WORLDWIDE PDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Aug 1, 2016 – 04:24 AM EDT

PDB ID	:	5JHL
Title	:	Crystal structure of zika virus envelope protein in complex with a flavivirus broadly-protective antibody
Authors	:	Dai, L.; Shi, Y.; Qi, J.; Gao, G.F.
Deposited on	:	2016-04-21
Resolution	:	3.00 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

|		
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027939
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027939

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 3.00 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	Percentile Ranks	Value
Rfree		0.263
Clashscore		13
Ramachandran outliers		4.4%
Sidechain outliers		9.4%
RSRZ outliers		2.6%

Worse   *Better*

▌ Percentile relative to all X-ray structures

◻ Percentile relative to X-ray structures of similar resolution
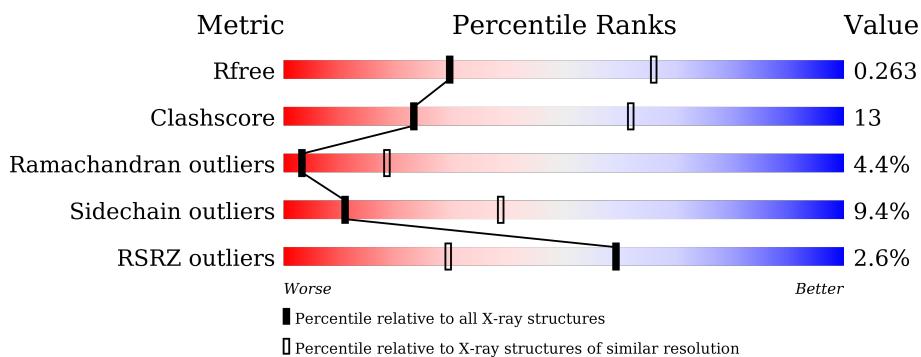
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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. 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	416	3% 57% 28% 6% · 7%
2	H	231	3% 68% 24% · 6%
3	L	216	75% 22% ··
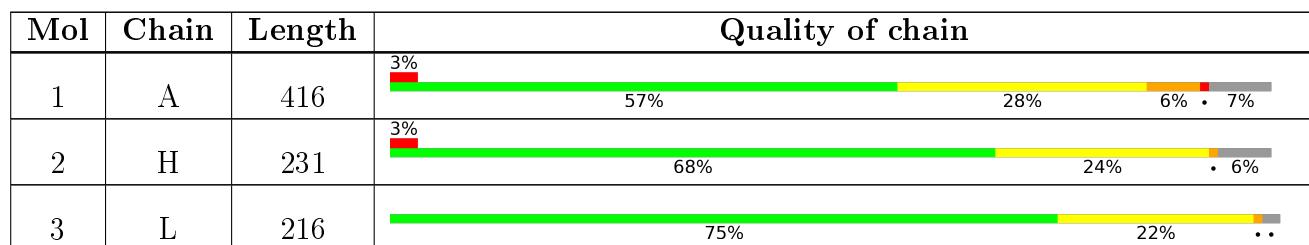
2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 6087 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 envelope protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	385	Total	C	N	O	S	0	0	0
			2853	1789	482	558	24			

- Molecule 2 is a protein called Antibody Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	216	Total	C	N	O	S	0	0	0
			1624	1022	269	326	7			

- Molecule 3 is a protein called antibody Light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	211	Total	C	N	O	S	0	0	0
			1610	1000	269	334	7			

