WORLDWIDE

wwPDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 05:55 am GMT

PDB ID	:	4NCC
Title	:	Neutralizing antibody to murine norovirus
Authors	:	Smith, T.; Li, M.
Deposited on	:	2013-10-24
Resolution	:	2.49 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 ⓘ symbol.

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

|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

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 2.49 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		0.271
Clashscore		12
Ramachandran outliers		1.2%
Sidechain outliers		8.9%
RSRZ outliers		1.4%

Worse ▬ *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
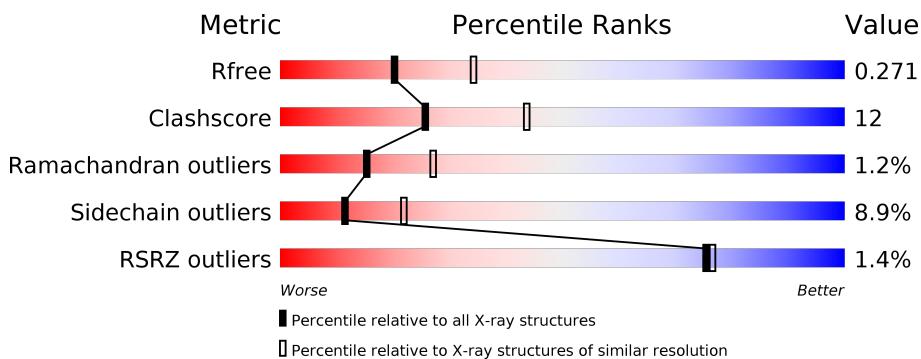
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	3846 (2.50-2.50)
Clashscore	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)
RSRZ outliers	101464	3876 (2.50-2.50)

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	1	211	% 77% 19% ·
1	L	211	79% 19% ·
2	2	221	2% 68% 28% · ·
2	H	221	2% 64% 31% · ·

WORLDWIDE wwPDB PROTEIN DATA BANK
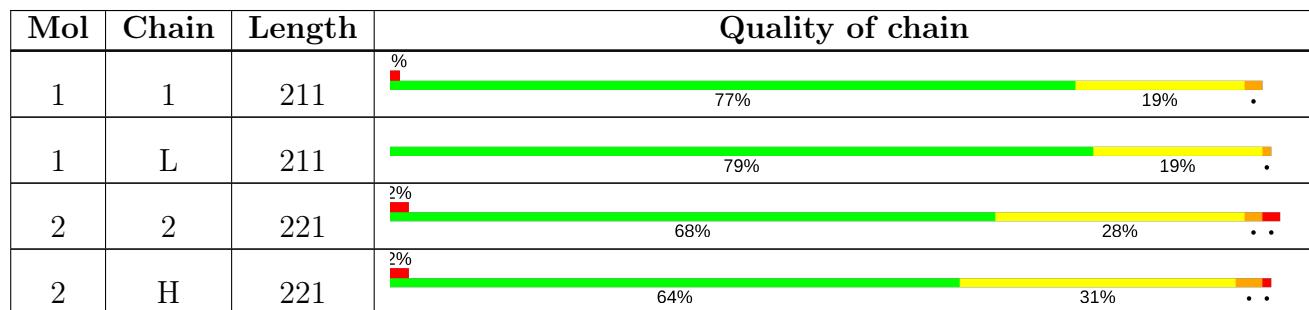
2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 6930 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 Fab fragment light.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	211	Total 1620	C 1010	N 272	O 330	S 8	0	0	0
1	1	210	Total 1612	C 1006	N 270	O 328	S 8	0	0	0

- Molecule 2 is a protein called Fab fragment heavy.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	220	Total 1664	C 1066	N 282	O 309	S 7	0	0	0
2	2	220	Total 1664	C 1066	N 282	O 309	S 7	0	0	0

- Molecule 3 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	L	84	Total 84	O 84	0	0
3	H	76	Total 76	O 76	0	0
3	1	113	Total 113	O 113	0	0
3	2	97	Total 97	O 97	0	0

