



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:55 PM GMT

PDB ID : 3V0V  
Title : Fab WN1 222-5 unliganded  
Authors : Gomery, K.; Evans, S.V.  
Deposited on : 2011-12-08  
Resolution : 2.13 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
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) : trunk26865

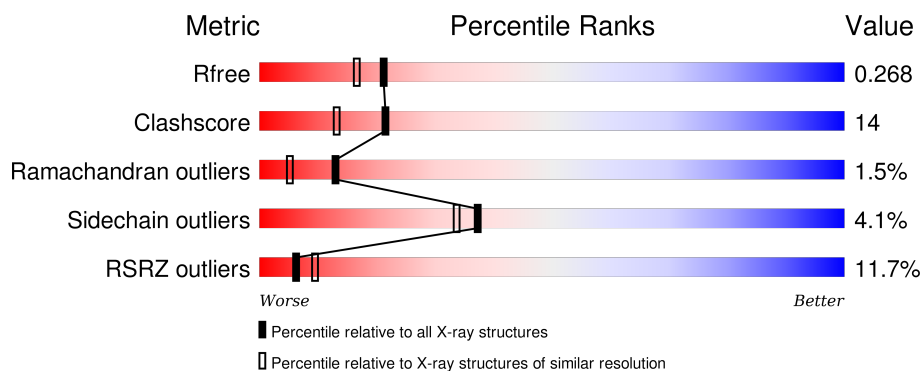
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.13 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))
$R_{free}$	91344	1693 (2.16-2.12)
Clashscore	102246	1824 (2.16-2.12)
Ramachandran outliers	100387	1798 (2.16-2.12)
Sidechain outliers	100360	1798 (2.16-2.12)
RSRZ outliers	91569	1699 (2.16-2.12)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	B	212	<div> <div>11%</div> <div>76%</div> <div>20%</div> <div>.</div> </div>
1	L	212	<div> <div>10%</div> <div>67%</div> <div>29%</div> <div>.</div> </div>
2	A	220	<div> <div>13%</div> <div>69%</div> <div>24%</div> <div>6%</div> <div>.</div> </div>
2	H	220	<div> <div>12%</div> <div>79%</div> <div>17%</div> <div>..</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7022 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 WN1 222-5 Fab (IgG2a) light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	212	Total	C	N	O	S	0	0	0
			1636	1021	278	331	6			
1	B	212	Total	C	N	O	S	0	0	0
			1637	1021	278	332	6			

- Molecule 2 is a protein called WN1 222-5 Fab (IgG2a) heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	214	Total	C	N	O	S	0	0	0
			1612	1017	273	316	6			
2	A	217	Total	C	N	O	S	0	0	0
			1634	1029	276	322	7			

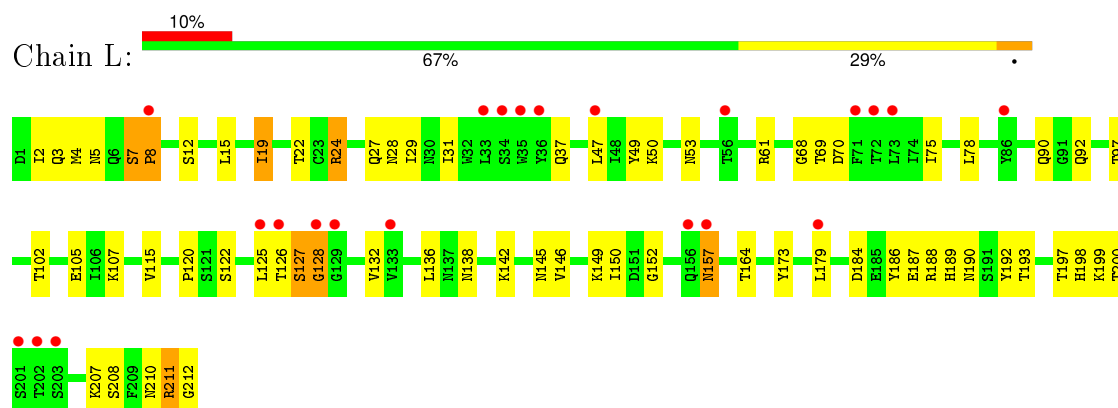
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	L	143	Total	O	0	0
			143	143		
3	H	98	Total	O	0	0
			98	98		
3	B	127	Total	O	0	0
			127	127		
3	A	135	Total	O	0	0
			135	135		