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: envelope protein
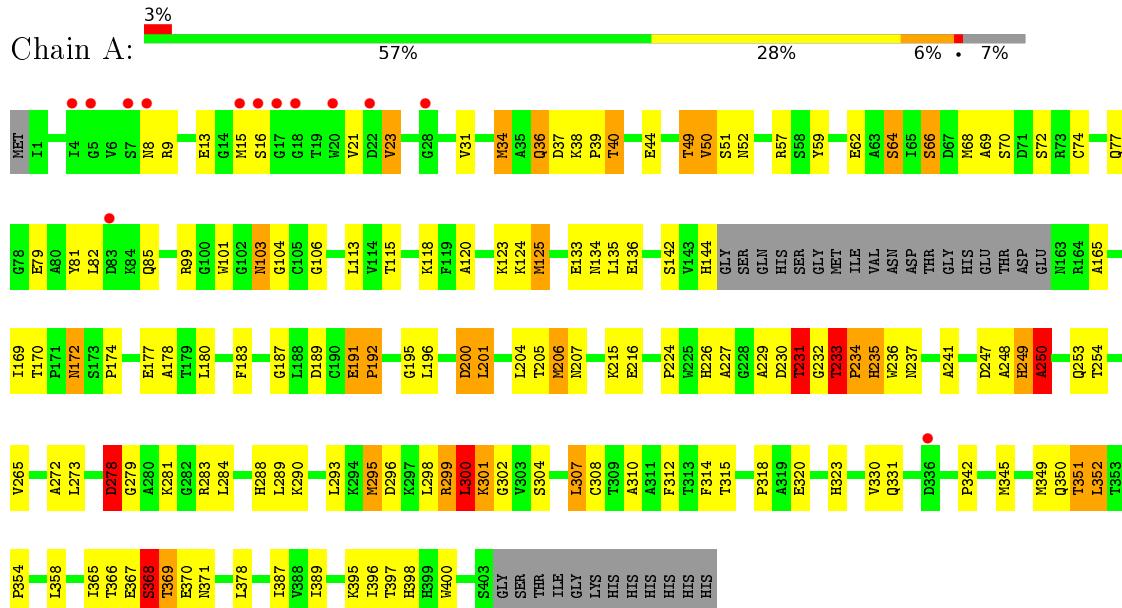
• Molecule 2: Antibody Heavy chain
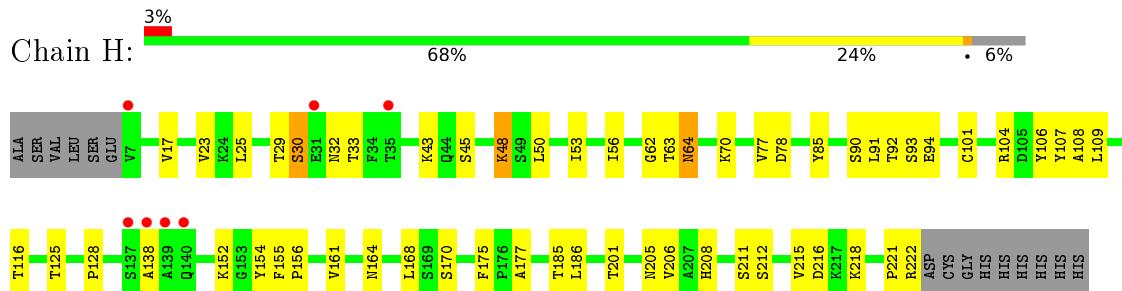
• Molecule 3: antibody Light chain

K148 W149 T165 D166 Q167 M176 T183 K184 D185 E186 Y187 Y193 E196 A197 T198 H199 P205 I206 V207 K208 S209 F210 N211 R212 ASN GLU CYS SER

4   Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	49.60Å 104.86Å 81.86Å 90.00° 102.70° 90.00°	Depositor
Resolution (Å)	30.69 – 3.00 30.69 – 2.99	Depositor EDS
% Data completeness (in resolution range)	97.7 (30.69-3.00) 88.6 (30.69-2.99)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.89 (at 3.00Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.228 , 0.269 0.226 , 0.263	Depositor DCC
R_{free} test set	748 reflections (5.09%)	DCC
Wilson B-factor (Å^2)	61.5	Xtriage
Anisotropy	0.684	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 34.2	EDS
L-test for twinning[2]	$< |L| > = 0.47, < L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	6087	wwPDB-VP
Average B, all atoms (Å^2)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.71% of the height of the origin peak. No significant pseudotranslation is detected.*

---

[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	0.34	0/2914	0.52	2/3966 (0.1%)
2	H	0.29	0/1666	0.46	0/2279
3	L	0.31	0/1647	0.47	1/2243 (0.0%)
All	All	0.32	0/6227	0.49	3/8488 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	L	53	ALA	CB-CA-C	-5.99	101.12	110.10
1	A	233	THR	C-N-CD	5.93	140.86	128.40
1	A	250	ALA	CB-CA-C	5.72	118.68	110.10

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	2853	0	2706	106	1
2	H	1624	0	1564	28	1
3	L	1610	0	1491	28	0
All	All	6087	0	5761	159	1

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 13.