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 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: Fab fragment light
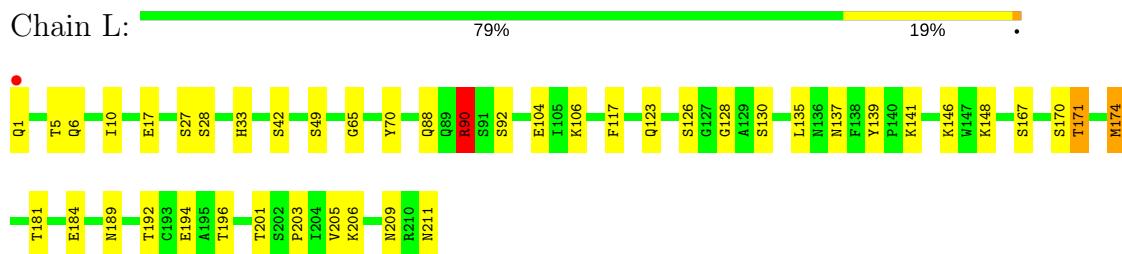
Chain L:

• Molecule 1: Fab fragment light

Chain 1:

• Molecule 2: Fab fragment heavy

Chain H:

• Molecule 2: Fab fragment heavy

Chain 2:

GLU V2 K3 L4 L5 E6 V12 L18 K19 L20 S21 C22 F29 S30 R31 Y32 W33 R38 E46 W47 I48 P53 S56 T57 Y60 S63 L64 R65 D66 K67 F68 I69 I70 A75 K76 N77 T78 Q82 M83 T84 T91 R98 L99 L100 R101 Y102 F103

Y104 D107 Q111 G112 A113 T116 S119 P124 A135 K149 F152 V156 T157 V158 F172 P173 L176 Q177 A178 A179 L180 Y181 S184 S185 S186 S191 W194 P195 T198 N202 V203 A204 T210 K211 A220 A221
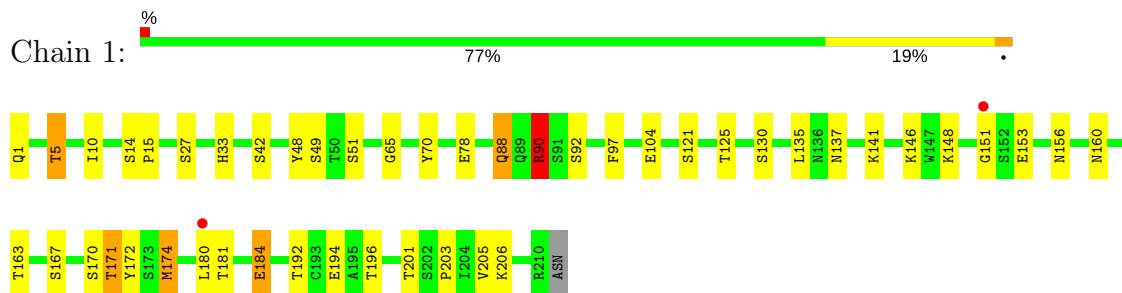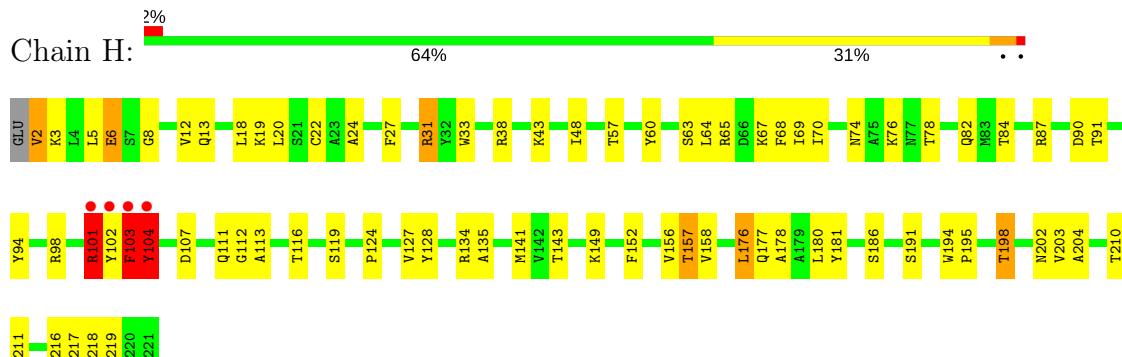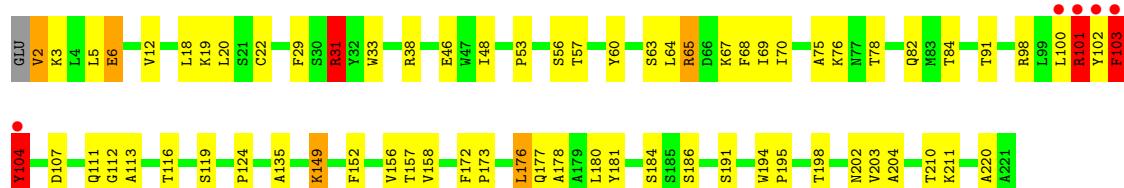
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	42.59Å 135.81Å 83.31Å 90.00° 93.93° 90.00°	Depositor
Resolution (Å)	42.49 – 2.49 52.59 – 2.49	Depositor EDS
% Data completeness (in resolution range)	71.4 (42.49-2.49) 71.3 (52.59-2.49)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.84 (at 2.48Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.8.2_1309)	Depositor
R, R_{free}	0.204 , 0.273 0.201 , 0.271	Depositor DCC
R_{free} test set	1136 reflections (4.83%)	DCC
Wilson B-factor (Å^2)	13.9	Xtriage
Anisotropy	0.331	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 49.6	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.82	EDS
Total number of atoms	6930	wwPDB-VP
Average B, all atoms (Å^2)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.73% 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 (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	1	0.57	2/1651 (0.1%)	0.74	5/2242 (0.2%)
1	L	0.57	1/1659 (0.1%)	0.71	5/2253 (0.2%)
2	2	0.55	2/1710 (0.1%)	0.89	7/2337 (0.3%)
2	H	0.63	5/1710 (0.3%)	0.95	7/2337 (0.3%)
All	All	0.58	10/6730 (0.1%)	0.83	24/9169 (0.3%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	184	GLU	CD-OE1	-13.48	1.10	1.25
1	L	184	GLU	CD-OE1	-13.13	1.11	1.25
2	H	101	ARG	CZ-NH1	6.44	1.41	1.33
2	H	103	PHE	CB-CG	6.33	1.62	1.51
2	H	31	ARG	CG-CD	-6.27	1.36	1.51
2	H	101	ARG	CD-NE	-6.07	1.36	1.46
2	2	103	PHE	CD1-CE1	5.85	1.50	1.39
1	1	184	GLU	CG-CD	-5.73	1.43	1.51
2	2	31	ARG	CG-CD	-5.59	1.38	1.51
2	H	103	PHE	CD1-CE1	5.40	1.50	1.39