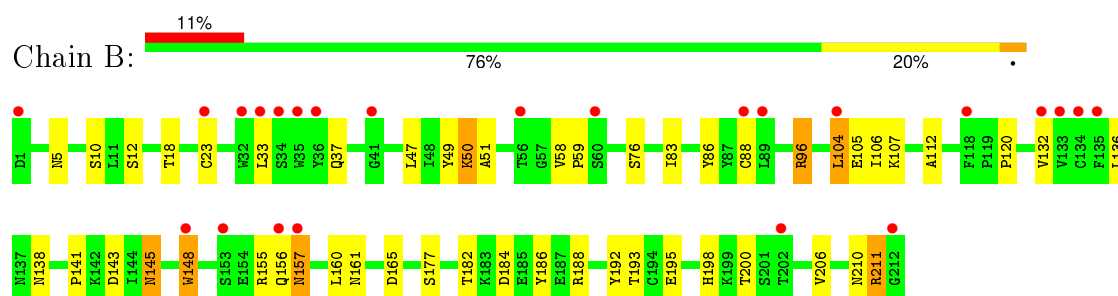
### 3 Residue-property plots

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.

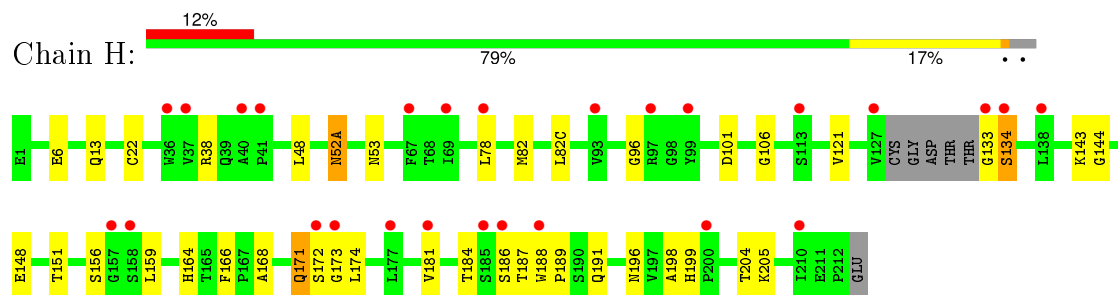
#### • Molecule 1: WN1 222-5 Fab (IgG2a) light chain



