



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 30, 2017 – 08:55 PM EST

PDB ID : 5WTG  
Title : Crystal structure of the Fab fragment of anti-HAV antibody R10  
Authors : Wang, X.; Zhu, L.; Dang, M.; Hu, Z.; Gao, Q.; Yuan, S.; Sun, Y.; Zhang, B.; Ren, J.; Walter, T.S.; Wang, J.; Fry, E.E.; Stuart, D.I.; Rao, Z.  
Deposited on : 2016-12-11  
Resolution : 2.91 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	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
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-20028442

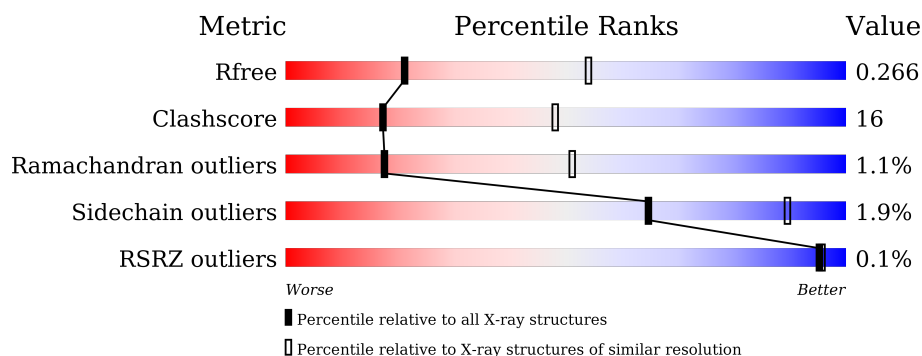
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.91 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	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (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 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	A	212	<div> <div>72%</div> <div>26%</div> <div>.</div> </div>
1	C	212	<div> <div>71%</div> <div>27%</div> <div>.</div> </div>
2	B	221	<div> <div>67%</div> <div>29%</div> <div>..</div> </div>
2	D	221	<div> <div>65%</div> <div>32%</div> <div>..</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6531 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 Light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	212	Total	C	N	O	S	0	0	0
			1630	1012	273	336	9			
1	C	212	Total	C	N	O	S	0	0	0
			1633	1013	273	338	9			

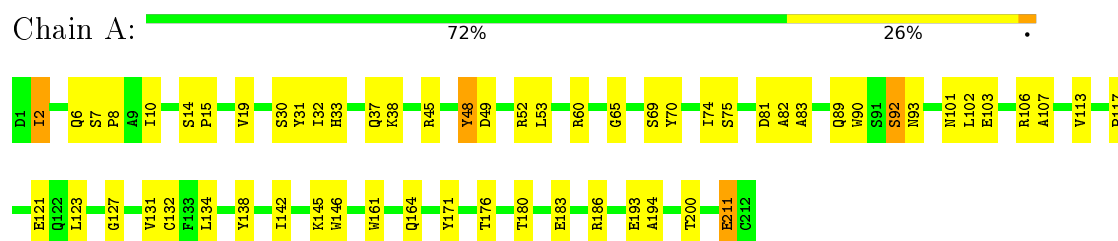
- Molecule 2 is a protein called FAB Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	217	Total	C	N	O	S	0	0	0
			1634	1040	268	318	8			
2	D	217	Total	C	N	O	S	0	0	0
			1634	1040	268	318	8			

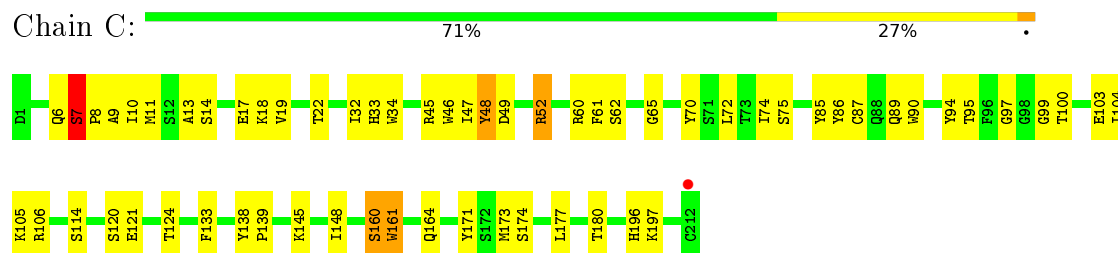
### 3 Residue-property plots

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.