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	101	ARG	NE-CZ-NH2	-20.31	110.15	120.30
2	2	101	ARG	NE-CZ-NH2	-16.94	111.83	120.30
2	H	101	ARG	NE-CZ-NH1	14.51	127.56	120.30
1	1	90	ARG	NE-CZ-NH1	13.25	126.92	120.30
1	L	90	ARG	NE-CZ-NH1	-12.73	113.94	120.30
1	1	90	ARG	NE-CZ-NH2	-12.17	114.22	120.30
1	L	90	ARG	NE-CZ-NH2	11.34	125.97	120.30
2	2	101	ARG	CG-CD-NE	-11.16	88.36	111.80
2	2	101	ARG	NE-CZ-NH1	10.59	125.59	120.30
2	H	101	ARG	CG-CD-NE	-9.34	92.20	111.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	184	GLU	CG-CD-OE2	7.60	133.50	118.30
2	H	103	PHE	CZ-CE2-CD2	7.60	129.22	120.10
2	2	103	PHE	CB-CG-CD1	7.49	126.05	120.80
1	L	184	GLU	CG-CD-OE2	7.27	132.83	118.30
2	2	104	TYR	N-CA-C	6.89	129.60	111.00
1	1	90	ARG	CD-NE-CZ	6.41	132.57	123.60
1	1	184	GLU	CG-CD-OE1	-6.26	105.78	118.30
2	H	134	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	L	184	GLU	CG-CD-OE1	-5.53	107.24	118.30
2	H	31	ARG	CB-CG-CD	-5.28	97.87	111.60
1	L	90	ARG	CD-NE-CZ	5.16	130.82	123.60
2	H	104	TYR	N-CA-C	5.12	124.83	111.00
2	2	104	TYR	CA-CB-CG	5.11	123.12	113.40
2	2	31	ARG	CB-CG-CD	-5.09	98.37	111.60

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	1	1612	0	1548	37	0
1	L	1620	0	1554	30	0
2	2	1664	0	1658	50	0
2	H	1664	0	1658	54	0
3	1	113	0	0	13	0
3	2	97	0	0	10	0
3	H	76	0	0	10	0
3	L	84	0	0	10	0
All	All	6930	0	6418	155	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 12.