All (159) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:331:GLN:CG	1:A:371:ASN:OD1	1.89	1.20
1:A:331:GLN:HG2	1:A:371:ASN:OD1	1.42	1.20
1:A:351:THR:HG22	1:A:352:LEU:HB2	1.12	1.09
1:A:50:VAL:HG12	1:A:135:LEU:HD23	1.41	1.01
1:A:231:THR:HG23	1:A:232:GLY:H	1.23	1.01
1:A:331:GLN:NE2	1:A:371:ASN:OD1	1.95	0.99
1:A:331:GLN:CD	1:A:371:ASN:OD1	2.00	0.99
1:A:351:THR:CG2	1:A:352:LEU:HB2	1.92	0.98
1:A:50:VAL:CG1	1:A:135:LEU:HD23	2.01	0.89
1:A:351:THR:HG22	1:A:352:LEU:CB	2.01	0.89
1:A:369:THR:OG1	1:A:370:GLU:HG2	1.78	0.83
1:A:74:CYS:HB2	1:A:77:GLN:HG3	1.66	0.78
2:H:43:LYS:HB2	2:H:53:ILE:HD11	1.67	0.76
2:H:205:ASN:ND2	2:H:216:ASP:OD1	2.23	0.72
1:A:232:GLY:O	1:A:233:THR:HG22	1.90	0.71
3:L:52:SER:O	3:L:53:ALA:HB3	1.89	0.71
1:A:231:THR:HG23	1:A:232:GLY:N	2.04	0.69
1:A:81:TYR:HB2	1:A:85:GLN:HE22	1.59	0.66
1:A:183:PHE:HA	1:A:299:ARG:O	1.97	0.65
1:A:349:MET:HA	1:A:352:LEU:HD12	1.80	0.64
1:A:15:MET:SD	1:A:16:SER:N	2.72	0.62
1:A:352:LEU:HG	1:A:352:LEU:O	1.99	0.62
1:A:125:MET:HB2	1:A:206:MET:HA	1.80	0.62
2:H:104:ARG:NH1	2:H:107:TYR:O	2.32	0.62
1:A:192:PRO:HD3	1:A:289:LEU:HD12	1.81	0.62
1:A:307:LEU:HD22	1:A:342:PRO:HG3	1.82	0.61
1:A:124:LYS:CD	1:A:236:TRP:HH2	2.14	0.61
1:A:124:LYS:HD2	1:A:236:TRP:HH2	1.66	0.60
1:A:358:LEU:HD22	1:A:378:LEU:HD22	1.83	0.59
3:L:52:SER:O	3:L:53:ALA:CB	2.50	0.59
2:H:63:THR:O	2:H:64:ASN:HB2	2.02	0.59
3:L:82:SER:O	3:L:85:LEU:HG	2.02	0.58
1:A:172:ASN:N	1:A:172:ASN:OD1	2.37	0.57
1:A:314:PHE:HE2	1:A:398:HIS:HB2	1.69	0.57
1:A:295:MET:HB2	1:A:298:LEU:HD12	1.84	0.57
1:A:50:VAL:O	1:A:50:VAL:HG23	2.03	0.57
1:A:183:PHE:CD2	1:A:300:LEU:O	2.57	0.57
1:A:308:CYS:HB2	1:A:342:PRO:HD3	1.86	0.56
1:A:170:THR:HG22	1:A:172:ASN:H	1.71	0.56
1:A:230:ASP:OD2	1:A:231:THR:N	2.32	0.55

