	1.99	0.45
2:E:139:VAL:O	2:E:227:LYS:NZ	2.50	0.45
1:D:215:ILE:HB	1:D:306:LEU:HD21	1.99	0.45
2:B:203:PRO:HG3	1:D:397:HIS:CE1	2.52	0.45
2:E:114:ASP:O	1:D:304:ARG:NH2	2.51	0.45
1:D:313:SER:OG	1:D:314:GLN:N	2.50	0.45
1:A:223:LYS:O	1:A:227:ASN:ND2	2.47	0.45
3:L:24:ALA:HB2	3:L:83:LEU:HD11	1.99	0.45
2:K:150:SER:OG	2:K:151:GLY:N	2.47	0.44
3:L:37:PHE:HB3	3:L:96:ARG:HG3	1.99	0.44
1:J:383:TYR:O	1:J:387:ARG:HG2	2.16	0.44
1:G:323:ASP:O	1:G:327:ILE:HG13	2.17	0.44
1:J:398:SER:O	1:J:402:VAL:HG12	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:164:PHE:HA	2:K:165:PRO:HA	1.78	0.44
1:G:169:THR:OG1	1:G:456:ASN:OD1	2.34	0.44
1:A:212:HIS:NE2	1:A:423:TYR:OH	2.40	0.44
2:E:11:GLU:HG3	2:E:101:CYS:HB2	2.00	0.44
3:F:147:ARG:HD2	3:F:178:TYR:CE1	2.53	0.44
1:A:344:ILE:HD11	1:A:385:ILE:HG23	2.00	0.44
2:K:107:ILE:HB	2:K:113:THR:HG23	2.00	0.44
3:L:187:SER:HB2	3:L:190:ASP:H	1.82	0.44
1:A:204:GLU:OE1	1:A:328:TYR:OH	2.22	0.44
1:J:418:ARG:HH22	2:E:234:CYS:HA	1.82	0.43
2:K:57:THR:O	2:K:77:ARG:NH1	2.50	0.43
2:K:72:ARG:NH1	2:K:90:SER:O	2.49	0.43
2:H:227:LYS:HE3	2:H:227:LYS:HB2	1.85	0.43
2:H:66:THR:HG22	2:H:69:VAL:HG22	2.01	0.43
1:J:448:ILE:HG22	1:J:452:LYS:HE2	2.01	0.43
1:D:421:GLU:O	1:D:425:ASN:HB2	2.19	0.43
2:H:210:GLN:HE21	2:H:210:GLN:HB2	1.61	0.43
1:A:283:GLY:O	1:A:287:ASN:ND2	2.52	0.43
3:I:110:GLU:OE2	3:I:178:TYR:OH	2.21	0.43
2:K:56:ILE:HG13	2:K:63:VAL:HG12	2.00	0.43
2:K:93:ALA:O	2:K:96:THR:HG23	2.19	0.43
1:J:393:GLN:NE2	2:E:211:THR:H	2.16	0.43
1:A:358:ILE:HD11	1:A:458:LEU:HD21	2.00	0.43
2:H:57:THR:O	2:H:77:ARG:NH1	2.51	0.43
1:G:175:ILE:HD11	1:G:244:LYS:HG3	2.01	0.43
2:E:39:MET:HB3	2:E:84:LEU:HD22	2.00	0.43
1:J:287:ASN:HA	1:J:290:ARG:HG3	2.01	0.42
1:G:195:HIS:CE1	1:G:237:ILE:HG13	2.54	0.42
2:E:98:VAL:HG22	2:E:126:LEU:HB2	2.01	0.42
3:F:8:VAL:HG12	3:F:31:SER:HB3	2.01	0.42
1:J:418:ARG:NH2	2:E:234:CYS:HA	2.35	0.42
2:B:188:LEU:HG	2:B:194:TYR:CE1	2.54	0.42
1:D:278:LYS:HE2	1:D:278:LYS:HB3	1.83	0.42
1:A:419:LEU:HD21	1:A:423:TYR:CZ	2.54	0.42
1:G:351:TYR:HB2	1:G:381:MET:HE2	2.02	0.42
1:G:351:TYR:O	1:G:355:VAL:HG23	2.20	0.42
1:J:374:ILE:HG23	1:J:454:VAL:HG13	2.00	0.42
3:C:7:ILE:HG23	3:C:32:GLN:HG3	2.02	0.42
3:C:118:PRO:HB3	3:C:144:PHE:HB3	2.01	0.42
1:A:267:TYR:CZ	1:A:372:ASN:HB3	2.55	0.42
2:H:27:CYS:O	2:H:83:SER:HA	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:421:GLU:O	1:G:425:ASN:HB2	2.19	0.42
2:E:177:LEU:HD21	2:E:200:VAL:HG21	2.00	0.42
2:K:142:LEU:HD11	2:K:159:LEU:HB2	2.02	0.42
1:J:332:PHE:CE2	1:J:402:VAL:HG11	2.54	0.42