All (155) 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)
1:1:42:SER:O	3:1:344:HOH:O	1.81	0.98
1:L:28:SER:O	3:L:318:HOH:O	1.83	0.96
2:H:127:VAL:O	3:H:305:HOH:O	1.89	0.90
1:L:126:SER:HB3	3:L:354:HOH:O	1.75	0.86
2:H:219:ARG:O	3:H:332:HOH:O	1.94	0.86
1:1:151:GLY:O	3:1:364:HOH:O	1.96	0.83
2:2:101:ARG:O	3:2:328:HOH:O	1.96	0.83
1:L:189:ASN:OD1	3:L:361:HOH:O	2.00	0.79
2:2:101:ARG:NH2	2:2:103:PHE:O	2.17	0.78
2:H:157:THR:O	3:H:371:HOH:O	2.03	0.75
2:2:220:ALA:O	3:2:327:HOH:O	2.04	0.75
2:2:2:VAL:N	3:2:382:HOH:O	2.20	0.74
1:L:130:SER:OG	2:H:149:LYS:NZ	2.22	0.73
3:L:381:HOH:O	2:H:141:MET:SD	2.48	0.71
1:1:160:ASN:O	3:1:341:HOH:O	2.07	0.71
1:L:17:GLU:OE1	3:L:309:HOH:O	2.07	0.71
2:H:158:VAL:HG22	2:H:203:VAL:HG22	1.72	0.70
1:L:42:SER:O	3:L:323:HOH:O	2.08	0.70
1:L:146:LYS:HD2	1:L:148:LYS:HE3	1.72	0.70
2:H:8:GLY:N	3:H:360:HOH:O	2.23	0.69
2:2:158:VAL:HG22	2:2:203:VAL:HG22	1.74	0.68
2:H:101:ARG:NH2	2:H:103:PHE:O	2.26	0.68
1:1:146:LYS:HD2	1:1:148:LYS:HE3	1.75	0.68
1:1:153:GLU:OE1	3:1:395:HOH:O	2.10	0.68
3:1:403:HOH:O	2:2:104:TYR:HD2	1.77	0.68
2:H:101:ARG:NH2	2:H:104:TYR:CZ	2.62	0.67
2:H:2:VAL:N	3:H:365:HOH:O	2.26	0.67
1:1:146:LYS:NZ	3:1:352:HOH:O	2.13	0.67
2:H:124:PRO:HD2	1:1:15:PRO:O	1.95	0.66
2:H:141:MET:HG2	3:H:312:HOH:O	1.96	0.66
1:1:194:GLU:HG3	1:1:205:VAL:HG22	1.78	0.65
2:2:38:ARG:HB3	2:2:48:ILE:HD11	1.78	0.65
2:2:64:LEU:HA	2:2:67:LYS:HG2	1.79	0.64
2:2:119:SER:O	3:2:305:HOH:O	2.15	0.64
1:L:194:GLU:HG3	1:L:205:VAL:HG22	1.80	0.64
2:H:64:LEU:HA	2:H:67:LYS:HG2	1.80	0.64
2:H:63:SER:O	2:H:64:LEU:HG	1.98	0.64
1:L:206:LYS:NZ	3:L:344:HOH:O	2.31	0.64
1:L:104:GLU:OE2	1:L:141:LYS:NZ	2.31	0.63
2:2:204:ALA:HB2	2:2:211:LYS:HD3	1.79	0.63
2:2:63:SER:O	2:2:64:LEU:HG	1.99	0.62
1:L:211:ASN:ND2	3:L:345:HOH:O	2.32	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:176:LEU:HG	2:H:181:TYR:CE1	2.35	0.62
2:2:56:SER:O	3:2:387:HOH:O	2.16	0.61
2:H:204:ALA:HB2	2:H:211:LYS:HD3	1.83	0.61
2:H:124:PRO:HG3	1:1:14:SER:HB2	1.81	0.61
1:L:189:ASN:ND2	3:L:377:HOH:O	2.09	0.60
1:L:33:HIS:CD2	1:L:49:SER:H	2.19	0.59
1:1:33:HIS:CD2	1:1:49:SER:H	2.21	0.58
1:1:5:THR:O	3:1:363:HOH:O	2.17	0.58
2:H:64:LEU:HD13	2:H:68:PHE:CD2	2.39	0.58
2:H:103:PHE:HD1	2:H:103:PHE:H	1.53	0.57
2:H:38:ARG:HB3	2:H:48:ILE:HD11	1.86	0.56
2:2:64:LEU:HD13	2:2:68:PHE:CD2	2.40	0.56