#### • Molecule 1: WN1 222-5 Fab (IgG2a) light chain

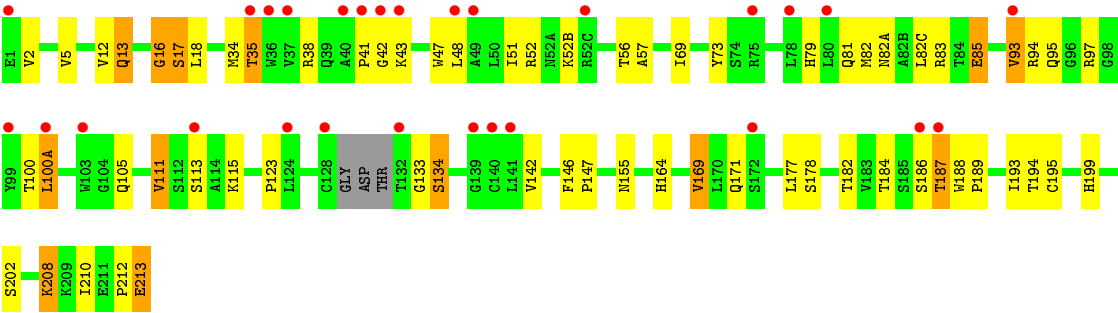


#### • Molecule 2: WN1 222-5 Fab (IgG2a) heavy chain



#### • Molecule 2: WN1 222-5 Fab (IgG2a) heavy chain





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	134.89Å 48.20Å 140.13Å 90.00° 110.55° 90.00°	Depositor
Resolution (Å)	19.98 – 2.13 19.99 – 2.20	Depositor EDS
% Data completeness (in resolution range)	92.3 (19.98-2.13) 92.1 (19.99-2.20)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.07 (at 2.19Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.238 , 0.284 0.224 , 0.268	Depositor DCC
$R_{free}$ test set	2063 reflections (5.17%)	DCC
Wilson B-factor (Å <sup>2</sup> )	43.8	Xtriage
Anisotropy	0.082	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 42.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 39916 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7022	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.43% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	B	0.23	0/1674	0.43	0/2272
1	L	0.24	0/1673	0.44	0/2272
2	A	0.23	0/1673	0.44	0/2281
2	H	0.22	0/1651	0.42	0/2251
All	All	0.23	0/6671	0.43	0/9076

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	B	1637	0	1583	40	0
1	L	1636	0	1583	57	0
2	A	1634	0	1601	64	0
2	H	1612	0	1583	37	0
3	A	135	0	0	1	0
3	B	127	0	0	2	0
3	H	98	0	0	1	0
3	L	143	0	0	5	0
All	All	7022	0	6350	182	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 14.