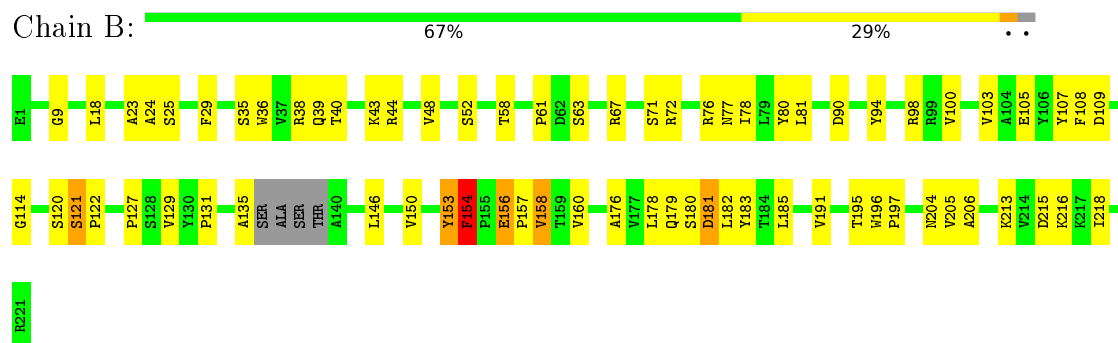
#### • Molecule 1: FAB Light chain



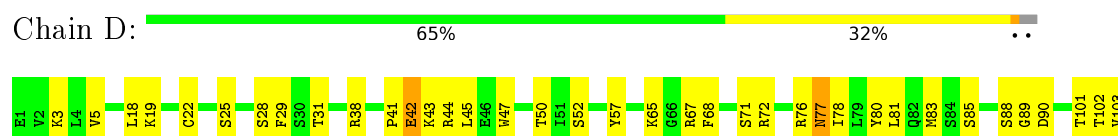
#### • Molecule 1: FAB Light chain



#### • Molecule 2: FAB Heavy chain



#### • Molecule 2: FAB Heavy chain





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	52.51Å 140.52Å 68.92Å 90.00° 110.36° 90.00°	Depositor
Resolution (Å)	49.23 – 2.91 49.23 – 2.91	Depositor EDS
% Data completeness (in resolution range)	97.2 (49.23-2.91) 97.2 (49.23-2.91)	Depositor EDS
$R_{merge}$	0.20	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.02 (at 2.91Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, $R_{free}$	0.201 , 0.266 0.201 , 0.266	Depositor DCC
$R_{free}$ test set	983 reflections (4.90%)	DCC
Wilson B-factor (Å <sup>2</sup> )	18.9	Xtriage
Anisotropy	0.840	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 1.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.054 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	6531	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.25% 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, 0.333 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	0.92	3/1669 (0.2%)	0.89	4/2267 (0.2%)
1	C	0.84	3/1672 (0.2%)	0.78	3/2271 (0.1%)
2	B	0.64	1/1678 (0.1%)	0.72	2/2292 (0.1%)
2	D	0.76	1/1678 (0.1%)	0.83	3/2292 (0.1%)
All	All	0.80	8/6697 (0.1%)	0.81	12/9122 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	41	PRO	N-CD	-15.92	1.25	1.47
1	A	138	TYR	CE1-CZ	-7.97	1.28	1.38
1	C	121	GLU	CD-OE1	-6.08	1.19	1.25
1	C	121	GLU	CD-OE2	-5.99	1.19	1.25
1	C	161	TRP	CE3-CZ3	-5.71	1.28	1.38
1	A	48	TYR	CE1-CZ	-5.28	1.31	1.38
1	A	200	THR	C-N	-5.26	1.22	1.34
2	B	153	TYR	CE2-CZ	-5.13	1.31	1.38