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:187:TYR:O	3:L:193:TYR:OH	2.23	0.55
3:L:50:ILE:HD13	3:L:56:ARG:HB3	1.88	0.55
1:A:230:ASP:C	1:A:231:THR:HG22	2.27	0.54
2:H:17:VAL:HG11	2:H:91:LEU:HD12	1.90	0.54
1:A:169:ILE:HG23	1:A:174:PRO:HA	1.89	0.54
2:H:152:LYS:HA	2:H:185:THR:HG23	1.89	0.54
2:H:29:THR:OG1	2:H:30:SER:N	2.40	0.53
1:A:200:ASP:OD2	1:A:201:LEU:N	2.34	0.53
1:A:23:VAL:HG12	1:A:31:VAL:HG11	1.90	0.52
3:L:85:LEU:HD22	3:L:167:GLN:HB3	1.91	0.52
3:L:15:THR:HG21	3:L:80:ILE:HD13	1.90	0.52
1:A:226:HIS:CD2	1:A:234:PRO:HB3	2.45	0.52
1:A:302:GLY:C	1:A:304:SER:H	2.13	0.51
3:L:92:GLN:NE2	3:L:96:TYR:O	2.44	0.51
1:A:206:MET:HE3	1:A:265:VAL:HB	1.92	0.51
1:A:62:GLU:OE1	1:A:123:LYS:NZ	2.36	0.51
1:A:39:PRO:HG3	1:A:300:LEU:HA	1.93	0.51
2:H:25:LEU:HD22	2:H:116:THR:HG21	1.92	0.51
2:H:164:ASN:HD22	2:H:168:LEU:HD13	1.76	0.51
1:A:351:THR:CB	1:A:352:LEU:HB2	2.42	0.50
1:A:345:MET:O	1:A:354:PRO:HA	2.12	0.50
3:L:137:LEU:HD13	3:L:176:MET:HG3	1.93	0.49
1:A:206:MET:CE	1:A:265:VAL:HB	2.41	0.49
1:A:299:ARG:O	1:A:300:LEU:C	2.51	0.49
2:H:206:VAL:HB	2:H:215:VAL:HG13	1.93	0.49
3:L:16:SER:OG	3:L:19:ASP:OD1	2.28	0.49
1:A:66:SER:HB2	1:A:118:LYS:HB3	1.95	0.49
1:A:72:SER:HB3	1:A:113:LEU:HD13	1.95	0.49
1:A:295:MET:HB2	1:A:298:LEU:CD1	2.42	0.49
2:H:177:ALA:HB2	2:H:186:LEU:HD23	1.95	0.48
1:A:387:ILE:O	1:A:397:THR:HA	2.13	0.48
3:L:108:LYS:HA	3:L:141:TYR:OH	2.13	0.48
1:A:224:PRO:HD3	1:A:241:ALA:HB3	1.95	0.48
1:A:278:ASP:HA	1:A:279:GLY:HA2	1.65	0.48
1:A:226:HIS:CG	1:A:234:PRO:HB3	2.49	0.48
1:A:314:PHE:CE2	1:A:398:HIS:HB2	2.49	0.48
1:A:187:GLY:O	1:A:293:LEU:HB2	2.14	0.47
2:H:208:HIS:ND1	2:H:211:SER:OG	2.44	0.47
1:A:226:HIS:CD2	1:A:234:PRO:CB	2.98	0.47
3:L:135:CYS:HB2	3:L:149:TRP:CH2	2.50	0.47
1:A:249:HIS:O	1:A:250:ALA:HB2	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:312:PHE:HE1	1:A:365:ILE:HD11	1.79	0.47
2:H:175:PHE:CD1	3:L:165:THR:HG23	2.49	0.47
1:A:206:MET:HE3	1:A:265:VAL:CG1	2.44	0.47
1:A:351:THR:CA	1:A:352:LEU:HB2	2.45	0.46
3:L:196:GLU:HG2	3:L:207:VAL:HG22	1.97	0.46
1:A:350:GLN:HA	1:A:351:THR:HG23	1.97	0.46
1:A:345:MET:HG2	1:A:387:ILE:HG22	1.97	0.46
2:H:93:SER:OG	2:H:94:GLU:OE2	2.31	0.46
1:A:34:MET:HG3	1:A:34:MET:H	1.41	0.46
1:A:9:ARG:HB2	1:A:323:HIS:NE2	2.30	0.46
1:A:125:MET:HG3	1:A:204:LEU:HD11	1.97	0.46
1:A:64:SER:HB2	1:A:120:ALA:HB3	1.98	0.46
1:A:124:LYS:CD	1:A:236:TRP:CH2	2.98	0.46
1:A:49:THR:HG21	1:A:281:LYS:HD3	1.98	0.46
3:L:120:PRO:HB3	3:L:210:PHE:CE2	2.51	0.46
2:H:125:THR:HG22	2:H:211:SER:HB3	1.98	0.46
1:A:101:TRP:NE1	1:A:106:GLY:O	2.47	0.45
1:A:295:MET:HG3	1:A:298:LEU:HD12	1.98	0.45