All (182) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:172:SER:HB2	2:H:173:GLY:HA3	1.17	1.15
2:H:172:SER:CB	2:H:173:GLY:HA3	1.85	1.04
2:A:51:ILE:HB	2:A:69:ILE:HD13	1.43	0.98
1:B:210:ASN:O	1:B:211:ARG:HB2	1.71	0.88
2:H:156:SER:H	2:H:196:ASN:HD21	1.24	0.85
1:L:127:SER:HB3	1:L:128:GLY:HA3	1.64	0.80
2:H:52(A):ASN:HD21	2:H:53:ASN:HD22	1.26	0.79
2:H:82:MET:HE2	2:H:82(C):LEU:HD21	1.66	0.78
1:B:138:ASN:HD21	2:A:164:HIS:HE1	1.32	0.77
2:H:171:GLN:HA	2:H:171:GLN:HE21	1.48	0.77
2:H:151:THR:HG22	2:H:198:ALA:HB3	1.67	0.76
1:L:210:ASN:O	1:L:211:ARG:HB2	1.84	0.76
1:L:2:ILE:O	1:L:97:THR:HG21	1.87	0.75
1:L:7:SER:HB3	1:L:8:PRO:CD	2.18	0.73
1:L:145:ASN:HD21	1:B:145:ASN:HD21	1.37	0.72
2:H:156:SER:H	2:H:196:ASN:ND2	1.88	0.72
1:B:155:ARG:HG2	1:B:156:GLN:O	1.90	0.71
1:L:3:GLN:HE21	1:L:5:ASN:HD21	1.36	0.71
1:L:90:GLN:HE21	1:L:97:THR:HG22	1.55	0.70
1:L:28:ASN:OD1	1:L:68:GLY:HA2	1.91	0.70
1:L:12:SER:OG	1:L:107:LYS:HG2	1.91	0.70
1:L:188:ARG:NE	2:A:83:ARG:HD2	2.06	0.69
2:A:57:ALA:CB	2:A:69:ILE:HD11	2.25	0.67
2:H:184:THR:HG22	2:H:186:SER:H	1.60	0.67
1:B:18:THR:HG22	1:B:76:SER:O	1.96	0.66
1:B:49:TYR:HB2	2:A:100:THR:HG21	1.77	0.66
1:L:22:THR:HG22	3:L:432:HOH:O	1.95	0.65
2:H:172:SER:CB	2:H:173:GLY:CA	2.70	0.65
2:A:184:THR:HG22	2:A:186:SER:H	1.62	0.65
2:A:100:THR:O	2:A:100(A):LEU:HB2	1.97	0.65
2:A:199:HIS:HD2	2:A:202:SER:OG	1.80	0.64
1:L:7:SER:HB2	1:L:22:THR:CG2	2.28	0.63
2:H:172:SER:HB2	2:H:173:GLY:CA	2.11	0.63
2:A:79:HIS:HD2	3:A:382:HOH:O	1.81	0.62
2:A:35:THR:HG22	2:A:93:VAL:O	1.98	0.62
1:B:112:ALA:HA	1:B:200:THR:HG21	1.81	0.62
1:L:61:ARG:HD2	3:L:427:HOH:O	1.99	0.62
2:A:38:ARG:HD3	2:A:48:LEU:HD11	1.81	0.62
2:H:52(A):ASN:HD21	2:H:53:ASN:ND2	1.98	0.61
2:A:147:PRO:O	2:A:199:HIS:HE1	1.84	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:138:ASN:ND2	2:A:164:HIS:HE1	1.99	0.61
2:A:13:GLN:NE2	2:A:113:SER:HA	2.16	0.61
2:A:13:GLN:HE22	2:A:113:SER:HA	1.66	0.60
2:H:52(A):ASN:ND2	2:H:53:ASN:HD22	1.97	0.60
1:L:189:HIS:CE1	2:A:85:GLU:HG2	2.38	0.59
2:H:133:GLY:O	2:H:134:SER:HB3	2.01	0.59
1:B:141:PRO:O	1:B:198:HIS:HE1	1.85	0.59
1:L:19:ILE:HD11	1:L:75:ILE:HB	1.86	0.58
1:L:145:ASN:HB2	1:L:197:THR:HB	1.86	0.58
1:L:7:SER:O	1:L:8:PRO:C	2.40	0.58
1:L:184:ASP:O	1:L:188:ARG:HG3	2.03	0.58
1:B:184:ASP:O	1:B:188:ARG:HG3	2.04	0.58
2:A:142:VAL:HB	2:A:177:LEU:HB3	1.85	0.58
1:L:152:GLY:HA3	3:L:381:HOH:O	2.04	0.57
2:A:57:ALA:HB1	2:A:69:ILE:HD11	1.86	0.57
3:B:321:HOH:O	2:A:100:THR:HG22	2.03	0.57
1:L:122:SER:O	1:L:126:THR:HG23	2.04	0.57
1:L:29:ILE:HA	1:L:92:GLN:NE2	2.20	0.57
1:L:50:LYS:HB2	1:L:53:ASN:HD22	1.69	0.57
1:L:187:GLU:HA	1:L:212:GLY:C	2.25	0.56
2:A:52(B):LYS:HE3	2:A:73:TYR:CD2	2.40	0.56
2:A:57:ALA:HB2	2:A:69:ILE:HD11	1.87	0.56