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	211	GLU	O-C-N	-16.74	95.92	122.70
1	A	211	GLU	CA-C-N	11.63	142.78	117.20
2	D	43	LYS	N-CA-C	9.27	136.03	111.00
2	D	42	GLU	N-CA-C	-7.78	89.98	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	211	GLU	N-CA-C	-5.96	94.90	111.00
1	A	211	GLU	C-N-CA	5.89	136.43	121.70
2	B	156	GLU	N-CA-C	5.86	126.83	111.00
1	C	7	SER	C-N-CD	5.82	140.62	128.40
1	C	52	ARG	N-CA-C	5.47	125.78	111.00
1	C	48	TYR	N-CA-C	5.25	125.17	111.00
2	D	152	GLY	N-CA-C	5.23	126.18	113.10
2	B	154	PHE	C-N-CD	5.00	138.91	128.40

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	211	GLU	Mainchain,Peptide
1	A	6	GLN	Peptide

## 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	1630	0	1537	43	1
1	C	1633	0	1541	66	0
2	B	1634	0	1601	64	0
2	D	1634	0	1601	53	1
All	All	6531	0	6280	206	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 16.

All (206) 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:52:ARG:HH12	2:B:103:VAL:CG2	1.26	1.45
1:A:89:GLN:NE2	1:A:93:ASN:O	1.65	1.28
1:A:52:ARG:NH1	2:B:103:VAL:CG2	2.05	1.19