3:F:145:TYR:CG	3:F:146:PRO:HA	2.54	0.42
2:H:57:THR:OG1	2:H:58:GLY:N	2.51	0.42
2:K:141:PRO:HB3	2:K:229:VAL:HG22	2.02	0.42
1:J:315:ASP:OD1	1:J:315:ASP:N	2.53	0.41
2:K:162:ASP:OD1	2:K:189:GLN:NE2	2.53	0.41
1:G:235:ARG:O	1:G:239:ILE:HG13	2.20	0.41
2:E:11:GLU:CG	2:E:101:CYS:HB2	2.50	0.41
3:I:12:SER:HA	3:I:13:PRO:HA	1.91	0.41
2:K:45:ALA:HB3	2:K:48:LYS:HB2	2.01	0.41
3:L:202:THR:HG23	3:L:209:PRO:HG3	2.02	0.41
1:D:370:THR:O	1:D:374:ILE:HG13	2.21	0.41
1:A:362:GLU:HG3	1:A:371:ILE:HG21	2.03	0.41
2:H:112:ILE:HG22	1:G:297:LYS:HG3	2.03	0.41
2:K:7:VAL:HG13	2:K:32:PHE:HD1	1.86	0.41
1:G:263:GLN:HE22	1:G:265:GLU:HG3	1.86	0.41
1:A:340:TYR:HD1	1:A:388:PHE:HZ	1.68	0.41
2:E:65:TYR:CE1	2:E:75:VAL:HG23	2.56	0.41
3:L:181:SER:O	3:L:181:SER:OG	2.36	0.41
3:L:118:PRO:HB3	3:L:144:PHE:HB3	2.03	0.41
2:H:38:SER:HB3	2:H:57:THR:HA	2.03	0.40
2:K:116:TRP:HB2	3:L:96:ARG:HB2	2.03	0.40
2:E:90:SER:O	2:E:90:SER:OG	2.39	0.40
1:J:278:LYS:NZ	1:J:279:GLU:OE1	2.54	0.40
2:B:88:MET:HE1	2:B:127:VAL:HG21	2.04	0.40
1:D:319:ASN:OD1	1:D:319:ASN:N	2.54	0.40
2:B:114:ASP:HB3	1:A:301:ASN:HD21	1.85	0.40
2:E:172:TRP:CH2	2:E:214:CYS:HB3	2.56	0.40
3:F:110:GLU:HG2	3:F:111:ILE:N	2.37	0.40
1:D:212:HIS:HB2	1:D:215:ILE:HG12	2.02	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	294/307 (96%)	284 (97%)	10 (3%)	0	100	100
1	D	294/307 (96%)	288 (98%)	6 (2%)	0	100	100
1	G	296/307 (96%)	287 (97%)	9 (3%)	0	100	100
1	J	295/307 (96%)	284 (96%)	11 (4%)	0	100	100
2	B	225/241 (93%)	218 (97%)	7 (3%)	0	100	100
2	E	227/241 (94%)	220 (97%)	7 (3%)	0	100	100
2	H	225/241 (93%)	217 (96%)	8 (4%)	0	100	100
2	K	224/241 (93%)	215 (96%)	9 (4%)	0	100	100
3	C	211/219 (96%)	198 (94%)	13 (6%)	0	100	100
3	F	211/219 (96%)	202 (96%)	9 (4%)	0	100	100
3	I	211/219 (96%)	204 (97%)	7 (3%)	0	100	100
3	L	211/219 (96%)	198 (94%)	13 (6%)	0	100	100
All	All	2924/3068 (95%)	2815 (96%)	109 (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	253/286 (88%)	249 (98%)	4 (2%)	62	86
1	D	248/286 (87%)	243 (98%)	5 (2%)	55	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	G	252/286 (88%)	249 (99%)	3 (1%)	71 91
1	J	238/286 (83%)	235 (99%)	3 (1%)	69 90
2	B	180/207 (87%)	178 (99%)	2 (1%)	73 92
2	E	178/207 (86%)	174 (98%)	4 (2%)	52 81
2	H	180/207 (87%)	178 (99%)	2 (1%)	73 92
2	K	179/207 (86%)	176 (98%)	3 (2%)	60 86
3	C	174/189 (92%)	168 (97%)	6 (3%)	37 71
3	F	172/189 (91%)	166 (96%)	6 (4%)	36 70
3	I	170/189 (90%)	167 (98%)	3 (2%)	59 85
3	L	169/189 (89%)	161 (95%)	8 (5%)	26 59
All	All	2393/2728 (88%)	2344 (98%)	49 (2%)	55 82