1:L:127:SER:CB	1:L:128:GLY:HA3	2.35	0.55
2:A:52:ARG:HD2	2:A:56:THR:OG1	2.06	0.55
1:B:148:TRP:HH2	1:B:177:SER:O	1.90	0.55
2:A:177:LEU:HD13	2:A:178:SER:N	2.21	0.55
2:H:171:GLN:HA	2:H:171:GLN:NE2	2.21	0.54
1:B:49:TYR:HB2	2:A:100:THR:CG2	2.36	0.54
2:A:155:ASN:ND2	2:A:194:THR:H	2.05	0.54
1:L:127:SER:HB3	1:L:128:GLY:CA	2.36	0.54
2:H:188:TRP:CG	2:H:189:PRO:HA	2.42	0.54
2:H:148:GLU:OE2	2:H:168:ALA:HB3	2.07	0.54
1:B:105:GLU:HG2	3:B:329:HOH:O	2.06	0.54
2:H:133:GLY:O	2:H:134:SER:CB	2.55	0.54
1:L:138:ASN:OD1	2:H:164:HIS:HE1	1.92	0.53
2:A:81:GLN:HE21	2:A:82(A):ASN:ND2	2.07	0.53
2:A:81:GLN:HE21	2:A:82(A):ASN:HD21	1.54	0.53
2:A:83:ARG:O	2:A:111:VAL:HG11	2.08	0.53
1:B:33:LEU:HD21	1:B:88:CYS:HB2	1.90	0.53
1:B:120:PRO:HD3	1:B:132:VAL:HG22	1.91	0.52
2:A:97:ARG:O	2:A:100:THR:HG23	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:83:ILE:HG13	1:B:106:ILE:HD11	1.89	0.52
2:A:5:VAL:HG13	2:A:105:GLN:NE2	2.24	0.52
2:A:12:VAL:HG21	2:A:18:LEU:HD13	1.91	0.52
2:A:212:PRO:O	2:A:213:GLU:C	2.47	0.52
1:L:31:ILE:HG22	1:L:31:ILE:O	2.09	0.52
1:B:10:SER:HB2	1:B:105:GLU:OE1	2.10	0.51
1:L:7:SER:CB	1:L:8:PRO:CD	2.88	0.51
2:A:69:ILE:HD12	2:A:69:ILE:O	2.09	0.51
1:B:182:THR:HG22	1:B:184:ASP:H	1.75	0.51
1:B:160:LEU:HD23	2:A:171:GLN:OE1	2.11	0.51
1:B:148:TRP:CD1	1:B:193:THR:O	2.64	0.50
1:B:198:HIS:HD2	1:B:200:THR:HB	1.76	0.50
2:H:22:CYS:HB3	2:H:78:LEU:HB3	1.93	0.50
2:A:82:MET:HE2	2:A:82(C):LEU:HD21	1.94	0.50
1:L:164:THR:HG23	2:H:166:PHE:CD2	2.47	0.50
1:B:160:LEU:HD21	2:A:169:VAL:CG1	2.42	0.49
1:L:142:LYS:HG2	1:L:173:TYR:CZ	2.47	0.49
1:B:198:HIS:CD2	1:B:200:THR:HB	2.48	0.49
2:A:34:MET:HE1	2:A:94:ARG:HG3	1.95	0.49
1:B:12:SER:OG	1:B:107:LYS:HG3	2.12	0.49
2:A:184:THR:HB	2:A:187:THR:HG23	1.95	0.49
2:H:143:LYS:HG3	3:H:375:HOH:O	2.13	0.49
1:L:189:HIS:NE2	2:A:85:GLU:HG2	2.29	0.48
2:H:199:HIS:HB3	2:H:204:THR:HB	1.94	0.48
2:A:42:GLY:C	2:A:43:LYS:HE2	2.33	0.48
2:A:188:TRP:CG	2:A:189:PRO:HA	2.49	0.48
1:B:5:ASN:O	1:B:23:CYS:HA	2.13	0.48
1:B:50:LYS:O	1:B:51:ALA:HB3	2.14	0.48
2:A:100:THR:O	2:A:100(A):LEU:CB	2.61	0.48
1:L:8:PRO:O	1:L:102:THR:HG23	2.14	0.48
1:L:7:SER:HB3	1:L:8:PRO:HD2	1.96	0.48
2:A:133:GLY:O	2:A:134:SER:CB	2.62	0.48
2:A:12:VAL:O	2:A:111:VAL:HA	2.14	0.48
3:L:361:HOH:O	2:H:164:HIS:HD2	1.95	0.47
2:A:5:VAL:HG13	2:A:105:GLN:HE22	1.77	0.47
2:A:42:GLY:O	2:A:43:LYS:HE2	2.14	0.47
2:H:52(A):ASN:HD22	2:H:52(A):ASN:H	1.61	0.47
2:A:94:ARG:O	2:A:100(A):LEU:HA	2.15	0.47
2:H:144:GLY:HA2	2:H:174:LEU:HD23	1.97	0.47
1:L:37:GLN:HB2	1:L:47:LEU:HD11	1.97	0.47
1:L:24:ARG:HA	1:L:69:THR:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:19:ILE:CD1	1:L:75:ILE:HB	2.44	0.47
1:L:190:ASN:ND2	1:L:211:ARG:HA	2.30	0.46
2:A:155:ASN:HD21	2:A:193:ILE:HA	1.80	0.46