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:ARG:NH1	2:B:103:VAL:HG21	1.58	1.17
1:C:49:ASP:OD1	2:D:102:THR:CG2	1.94	1.15
1:A:113:VAL:HG22	1:A:134:LEU:HD22	1.33	1.10
2:B:158:VAL:HG11	2:B:185:LEU:HD21	1.38	1.05
2:B:100:VAL:HG11	2:B:109:ASP:OD2	1.56	1.03
1:A:52:ARG:NH1	2:B:103:VAL:HG23	1.81	0.94
2:D:120:SER:OG	2:D:122:PRO:HD3	1.68	0.93
1:C:9:ALA:O	1:C:10:ILE:HD13	1.68	0.93
1:A:52:ARG:HH12	2:B:103:VAL:HG21	0.76	0.92
2:D:204:ASN:ND2	2:D:215:ASP:OD1	2.02	0.91
1:C:49:ASP:OD1	2:D:102:THR:HG21	1.67	0.90
1:C:33:HIS:ND1	1:C:48:TYR:O	2.05	0.90
1:C:11:MET:HE3	1:C:100:THR:HG21	1.57	0.86
1:A:45:ARG:NH2	2:B:109:ASP:OD1	2.10	0.84
1:C:8:PRO:HG2	1:C:11:MET:HE2	1.58	0.83
2:B:181:ASP:HB2	1:C:180:THR:HG21	1.60	0.82
2:B:158:VAL:CG1	2:B:185:LEU:HD21	2.09	0.81
1:C:7:SER:HB2	1:C:22:THR:H	1.47	0.78
1:C:103:GLU:OE1	1:C:171:TYR:OH	2.04	0.75
1:C:61:PHE:CZ	1:C:74:ILE:HD12	2.22	0.75
2:B:204:ASN:ND2	2:B:215:ASP:OD1	2.19	0.74
2:D:127:PRO:HB3	2:D:153:TYR:HB3	1.71	0.73
2:B:100:VAL:CG1	2:B:109:ASP:OD2	2.33	0.73
2:B:52:SER:O	2:B:72:ARG:NH2	2.21	0.73
1:A:186:ARG:NH2	2:D:42:GLU:OE2	2.19	0.73
2:B:23:ALA:HA	2:B:78:ILE:HG22	1.71	0.73
2:D:67:ARG:NH1	2:D:90:ASP:OD2	2.22	0.73
1:C:7:SER:CB	1:C:22:THR:H	2.02	0.73
2:B:39:GLN:HA	2:B:44:ARG:O	1.90	0.72
2:B:24:ALA:HB3	2:B:77:ASN:HB3	1.72	0.72
2:B:9:GLY:HA2	2:B:18:LEU:HD21	1.72	0.72
2:D:38:ARG:HH22	2:D:90:ASP:HA	1.55	0.72
2:B:206:ALA:CB	2:B:213:LYS:HG2	2.20	0.71
1:C:8:PRO:CG	1:C:11:MET:HE2	2.20	0.70
1:C:11:MET:HE3	1:C:100:THR:CG2	2.20	0.70
1:C:148:ILE:HD11	1:C:177:LEU:HD21	1.74	0.70
2:D:150:VAL:HB	2:D:185:LEU:HB3	1.73	0.69
2:B:129:VAL:O	2:B:216:LYS:NZ	2.27	0.67
1:A:48:TYR:HB3	2:B:107:TYR:CE2	2.29	0.66
1:A:92:SER:OG	1:A:93:ASN:N	2.29	0.66
2:D:3:LYS:HB2	2:D:25:SER:HB3	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:ARG:NH1	1:A:81:ASP:OD2	2.29	0.65
1:A:32:ILE:O	1:A:49:ASP:O	2.14	0.65
1:C:8:PRO:HG2	1:C:11:MET:CE	2.25	0.65
1:A:2:ILE:HG21	1:A:92:SER:OG	1.97	0.64
1:C:49:ASP:OD1	2:D:102:THR:HG22	1.92	0.64
2:D:192:PRO:HG2	2:D:195:THR:OG1	1.98	0.63
1:C:11:MET:CE	1:C:100:THR:HG21	2.29	0.62
1:C:138:TYR:CD1	1:C:139:PRO:HA	2.34	0.62
1:C:196:HIS:CD2	1:C:197:LYS:H	2.18	0.61
2:B:48:VAL:HA	2:B:61:PRO:HG3	1.82	0.61
1:C:7:SER:HB2	1:C:22:THR:N	2.14	0.61
1:A:7:SER:HB2	1:A:8:PRO:HD3	1.83	0.61
1:A:113:VAL:CG2	1:A:134:LEU:HD22	2.22	0.61
2:B:131:PRO:HG3	2:B:216:LYS:HD2	1.83	0.60
1:C:138:TYR:CG	1:C:139:PRO:HA	2.36	0.60
1:A:90:TRP:HB2	2:B:105:GLU:OE1	2.02	0.60
1:C:6:GLN:HE22	1:C:86:TYR:HA	1.67	0.60
2:D:120:SER:OG	2:D:122:PRO:CD	2.48	0.59
1:C:8:PRO:CG	1:C:11:MET:CE	2.79	0.59
1:C:49:ASP:OD1	2:D:102:THR:HG23	1.98	0.58
1:C:7:SER:HB3	1:C:8:PRO:CD	2.33	0.58
1:A:121:GLU:OE1	2:B:216:LYS:NZ	2.34	0.57
2:B:122:PRO:HG2	2:B:154:PHE:CE1	2.38	0.57
2:D:121:SER:N	2:D:122:PRO:HD3	2.19	0.57
2:B:156:GLU:OE1	2:B:176:ALA:HB3	2.04	0.56
1:A:19:VAL:HB	1:A:74:ILE:HB	1.87	0.56
2:D:158:VAL:CG1	2:D:185:LEU:HD22	2.35	0.56