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	197	SER
1	J	268	ASP
1	J	331	ASP
2	E	23	LEU
2	E	156	LEU
2	E	179	SER
2	E	190	SER
3	F	15	THR
3	F	72	SER
3	F	82	SER
3	F	96	ARG
3	F	161	SER
3	F	181	SER
2	B	195	SER
2	B	215	ASN
3	C	19	SER
3	C	27	SER
3	C	61	THR
3	C	70	SER
3	C	75	ASP
3	C	208	SER
1	D	267	TYR
1	D	304	ARG

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Mol	Chain	Res	Type
1	D	340	TYR
1	D	357	MET
1	D	406	SER
1	A	190	SER
1	A	335	MET
1	A	353	SER
1	A	418	ARG
2	H	12	SER
2	H	67	ASP
3	I	55	ASP
3	I	167	SER
3	I	208	SER
2	K	145	SER
2	K	190	SER
2	K	198	SER
3	L	23	ARG
3	L	75	ASP
3	L	97	SER
3	L	147	ARG
3	L	164	SER
3	L	175	ASP
3	L	181	SER
3	L	207	SER
1	G	340	TYR
1	G	350	SER
1	G	351	TYR

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

Mol	Chain	Res	Type
1	J	393	GLN
3	F	160	GLN
1	D	245	ASN
2	H	210	GLN
3	I	165	GLN

5.3.3 RNA

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, 95^{th} 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	296/307 (96%)	0.06	1 (0%) 94 94	44, 60, 82, 96	0
1	D	296/307 (96%)	0.06	2 (0%) 87 87	44, 58, 82, 93	0
1	G	298/307 (97%)	0.11	3 (1%) 82 82	45, 61, 78, 95	0
1	J	297/307 (96%)	0.12	2 (0%) 87 87	45, 69, 89, 103	0
2	B	227/241 (94%)	0.10	0 100 100	39, 56, 74, 91	0
2	E	229/241 (95%)	0.20	3 (1%) 77 77	44, 61, 81, 92	0
2	H	227/241 (94%)	0.19	4 (1%) 68 67	43, 63, 85, 92	0
2	K	226/241 (93%)	0.13	3 (1%) 77 77	43, 61, 85, 106	0
3	C	213/219 (97%)	-0.02	0 100 100	41, 58, 71, 93	0
3	F	213/219 (97%)	0.03	1 (0%) 91 91	45, 56, 76, 82	0
3	I	213/219 (97%)	0.06	2 (0%) 84 84	42, 55, 82, 90	0
3	L	213/219 (97%)	0.17	6 (2%) 53 49	45, 63, 86, 99	0
All	All	2948/3068 (96%)	0.10	27 (0%) 84 84	39, 60, 83, 106	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	L	191	TYR	4.5
3	L	198	ALA	3.7
2	H	167	PRO	3.4
3	I	134	THR	3.1
3	L	197	TYR	2.9
1	J	462	PHE	2.8
1	D	358	ILE	2.7
2	K	150	SER	2.6
3	I	186	LEU	2.5
1	G	329	LEU	2.5
3	F	183	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	G	322	PHE	2.3
2	E	16	LEU	2.3
2	K	142	LEU	2.3
2	H	148	SER	2.2
3	L	153	TRP	2.2
1	J	274	TYR	2.2
3	L	137	VAL	2.2
2	E	130	SER	2.2
1	G	205	PHE	2.1
2	K	143	ALA	2.1
2	E	137	PRO	2.1
2	H	168	VAL	2.1
3	L	134	THR	2.1
2	H	127	VAL	2.1
1	A	319	ASN	2.0
1	D	267	TYR	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.