2:H:6:GLU:CD	2:H:106:GLY:H	2.19	0.45
1:L:193:THR:HG22	1:L:208:SER:HB2	1.98	0.45
1:L:127:SER:CB	1:L:128:GLY:CA	2.93	0.45
1:L:210:ASN:O	1:L:211:ARG:CB	2.60	0.45
1:B:160:LEU:HD21	2:A:169:VAL:CG2	2.45	0.45
1:B:195:GLU:HG2	1:B:206:VAL:HG22	1.99	0.45
2:A:41:PRO:O	2:A:43:LYS:HE3	2.17	0.45
2:H:52(A):ASN:HD22	2:H:52(A):ASN:N	2.15	0.45
1:L:7:SER:CB	1:L:8:PRO:HD2	2.46	0.45
1:B:138:ASN:ND2	2:A:164:HIS:CE1	2.84	0.45
1:L:4:MET:HG2	1:L:97:THR:HG23	1.99	0.45
2:H:184:THR:HG22	2:H:186:SER:N	2.31	0.44
1:B:186:TYR:HA	1:B:192:TYR:OH	2.17	0.44
1:B:96:ARG:HG3	2:A:47:TRP:CD1	2.52	0.44
1:B:161:ASN:ND2	1:B:177:SER:OG	2.50	0.44
1:L:149:LYS:HB2	1:L:193:THR:OG1	2.17	0.44
2:H:52(A):ASN:H	2:H:52(A):ASN:ND2	2.16	0.44
2:A:35:THR:CG2	2:A:93:VAL:HG13	2.48	0.44
1:L:193:THR:HG22	1:L:208:SER:CB	2.48	0.44
1:L:78:LEU:HA	3:L:427:HOH:O	2.18	0.43
2:A:82:MET:HB3	2:A:82(C):LEU:HD21	1.99	0.43
2:A:52(B):LYS:HG3	2:A:73:TYR:CZ	2.53	0.43
2:H:144:GLY:CA	2:H:174:LEU:HD23	2.48	0.43
1:B:148:TRP:CH2	1:B:177:SER:O	2.71	0.43
1:B:160:LEU:HD11	2:A:169:VAL:CG1	2.48	0.43
1:L:24:ARG:HD2	1:L:70:ASP:OD1	2.19	0.43
1:L:126:THR:N	1:L:127:SER:HA	2.34	0.43
2:A:16:GLY:O	2:A:17:SER:CB	2.67	0.42
1:L:50:LYS:HB2	1:L:53:ASN:ND2	2.33	0.42
1:L:115:VAL:O	1:L:207:LYS:HE3	2.19	0.42
1:B:37:GLN:HB2	1:B:47:LEU:HD11	2.01	0.42
1:L:136:LEU:CD2	1:L:146:VAL:HG22	2.49	0.42
2:A:35:THR:HG23	2:A:93:VAL:HG13	2.01	0.42
2:A:13:GLN:HE21	2:A:13:GLN:HA	1.85	0.42
1:L:198:HIS:HD2	1:L:200:THR:OG1	2.03	0.42
2:H:187:THR:O	2:H:191:GLN:HB2	2.19	0.42
2:H:144:GLY:HA2	2:H:174:LEU:HB3	2.02	0.42
2:H:96:GLY:HA3	2:H:101:ASP:OD1	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:95:GLN:HB2	2:A:100(A):LEU:HD23	2.02	0.42
1:B:86:TYR:CE1	1:B:104:LEU:HD22	2.55	0.42
2:A:194:THR:HG23	2:A:208:LYS:C	2.40	0.41
2:A:199:HIS:HD2	2:A:202:SER:CB	2.32	0.41
1:B:96:ARG:H	1:B:96:ARG:HG2	1.62	0.41
1:L:198:HIS:CG	1:L:199:LYS:N	2.88	0.41
1:B:58:VAL:HA	1:B:59:PRO:HD3	1.87	0.41
2:H:159:LEU:HD21	2:H:181:VAL:HG21	2.03	0.41
1:B:136:LEU:HD12	1:B:136:LEU:N	2.36	0.41
2:H:13:GLN:HG2	2:H:13:GLN:H	1.70	0.41
2:A:146:PHE:HA	2:A:147:PRO:HA	1.87	0.41
1:L:49:TYR:O	1:L:53:ASN:HB2	2.21	0.41
1:L:120:PRO:HD3	1:L:132:VAL:HG22	2.03	0.41
2:H:38:ARG:HD3	2:H:48:LEU:HD11	2.02	0.41
1:L:27:GLN:O	1:L:29:ILE:HG23	2.21	0.41
1:L:150:ILE:HD11	1:L:179:LEU:HD21	2.03	0.41
2:A:123:PRO:HB3	2:A:210:ILE:HD13	2.03	0.40
1:B:156:GLN:O	1:B:157:ASN:O	2.39	0.40
1:L:186:TYR:HA	1:L:192:TYR:OH	2.22	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	B	210/212 (99%)	195 (93%)	13 (6%)	2 (1%)	19	10
1	L	210/212 (99%)	195 (93%)	10 (5%)	5 (2%)	7	2
2	A	213/220 (97%)	205 (96%)	4 (2%)	4 (2%)	10	3
2	H	210/220 (96%)	201 (96%)	7 (3%)	2 (1%)	19	10
All	All	843/864 (98%)	796 (94%)	34 (4%)	13 (2%)	13	5