1:C:7:SER:CB	1:C:8:PRO:CD	2.82	0.56
2:B:40:THR:OG1	2:B:44:ARG:HB3	2.06	0.56
2:D:151:LYS:HA	2:D:184:THR:HG23	1.88	0.56
2:B:146:LEU:HD22	2:B:218:ILE:HG21	1.87	0.56
1:A:103:GLU:OE1	1:A:171:TYR:OH	2.15	0.55
2:B:180:SER:OG	2:B:180:SER:O	2.20	0.55
2:B:63:SER:O	2:B:67:ARG:NH2	2.39	0.55
2:D:201:VAL:HG12	2:D:218:ILE:HD13	1.87	0.55
2:D:67:ARG:HG2	2:D:85:SER:HB2	1.89	0.55
2:B:179:GLN:O	2:B:180:SER:HB3	2.07	0.55
2:D:71:SER:HB2	2:D:80:TYR:HB2	1.87	0.55
1:C:33:HIS:CD2	1:C:90:TRP:HD1	2.24	0.55
2:D:158:VAL:HG13	2:D:185:LEU:HD22	1.89	0.54
1:A:48:TYR:HB3	2:B:107:TYR:CD2	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:191:VAL:HG13	2:D:195:THR:HB	1.88	0.54
1:C:60:ARG:NH1	1:C:74:ILE:HD11	2.22	0.54
2:D:5:VAL:HG13	2:D:113:GLN:NE2	2.23	0.54
2:D:217:LYS:HD2	2:D:219:VAL:CG1	2.38	0.54
2:D:101:THR:HG22	2:D:106:TYR:CE1	2.43	0.53
1:A:134:LEU:HD11	1:A:194:ALA:HB2	1.90	0.53
2:B:206:ALA:HB2	2:B:213:LYS:HG2	1.91	0.52
1:C:7:SER:OG	1:C:8:PRO:HD3	2.09	0.52
1:C:45:ARG:NH1	2:D:110:TYR:OH	2.43	0.52
2:B:191:VAL:HG13	2:B:195:THR:HB	1.92	0.52
1:C:104:ILE:O	1:C:164:GLN:NE2	2.41	0.52
2:B:121:SER:N	2:B:122:PRO:HD3	2.25	0.52
1:C:9:ALA:C	1:C:10:ILE:HD13	2.31	0.51
2:D:178:LEU:HD13	2:D:183:TYR:CE1	2.45	0.51
1:A:60:ARG:HB2	1:A:75:SER:HB3	1.92	0.51
2:B:76:ARG:HD2	2:B:78:ILE:HD11	1.92	0.51
2:D:28:SER:O	2:D:31:THR:HG22	2.11	0.51
1:A:164:GLN:HG3	1:A:171:TYR:CZ	2.45	0.51
2:D:102:THR:HG22	2:D:103:VAL:H	1.75	0.51
1:C:120:SER:O	1:C:124:THR:HG23	2.10	0.51
1:C:7:SER:HB3	1:C:8:PRO:HD2	1.91	0.51
1:C:6:GLN:HE21	1:C:97:GLY:HA3	1.74	0.51
2:B:67:ARG:NH1	2:B:90:ASP:OD2	2.45	0.50
2:B:40:THR:HG23	2:B:44:ARG:HB3	1.94	0.50
1:C:14:SER:N	1:C:17:GLU:OE2	2.42	0.50
1:C:46:TRP:O	1:C:47:ILE:HD13	2.12	0.49
2:D:88:SER:C	2:D:90:ASP:H	2.16	0.49
1:C:19:VAL:HB	1:C:74:ILE:CG2	2.43	0.49
1:C:7:SER:HB2	1:C:22:THR:CA	2.44	0.48
2:B:120:SER:CB	2:B:122:PRO:HD3	2.43	0.48
2:B:178:LEU:HD12	2:B:182:LEU:O	2.14	0.48
2:B:40:THR:CG2	2:B:44:ARG:HB3	2.43	0.48
2:D:38:ARG:NH2	2:D:90:ASP:HA	2.27	0.48
1:C:114:SER:HB2	1:C:133:PHE:HB2	1.96	0.47
1:C:34:TRP:HB2	1:C:47:ILE:HB	1.97	0.47
1:A:142:ILE:HG22	1:A:161:TRP:HH2	1.78	0.47
1:C:62:SER:O	1:C:72:LEU:HD12	2.13	0.47
1:C:89:GLN:NE2	1:C:95:THR:H	2.12	0.47
1:C:14:SER:HB2	1:C:105:LYS:HB3	1.97	0.47
2:B:120:SER:C	2:B:122:PRO:HD3	2.34	0.47
1:A:65:GLY:HA3	1:A:70:TYR:HA	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:ALA:HA	1:A:102:LEU:HD23	1.97	0.47
1:A:33:HIS:CD2	1:A:90:TRP:HD1	2.32	0.47
2:B:196:TRP:CD1	2:B:197:PRO:HA	2.49	0.47
2:D:191:VAL:CG1	2:D:195:THR:HB	2.44	0.47
1:A:142:ILE:HG22	1:A:161:TRP:CH2	2.50	0.47
1:A:131:VAL:HG22	1:A:176:THR:HG23	1.97	0.47
2:B:35:SER:HB2	2:B:108:PHE:CE1	2.50	0.47
2:D:68:PHE:CE1	2:D:83:MET:HB3	2.50	0.47
2:D:103:VAL:HG13	2:D:104:ALA:N	2.30	0.46
1:A:117:PRO:HG2	2:B:135:ALA:HB2	1.98	0.46
1:A:145:LYS:HG3	1:A:193:GLU:HG3	1.97	0.46
1:A:38:LYS:HG2	1:A:83:ALA:HB2	1.98	0.46
