



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2018 – 03:46 pm GMT

PDB ID : 5B4M  
Title : Crystal structure of an Fab against human influenza A  
Authors : Yuan, Y.A.  
Deposited on : 2016-04-05  
Resolution : 2.40 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

<https://www.wwpdb.org/validation/2017/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  
Xtriage (Phenix) : 1.13  
EDS : trunk30967  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30967

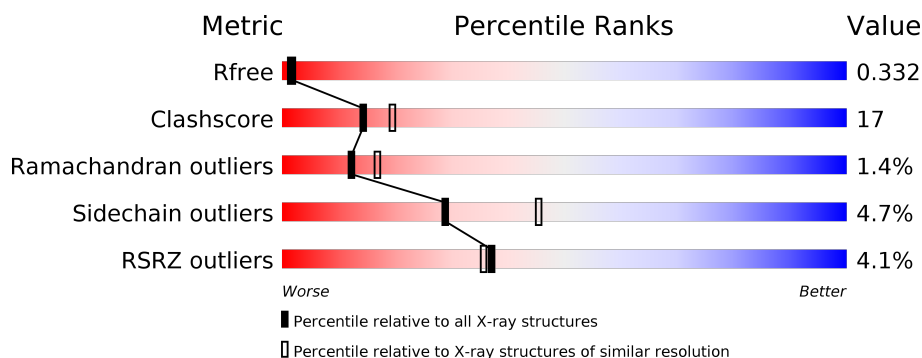
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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))
$R_{free}$	111664	3481 (2.40-2.40)
Clashscore	122126	3956 (2.40-2.40)
Ramachandran outliers	120053	3897 (2.40-2.40)
Sidechain outliers	120020	3898 (2.40-2.40)
RSRZ outliers	108989	3386 (2.40-2.40)

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	C	221	<div> <div>5%</div> <div> <div></div> <div>79%</div> <div>18%</div> <div>.</div> </div> </div>
1	H	221	<div> <div>3%</div> <div> <div></div> <div>74%</div> <div>22%</div> <div>.</div> </div> </div>
2	D	218	<div> <div>4%</div> <div> <div></div> <div>69%</div> <div>27%</div> <div>..</div> </div> </div>
2	L	218	<div> <div>4%</div> <div> <div></div> <div>68%</div> <div>28%</div> <div>..</div> </div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6738 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 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	221	Total	C	N	O	S	0	0	0
			1687	1068	284	328	7			
1	C	221	Total	C	N	O	S	0	0	0
			1687	1068	284	328	7			

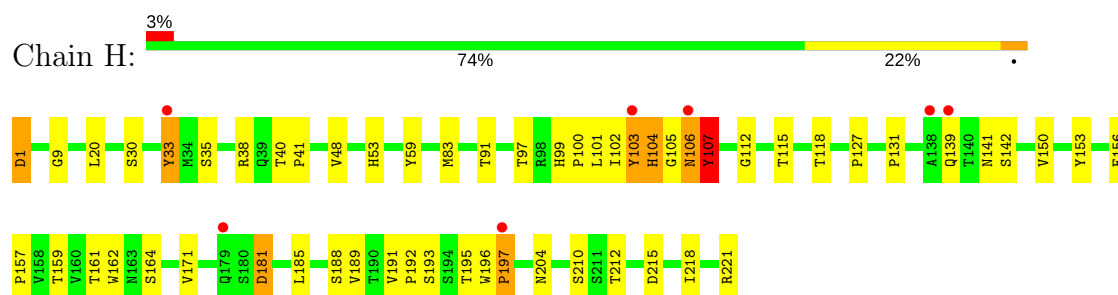
- Molecule 2 is a protein called Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	218	Total	C	N	O	S	0	0	0
			1682	1046	280	350	6			
2	D	218	Total	C	N	O	S	0	0	0
			1682	1046	280	350	6			