1:1:78:GLU:OE2	3:1:315:HOH:O	2.17	0.56
1:L:196:THR:HG22	1:L:203:PRO:HB3	1.87	0.55
2:2:75:ALA:O	3:2:375:HOH:O	2.18	0.55
1:1:90:ARG:CZ	2:2:104:TYR:HB3	2.37	0.54
1:1:104:GLU:OE2	1:1:141:LYS:NZ	2.40	0.54
2:H:69:ILE:HB	2:H:82:GLN:HB2	1.89	0.54
2:2:158:VAL:HA	2:2:202:ASN:O	2.08	0.53
2:H:216:ILE:O	3:H:330:HOH:O	2.19	0.53
2:2:60:TYR:CE1	2:2:70:ILE:HG13	2.44	0.53
2:H:60:TYR:CE1	2:H:70:ILE:HG13	2.44	0.53
1:L:33:HIS:HE1	2:H:104:TYR:HB2	1.74	0.53
1:1:33:HIS:CE1	2:2:104:TYR:HB2	2.44	0.53
2:H:158:VAL:HA	2:H:202:ASN:O	2.09	0.52
1:1:48:TYR:CD1	2:2:104:TYR:CE1	2.98	0.52
2:2:101:ARG:NH2	2:2:104:TYR:CZ	2.74	0.52
2:2:69:ILE:HB	2:2:82:GLN:HB2	1.89	0.52
2:H:101:ARG:NH2	2:H:104:TYR:CE1	2.77	0.52
2:H:198:THR:O	3:H:325:HOH:O	2.17	0.52
1:1:163:THR:HB	3:1:312:HOH:O	2.09	0.52
1:1:104:GLU:OE1	1:1:172:TYR:OH	2.19	0.51
2:H:91:THR:HG23	2:H:116:THR:HA	1.91	0.51
1:1:196:THR:HG22	1:1:203:PRO:HB3	1.93	0.51
2:2:6:GLU:HB2	2:2:113:ALA:HB2	1.93	0.50
1:L:106:LYS:HA	1:L:139:TYR:OH	2.12	0.50
2:2:194:TRP:O	3:2:363:HOH:O	2.20	0.50
2:2:101:ARG:NH2	2:2:104:TYR:CE1	2.79	0.50
1:L:135:LEU:HD13	1:L:174:MET:HG3	1.93	0.50
1:1:135:LEU:HD13	1:1:174:MET:HG3	1.94	0.50
2:2:101:ARG:HD2	2:2:103:PHE:CD1	2.46	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:98:ARG:NH2	2:H:107:ASP:OD2	2.33	0.50
2:H:194:TRP:CG	2:H:195:PRO:HA	2.47	0.49
1:L:33:HIS:CE1	2:H:104:TYR:HB2	2.46	0.49
2:2:103:PHE:H	2:2:103:PHE:HD1	1.60	0.49
2:2:98:ARG:NH2	2:2:107:ASP:OD2	2.34	0.49
2:2:6:GLU:OE1	2:2:112:GLY:N	2.45	0.48
2:2:184:SER:OG	3:2:379:HOH:O	2.17	0.48
1:L:90:ARG:CZ	2:H:104:TYR:HB3	2.44	0.48
1:L:137:ASN:HA	1:L:171:THR:CG2	2.43	0.48
1:1:156:ASN:O	3:1:411:HOH:O	2.20	0.48
2:H:33:TRP:CE2	2:H:102:TYR:HD1	2.31	0.48
1:1:137:ASN:HA	1:1:171:THR:CG2	2.43	0.48
2:2:194:TRP:CG	2:2:195:PRO:HA	2.48	0.48
1:1:33:HIS:HE1	2:2:104:TYR:HB2	1.77	0.48
2:H:143:THR:O	3:H:327:HOH:O	2.20	0.48
1:1:180:LEU:HD23	1:1:184:GLU:HG2	1.94	0.48
2:2:38:ARG:NE	2:2:46:GLU:OE1	2.41	0.48
2:H:101:ARG:HD2	2:H:103:PHE:CD1	2.49	0.47
1:1:10:ILE:HD11	1:1:104:GLU:OE2	2.14	0.47
2:H:6:GLU:OE1	2:H:112:GLY:N	2.45	0.47
2:2:33:TRP:CE2	2:2:102:TYR:HD1	2.32	0.47
2:2:91:THR:HG23	2:2:116:THR:HA	1.96	0.47
3:1:320:HOH:O	2:2:173:PRO:HG2	2.14	0.47
1:1:148:LYS:HB2	1:1:192:THR:HB	1.96	0.46
2:2:33:TRP:HB2	3:2:328:HOH:O	2.15	0.46