1:C:19:VAL:HB	1:C:74:ILE:HG23	1.98	0.46
2:B:29:PHE:CD2	2:B:77:ASN:HA	2.51	0.46
1:C:33:HIS:O	1:C:87:CYS:HA	2.16	0.45
1:C:160:SER:HB3	2:D:174:PHE:HB3	1.98	0.45
1:A:106:ARG:NE	1:A:107:ALA:O	2.45	0.45
1:A:30:SER:HB3	1:A:31:TYR:CD1	2.52	0.45
1:C:33:HIS:CD2	1:C:90:TRP:CD1	3.04	0.45
2:D:149:LEU:HD12	2:D:185:LEU:O	2.17	0.45
2:D:217:LYS:HD2	2:D:219:VAL:HG13	1.99	0.45
2:B:181:ASP:O	2:B:182:LEU:HD23	2.17	0.45
1:C:11:MET:HB2	1:C:11:MET:HE2	1.80	0.45
1:C:7:SER:HB2	1:C:22:THR:CB	2.47	0.45
2:D:127:PRO:CB	2:D:153:TYR:HB3	2.44	0.45
2:D:52:SER:O	2:D:72:ARG:NH2	2.50	0.45
2:D:68:PHE:HB3	2:D:81:LEU:HD11	1.99	0.45
1:C:7:SER:HB2	1:C:22:THR:HB	1.98	0.44
2:D:47:TRP:HE1	2:D:50:THR:HG1	1.63	0.44
1:C:196:HIS:CD2	1:C:197:LYS:N	2.86	0.44
2:D:67:ARG:C	2:D:68:PHE:HD1	2.20	0.44
2:D:77:ASN:N	2:D:77:ASN:OD1	2.49	0.44
2:D:181:ASP:O	2:D:182:LEU:HD23	2.17	0.44
2:B:127:PRO:HB3	2:B:153:TYR:HB3	2.00	0.44
2:B:156:GLU:OE1	2:B:176:ALA:CB	2.66	0.44
1:C:65:GLY:HA3	1:C:70:TYR:CD2	2.53	0.44
1:A:180:THR:HG21	2:D:181:ASP:OD2	2.18	0.44
2:D:29:PHE:CD2	2:D:77:ASN:HA	2.53	0.43
1:C:18:LYS:HG2	1:C:75:SER:HA	2.00	0.43
2:D:76:ARG:O	2:D:78:ILE:HG13	2.18	0.43
2:B:154:PHE:O	2:B:183:TYR:HD2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:36:TRP:NE1	2:B:81:LEU:HB2	2.33	0.43
1:C:33:HIS:CE1	1:C:48:TYR:O	2.70	0.43
1:C:48:TYR:CE2	1:C:52:ARG:HB3	2.53	0.43
1:A:180:THR:H	1:A:183:GLU:HB3	1.83	0.43
2:D:3:LYS:HB3	2:D:3:LYS:HE3	1.79	0.43
2:B:154:PHE:O	2:B:183:TYR:CD2	2.72	0.43
2:D:18:LEU:HG	2:D:19:LYS:H	1.84	0.43
2:B:196:TRP:CG	2:B:197:PRO:HA	2.54	0.43
1:C:173:MET:HG2	1:C:174:SER:N	2.34	0.43
1:A:14:SER:OG	1:A:15:PRO:HD2	2.18	0.42
2:B:100:VAL:HG21	2:B:109:ASP:OD2	2.19	0.42
2:D:180:SER:OG	2:D:180:SER:O	2.31	0.42
2:B:38:ARG:HG2	2:B:48:VAL:CG1	2.49	0.42
1:C:65:GLY:HA3	1:C:70:TYR:HA	2.01	0.42
2:D:196:TRP:CG	2:D:197:PRO:HA	2.54	0.42
1:C:60:ARG:HB2	1:C:60:ARG:HH11	1.85	0.42
2:D:44:ARG:HG2	2:D:45:LEU:N	2.33	0.42
2:D:102:THR:HG22	2:D:103:VAL:N	2.34	0.42
1:C:32:ILE:O	1:C:49:ASP:O	2.38	0.42
1:C:33:HIS:HD2	1:C:90:TRP:HD1	1.66	0.42
2:B:146:LEU:HD13	2:B:218:ILE:HG21	2.02	0.41
1:A:32:ILE:HB	1:A:70:TYR:CD1	2.55	0.41
1:A:132:CYS:HB2	1:A:146:TRP:CZ2	2.55	0.41
1:C:160:SER:O	1:C:173:MET:HA	2.21	0.41
2:B:40:THR:O	2:B:43:LYS:N	2.49	0.41
2:B:71:SER:HB2	2:B:80:TYR:HB2	2.01	0.41
2:B:94:TYR:O	2:B:114:GLY:HA2	2.21	0.41
2:B:76:ARG:HB2	2:B:78:ILE:HG12	2.03	0.41
2:B:98:ARG:O	2:B:108:PHE:HA	2.21	0.41
2:B:122:PRO:HG2	2:B:154:PHE:CZ	2.55	0.41
1:C:74:ILE:HG23	1:C:74:ILE:O	2.21	0.41
1:A:123:LEU:HA	1:A:127:GLY:O	2.20	0.41
1:C:89:GLN:O	1:C:94:TYR:HA	2.21	0.41
1:A:37:GLN:O	1:A:83:ALA:HB1	2.21	0.40
1:C:13:ALA:O	1:C:105:LYS:N	2.43	0.40
2:B:160:VAL:HG22	2:B:205:VAL:HG22	2.03	0.40
2:B:150:VAL:HB	2:B:185:LEU:CD1	2.51	0.40
1:A:10:ILE:HG12	1:A:101:ASN:HB2	2.02	0.40
1:C:85:TYR:O	1:C:99:GLY:HA2	2.21	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:53:LEU:O	2:D:169:SER:OG[2_747]	2.19	0.01