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	7	SER
1	L	8	PRO
1	L	157	ASN
2	H	134	SER
1	B	211	ARG
2	A	17	SER
2	A	134	SER
1	L	211	ARG
1	B	157	ASN
2	A	16	GLY
2	A	100(A)	LEU
2	H	121	VAL
1	L	128	GLY

### 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	B	188/188 (100%)	181 (96%)	7 (4%)	41	38
1	L	188/188 (100%)	181 (96%)	7 (4%)	41	38
2	A	183/185 (99%)	170 (93%)	13 (7%)	18	12
2	H	180/185 (97%)	177 (98%)	3 (2%)	68	72
All	All	739/746 (99%)	709 (96%)	30 (4%)	37	34

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

Mol	Chain	Res	Type
1	L	15	LEU
1	L	19	ILE
1	L	24	ARG
1	L	105	GLU
1	L	125	LEU
1	L	127	SER
1	L	157	ASN

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Mol	Chain	Res	Type
2	H	52(A)	ASN
2	H	171	GLN
2	H	205	LYS
1	B	50	LYS
1	B	96	ARG
1	B	104	LEU
1	B	143	ASP
1	B	145	ASN
1	B	148	TRP
1	B	165	ASP
2	A	2	VAL
2	A	13	GLN
2	A	35	THR
2	A	85	GLU
2	A	93	VAL
2	A	111	VAL
2	A	115	LYS
2	A	169	VAL
2	A	182	THR
2	A	187	THR
2	A	195	CYS
2	A	208	LYS
2	A	213	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	5	ASN
1	L	6	GLN
1	L	27	GLN
1	L	42	ASN
1	L	53	ASN
1	L	145	ASN
1	L	190	ASN
1	L	198	HIS
2	H	52(A)	ASN
2	H	79	HIS
2	H	164	HIS
2	H	171	GLN
2	H	196	ASN
1	B	3	GLN
1	B	6	GLN

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Mol	Chain	Res	Type
1	B	37	GLN
1	B	138	ASN
1	B	161	ASN
1	B	190	ASN
1	B	198	HIS
1	B	210	ASN
2	A	13	GLN
2	A	82(A)	ASN
2	A	155	ASN
2	A	164	HIS
2	A	199	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 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	B	212/212 (100%)	0.68	24 (11%) <b>7</b> <b>10</b>	26, 39, 54, 64	0
1	L	212/212 (100%)	0.68	22 (10%) <b>8</b> <b>12</b>	27, 41, 55, 63	0
2	A	217/220 (98%)	0.61	28 (12%) <b>5</b> <b>7</b>	27, 40, 58, 78	0
2	H	214/220 (97%)	0.76	26 (12%) <b>6</b> <b>8</b>	29, 41, 58, 68	0
All	All	855/864 (98%)	0.68	100 (11%) <b>6</b> <b>9</b>	26, 40, 57, 78	0