1:A:39:PRO:N	1:A:300:LEU:HD12	2.31	0.45
1:A:49:THR:O	1:A:50:VAL:HG13	2.16	0.45
1:A:57:ARG:NH1	1:A:59:TYR:OH	2.49	0.45
1:A:69:ALA:O	1:A:115:THR:HG23	2.17	0.45
2:H:63:THR:O	2:H:64:ASN:CB	2.63	0.45
2:H:155:PHE:HA	2:H:156:PRO:HA	1.73	0.45
3:L:50:ILE:HA	3:L:56:ARG:HA	1.99	0.45
3:L:209:SER:OG	3:L:210:PHE:N	2.49	0.45
2:H:208:HIS:CE1	2:H:211:SER:HG	2.35	0.44
3:L:30:HIS:CD2	3:L:70:GLY:HA2	2.53	0.44
1:A:312:PHE:C	1:A:396:ILE:HD11	2.37	0.44
3:L:198:THR:HG23	3:L:205:PRO:HB3	1.98	0.44
2:H:128:PRO:HD3	2:H:208:HIS:ND1	2.33	0.43
2:H:23:VAL:HG12	2:H:91:LEU:HD11	2.00	0.43
1:A:231:THR:CG2	1:A:232:GLY:H	2.05	0.43
1:A:40:THR:HG23	1:A:144:HIS:HB3	2.01	0.43
3:L:48:LEU:HB3	3:L:57:TYR:CD2	2.53	0.43
2:H:128:PRO:HB3	2:H:154:TYR:HB3	2.00	0.43
1:A:235:HIS:O	1:A:235:HIS:CG	2.70	0.43
1:A:330:VAL:HG11	1:A:389:ILE:HG21	2.00	0.43
2:H:78:ASP:HB2	2:H:85:TYR:HE1	1.83	0.43
1:A:366:THR:O	1:A:367:GLU:C	2.55	0.43
1:A:106:GLY:HA2	2:H:104:ARG:HD3	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:295:MET:HB2	1:A:298:LEU:HG	2.01	0.43
1:A:224:PRO:HA	1:A:237:ASN:O	2.19	0.42
1:A:192:PRO:HG3	1:A:290:LYS:H	1.83	0.42
3:L:68:GLY:HA3	3:L:73:PHE:HA	2.01	0.42
1:A:300:LEU:HD12	1:A:300:LEU:HA	1.87	0.42
2:H:161:VAL:HA	2:H:205:ASN:O	2.20	0.42
3:L:211:ASN:HB3	3:L:212:ARG:H	1.65	0.42
1:A:36:GLN:C	1:A:38:LYS:H	2.23	0.42
1:A:295:MET:HB2	1:A:298:LEU:CG	2.49	0.42
1:A:235:HIS:ND1	1:A:235:HIS:C	2.73	0.42
1:A:74:CYS:O	1:A:77:GLN:HB2	2.20	0.42
1:A:21:VAL:HG23	1:A:23:VAL:HG22	2.01	0.42
1:A:191:GLU:HA	1:A:192:PRO:HD3	1.85	0.42
1:A:368:SER:HB2	1:A:369:THR:H	1.74	0.42
3:L:63:ARG:HB3	3:L:78:SER:O	2.20	0.42
1:A:99:ARG:HA	1:A:103:ASN:OD1	2.20	0.42
1:A:38:LYS:HA	1:A:300:LEU:HD13	2.01	0.41
1:A:206:MET:CE	1:A:265:VAL:HG11	2.50	0.41
1:A:165:ALA:HB3	1:A:178:ALA:HB1	2.03	0.41
1:A:51:SER:O	1:A:52:ASN:HB2	2.20	0.41
2:H:32:ASN:OD1	2:H:33:THR:N	2.53	0.41
3:L:135:CYS:HB2	3:L:149:TRP:CZ2	2.56	0.41
1:A:124:LYS:HD2	1:A:236:TRP:CH2	2.50	0.41
1:A:320:GLU:HB2	1:A:400:TRP:CZ2	2.56	0.41
1:A:349:MET:CA	1:A:352:LEU:HD12	2.49	0.41
1:A:200:ASP:HA	1:A:215:LYS:HD2	2.03	0.41
2:H:56:ILE:HA	2:H:62:GLY:O	2.21	0.41
1:A:49:THR:O	1:A:50:VAL:CG1	2.69	0.41
1:A:51:SER:O	1:A:134:ASN:ND2	2.54	0.41
2:H:201:THR:HA	2:H:218:LYS:HE3	2.02	0.41
3:L:141:TYR:O	3:L:199:HIS:HE1	2.04	0.41
3:L:108:LYS:HE3	3:L:108:LYS:HB2	1.86	0.40
1:A:101:TRP:HB2	3:L:93:TYR:HB2	2.02	0.40
1:A:82:LEU:O	1:A:85:GLN:NE2	2.54	0.40
1:A:248:ALA:HA	1:A:253:GLN:HA	2.03	0.40
2:H:43:LYS:HE2	2:H:45:SER:OG	2.22	0.40
3:L:50:ILE:HG21	3:L:66:GLY:HA3	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279:GLY:O	2:H:212:SER:OG[2_444]	2.18	0.02