## 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	210/212 (99%)	193 (92%)	16 (8%)	1 (0%)	34	71
1	C	210/212 (99%)	192 (91%)	17 (8%)	1 (0%)	34	71
2	B	213/221 (96%)	192 (90%)	18 (8%)	3 (1%)	14	44
2	D	213/221 (96%)	187 (88%)	22 (10%)	4 (2%)	10	35
All	All	846/866 (98%)	764 (90%)	73 (9%)	9 (1%)	17	51

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	7	SER
1	A	2	ILE
2	D	65	LYS
2	B	181	ASP
2	D	154	PHE
2	B	154	PHE
2	B	121	SER
2	D	89	GLY
2	D	121	SER

### 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	185/186 (100%)	183 (99%)	2 (1%)	80	95
1	C	186/186 (100%)	182 (98%)	4 (2%)	60	88
2	B	183/187 (98%)	179 (98%)	4 (2%)	60	88
2	D	183/187 (98%)	179 (98%)	4 (2%)	60	88
All	All	737/746 (99%)	723 (98%)	14 (2%)	65	89

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	SER
1	A	92	SER
2	B	25	SER
2	B	58	THR
2	B	157	PRO
2	B	158	VAL
1	C	106	ARG
1	C	145	LYS
1	C	160	SER
1	C	161	TRP
2	D	22	CYS
2	D	57	TYR
2	D	77	ASN
2	D	186	SER

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

Mol	Chain	Res	Type
1	C	6	GLN
1	C	196	HIS
1	C	210	ASN
2	D	113	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 [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, 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	A	212/212 (100%)	-0.65	0 100 100	9, 20, 36, 63	0
1	C	212/212 (100%)	-0.71	1 (0%) 91 90	9, 20, 34, 72	0
2	B	217/221 (98%)	-0.62	0 100 100	10, 19, 35, 49	0
2	D	217/221 (98%)	-0.68	0 100 100	9, 18, 35, 51	0
All	All	858/866 (99%)	-0.66	1 (0%) 95 96	9, 19, 35, 72	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	212	CYS	2.2

### 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.