2:H:13:GLN:OE1	2:H:119:SER:HA	2.14	0.46
2:H:6:GLU:HB2	2:H:113:ALA:HB2	1.97	0.46
2:2:176:LEU:HD22	2:2:181:TYR:CE1	2.52	0.45
1:L:10:ILE:HD11	1:L:104:GLU:OE2	2.16	0.45
2:H:60:TYR:HE1	2:H:70:ILE:HG13	1.82	0.45
2:2:12:VAL:HG21	2:2:18:LEU:HD22	1.99	0.45
2:2:31:ARG:HH11	2:2:31:ARG:HD2	1.60	0.44
1:L:209:ASN:ND2	3:L:377:HOH:O	2.51	0.44
1:L:148:LYS:HB2	1:L:192:THR:HB	2.00	0.44
1:1:121:SER:O	1:1:125:THR:HG23	2.17	0.44
2:2:65:ARG:O	3:2:320:HOH:O	2.21	0.44
2:H:94:TYR:O	2:H:112:GLY:HA2	2.17	0.44
2:2:33:TRP:CD1	2:2:53:PRO:HD3	2.53	0.43
2:H:31:ARG:HD3	2:H:31:ARG:HH11	1.51	0.43
2:H:24:ALA:HB1	2:H:27:PHE:CE1	2.53	0.43
2:H:74:ASN:ND2	3:H:375:HOH:O	2.51	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:65:GLY:HA3	1:L:70:TYR:HA	1.99	0.43
2:2:100:LEU:HD23	2:2:101:ARG:HG2	1.99	0.43
1:1:130:SER:OG	2:2:149:LYS:NZ	2.51	0.43
1:L:6:GLN:HE21	1:L:6:GLN:HB3	1.64	0.43
1:1:137:ASN:HA	1:1:171:THR:HG21	2.00	0.43
1:L:117:PHE:HZ	2:H:143:THR:HG22	1.84	0.43
2:2:76:LYS:O	2:2:78:THR:HG23	2.19	0.43
1:L:137:ASN:HA	1:L:171:THR:HG21	2.01	0.42
2:H:12:VAL:HG21	2:H:18:LEU:HD22	2.01	0.42
1:1:88:GLN:HG3	1:1:97:PHE:CE1	2.54	0.42
2:2:60:TYR:HE1	2:2:70:ILE:HG13	1.83	0.42
1:L:123:GLN:HG2	1:L:128:GLY:O	2.19	0.42
2:2:152:PHE:HB2	2:2:180:LEU:HD23	2.01	0.42
2:H:87:ARG:N	2:H:90:ASP:OD2	2.42	0.41
1:L:123:GLN:HG3	2:H:128:TYR:CZ	2.55	0.41
1:1:51:SER:OG	3:1:356:HOH:O	2.15	0.41
2:H:152:PHE:HB2	2:H:180:LEU:HD23	2.02	0.41
2:2:29:PHE:C	2:2:31:ARG:H	2.24	0.41
1:1:163:THR:HG23	2:2:172:PHE:CD2	2.56	0.41
1:1:205:VAL:O	1:1:206:LYS:HD3	2.21	0.41
1:1:65:GLY:HA3	1:1:70:TYR:HA	2.02	0.41
2:H:101:ARG:NH1	2:H:103:PHE:CE1	2.89	0.41
1:1:90:ARG:NH2	2:2:104:TYR:HB3	2.36	0.40
2:2:124:PRO:HB3	2:2:210:THR:HG21	2.03	0.40
2:H:124:PRO:HB3	2:H:210:THR:HG21	2.03	0.40
2:H:217:VAL:HA	2:H:218:PRO:HD3	1.95	0.40
1:L:123:GLN:HA	2:H:128:TYR:CE1	2.57	0.40
2:H:76:LYS:O	2:H:78:THR:HG23	2.21	0.40
1:1:125:THR:CG2	3:1:357:HOH:O	2.70	0.40
1:1:10:ILE:HD11	1:1:141:LYS:NZ	2.36	0.40
2:H:6:GLU:HG2	2:H:6:GLU:H	1.32	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	1	208/211 (99%)	200 (96%)	8 (4%)	0	100	100
1	L	209/211 (99%)	202 (97%)	7 (3%)	0	100	100
2	2	218/221 (99%)	203 (93%)	10 (5%)	5 (2%)	7	11
2	H	218/221 (99%)	204 (94%)	9 (4%)	5 (2%)	7	11
All	All	853/864 (99%)	809 (95%)	34 (4%)	10 (1%)	15	27