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	381/416 (92%)	311 (82%)	41 (11%)	29 (8%)	1	6
2	H	214/231 (93%)	195 (91%)	13 (6%)	6 (3%)	6	30
3	L	209/216 (97%)	197 (94%)	12 (6%)	0	100	100
All	All	804/863 (93%)	703 (87%)	66 (8%)	35 (4%)	3	18

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	227	ALA
1	A	231	THR
1	A	247	ASP
1	A	288	HIS
2	H	64	ASN
1	A	36	GLN
1	A	201	LEU
1	A	250	ALA
1	A	278	ASP
1	A	300	LEU
1	A	301	LYS
1	A	368	SER
2	H	221	PRO
1	A	192	PRO
1	A	207	ASN
1	A	233	THR
1	A	234	PRO
1	A	352	LEU
2	H	48	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	H	108	ALA
2	H	138	ALA
1	A	191	GLU
1	A	195	GLY
1	A	272	ALA
1	A	273	LEU
1	A	318	PRO
2	H	30	SER
1	A	70	SER
1	A	200	ASP
1	A	229	ALA
1	A	310	ALA
1	A	8	ASN
1	A	104	GLY
1	A	196	LEU
1	A	50	VAL

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	302/348 (87%)	260 (86%)	42 (14%)	4	19
2	H	184/200 (92%)	173 (94%)	11 (6%)	24	62
3	L	181/192 (94%)	171 (94%)	10 (6%)	27	65
All	All	667/740 (90%)	604 (91%)	63 (9%)	11	39

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	GLU
1	A	23	VAL
1	A	34	MET
1	A	37	ASP
1	A	40	THR
1	A	44	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	49	THR
1	A	64	SER
1	A	66	SER
1	A	68	MET
1	A	79	GLU
1	A	103	ASN
1	A	125	MET
1	A	133	GLU
1	A	136	GLU
1	A	142	SER
1	A	172	ASN
1	A	177	GLU
1	A	180	LEU
1	A	189	ASP
1	A	205	THR
1	A	206	MET
1	A	216	GLU
1	A	231	THR
1	A	233	THR
1	A	235	HIS
1	A	249	HIS
1	A	254	THR
1	A	278	ASP
1	A	283	ARG
1	A	284	LEU
1	A	295	MET
1	A	296	ASP
1	A	299	ARG
1	A	300	LEU
1	A	301	LYS
1	A	307	LEU
1	A	315	THR
1	A	351	THR
1	A	368	SER
1	A	369	THR
1	A	395	LYS
2	H	48	LYS
2	H	50	LEU
2	H	70	LYS
2	H	77	VAL
2	H	90	SER
2	H	92	THR

Continued on next page...

Full wwPDB X-ray Structure Validation Report

Continued from previous page...

Mol	Chain	Res	Type
2	H	101	CYS
2	H	106	TYR
2	H	109	LEU
2	H	170	SER
2	H	222	ARG
3	L	48	LEU
3	L	58	THR
3	L	84	ASP
3	L	85	LEU
3	L	106	GLU
3	L	123	SER
3	L	147	VAL
3	L	183	THR
3	L	185	ASP
3	L	186	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	85	GLN
1	A	226	HIS
3	L	30	HIS
3	L	39	GLN

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 carbohydrates 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 (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	385/416 (92%)	-0.07	13 (3%)	49 21	46, 75, 114, 166	0
2	H	216/231 (93%)	-0.22	7 (3%)	51 23	39, 63, 108, 155	0
3	L	211/216 (97%)	-0.31	1 (0%)	91 76	38, 68, 85, 107	0
All	All	812/863 (94%)	-0.18	21 (2%)	59 29	38, 69, 108, 166	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	31	GLU	8.0
1	A	18	GLY	5.0
2	H	137	SER	4.9
1	A	16	SER	4.8
1	A	22	ASP	4.5
1	A	5	GLY	3.5
1	A	28	GLY	3.1
2	H	7	VAL	3.1
1	A	20	TRP	3.1
1	A	8	ASN	3.0
1	A	7	SER	2.9
2	H	139	ALA	2.6
2	H	35	THR	2.6
2	H	138	ALA	2.5
1	A	83	ASP	2.5
1	A	336	ASP	2.4
1	A	15	MET	2.4
3	L	106	GLU	2.3
1	A	4	ILE	2.1
2	H	140	GLN	2.1
1	A	17	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 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.