All (100) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	35	TRP	5.5
2	H	172	SER	5.4
2	H	173	GLY	4.9
2	A	132	THR	4.5
1	B	33	LEU	4.2
2	H	157	GLY	4.1
1	L	203	SER	4.0
1	B	132	VAL	4.0
1	L	129	GLY	3.9
2	A	186	SER	3.9
2	H	40	ALA	3.8
2	A	93	VAL	3.7
2	A	35	THR	3.6
2	A	41	PRO	3.6
2	A	42	GLY	3.6
2	H	97	ARG	3.6
2	A	172	SER	3.5
2	H	134	SER	3.5
1	B	133	VAL	3.5
2	H	138	LEU	3.5
2	H	37	VAL	3.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	L	126	THR	3.4
1	L	33	LEU	3.4
1	B	153	SER	3.4
1	L	128	GLY	3.4
2	H	200	PRO	3.3
1	B	32	TRP	3.3
1	B	89	LEU	3.2
2	A	36	TRP	3.2
1	B	36	TYR	3.2
1	L	35	TRP	3.2
2	H	186	SER	3.1
1	L	133	VAL	3.1
1	B	34	SER	3.0
2	A	140	CYS	3.0
2	A	52(C)	ARG	3.0
1	L	56	THR	3.0
2	A	78	LEU	3.0
1	L	73	LEU	3.0
1	L	157	ASN	2.9
2	H	93	VAL	2.9
1	B	41	GLY	2.9
2	A	1	GLU	2.9
1	L	8	PRO	2.9
1	B	56	THR	2.9
2	H	99	TYR	2.8
1	L	34	SER	2.8
2	A	40	ALA	2.7
1	L	156	GLN	2.7
1	B	88	CYS	2.7
2	A	113	SER	2.6
2	H	188	TRP	2.6
2	H	133	GLY	2.6
1	B	157	ASN	2.6
2	A	141	LEU	2.5
1	B	156	GLN	2.5
2	A	43	LYS	2.5
2	A	187	THR	2.5
1	L	201	SER	2.5
1	B	212	GLY	2.5
1	B	104	LEU	2.5
2	H	177	LEU	2.4
1	B	134	CYS	2.4

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Mol	Chain	Res	Type	RSRZ
2	A	124	LEU	2.4
1	B	1	ASP	2.4
1	L	125	LEU	2.4
2	A	100(A)	LEU	2.4
2	A	103	TRP	2.4
1	L	72	THR	2.3
1	L	179	LEU	2.3
2	A	48	LEU	2.3
1	L	202	THR	2.3
1	B	23	CYS	2.3
1	B	60	SER	2.3
1	B	135	PHE	2.2
2	H	127	VAL	2.2
2	A	139	GLY	2.2
1	L	36	TYR	2.2
2	H	36	TRP	2.2
2	H	181	VAL	2.2
2	A	49	ALA	2.2
2	H	113	SER	2.2
2	H	210	ILE	2.2
1	L	47	LEU	2.2
2	H	67	PHE	2.2
2	A	75	ARG	2.1
2	A	80	LEU	2.1
1	B	118	PHE	2.1
2	H	69	ILE	2.1
2	A	128	CYS	2.1
2	H	41	PRO	2.1
2	H	158	SER	2.1
2	H	185	SER	2.1
1	B	202	THR	2.1
1	L	86	TYR	2.1
1	B	148	TRP	2.0
2	H	78	LEU	2.0
2	A	37	VAL	2.0
1	L	71	PHE	2.0
2	A	99	TYR	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.

### 6.4 Ligands

There are no ligands in this entry.

### 6.5 Other polymers

There are no such residues in this entry.