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	101	ARG
2	H	104	TYR
2	H	177	GLN
2	2	177	GLN
2	H	135	ALA
2	H	178	ALA
2	2	101	ARG
2	2	104	TYR
2	2	135	ALA
2	2	178	ALA

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	1	184/185 (100%)	172 (94%)	12 (6%)	20	37
1	L	185/185 (100%)	173 (94%)	12 (6%)	20	37
2	2	180/181 (99%)	159 (88%)	21 (12%)	6	12
2	H	180/181 (99%)	160 (89%)	20 (11%)	7	13
All	All	729/732 (100%)	664 (91%)	65 (9%)	11	22

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	1	GLN
1	L	5	THR
1	L	27	SER
1	L	88	GLN
1	L	90	ARG
1	L	92	SER
1	L	167	SER
1	L	170	SER
1	L	171	THR
1	L	174	MET
1	L	181	THR
1	L	201	THR
2	H	2	VAL
2	H	3	LYS
2	H	5	LEU
2	H	6	GLU
2	H	19	LYS
2	H	20	LEU
2	H	22	CYS
2	H	43	LYS
2	H	57	THR
2	H	65	ARG
2	H	84	THR
2	H	101	ARG
2	H	103	PHE
2	H	111	GLN
2	H	156	VAL
2	H	157	THR
2	H	176	LEU
2	H	186	SER
2	H	191	SER
2	H	198	THR
1	1	1	GLN
1	1	5	THR
1	1	27	SER
1	1	88	GLN
1	1	90	ARG
1	1	92	SER
1	1	167	SER
1	1	170	SER
1	1	171	THR
1	1	174	MET
1	1	181	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	201	THR
2	2	2	VAL
2	2	3	LYS
2	2	5	LEU
2	2	6	GLU
2	2	19	LYS
2	2	20	LEU
2	2	22	CYS
2	2	31	ARG
2	2	57	THR
2	2	65	ARG
2	2	84	THR
2	2	101	ARG
2	2	103	PHE
2	2	111	GLN
2	2	149	LYS
2	2	156	VAL
2	2	157	THR
2	2	176	LEU
2	2	186	SER
2	2	191	SER
2	2	198	THR

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

Mol	Chain	Res	Type
1	L	88	GLN
1	L	211	ASN
2	H	170	HIS
1	1	88	GLN
2	2	82	GLN

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 (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 ⓘ

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	1	210/211 (99%)	0.05	2 (0%)	82	83	7, 17, 32, 51	0
1	L	211/211 (100%)	-0.07	1 (0%)	90	91	8, 15, 27, 44	0
2	2	220/221 (99%)	0.20	5 (2%)	61	63	12, 20, 36, 63	0
2	H	220/221 (99%)	0.10	4 (1%)	69	70	8, 17, 37, 73	0
All	All	861/864 (99%)	0.07	12 (1%)	75	76	7, 17, 32, 73	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	102	TYR	4.9
2	2	103	PHE	4.4
2	2	102	TYR	4.0
2	H	103	PHE	3.9
2	H	101	ARG	3.9
2	2	101	ARG	3.4
1	L	1	GLN	2.8
2	H	104	TYR	2.7
1	1	151	GLY	2.6
2	2	104	TYR	2.5
2	2	100	LEU	2.1
1	1	180	LEU	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

WORLDWIDE
wwPDB
PROTEIN DATA BANK

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.