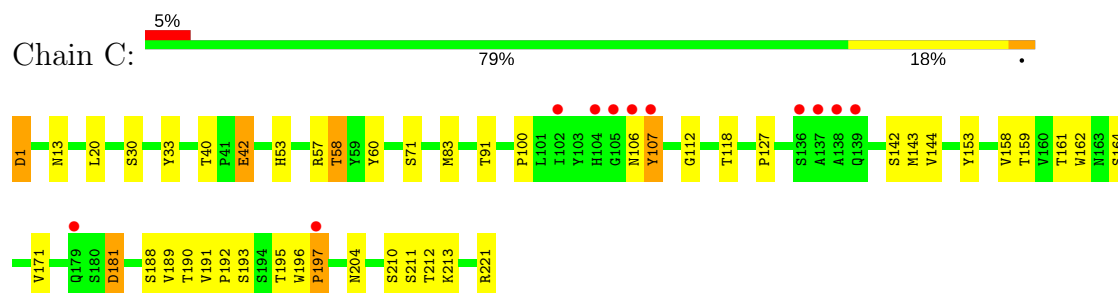
### 3 Residue-property plots

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.

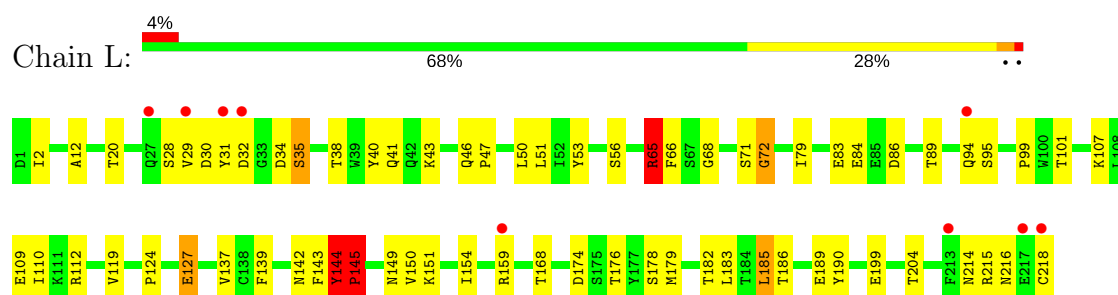
- Molecule 1: Fab heavy chain



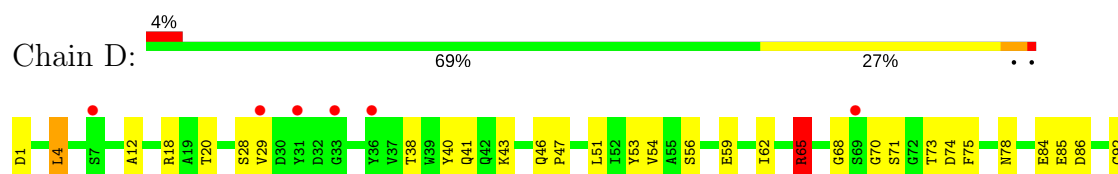
- Molecule 1: Fab heavy chain

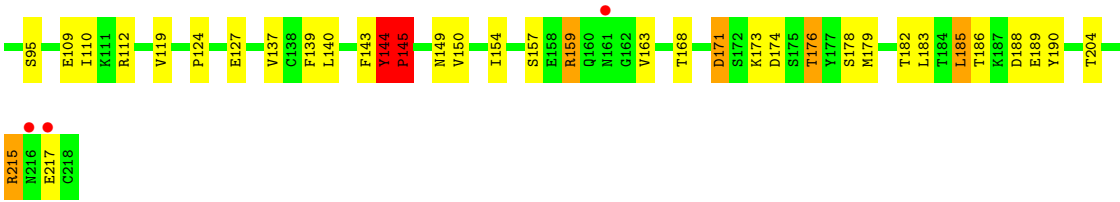


- Molecule 2: Fab light chain



- Molecule 2: Fab light chain





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	51.59Å 90.94Å 81.44Å 90.00° 92.21° 90.00°	Depositor
Resolution (Å)	81.38 – 2.40 31.74 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.5 (81.38-2.40) 98.5 (31.74-2.40)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.86 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, $R_{free}$	0.285 , 0.338 0.282 , 0.332	Depositor DCC
$R_{free}$ test set	1477 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	32.6	Xtriage
Anisotropy	0.930	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 10.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.059 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	6738	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.57% 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	C	0.55	0/1730	0.75	0/2363
1	H	0.59	0/1730	0.76	1/2363 (0.0%)
2	D	0.61	0/1721	0.81	6/2343 (0.3%)
2	L	0.64	0/1721	0.81	4/2343 (0.2%)
All	All	0.60	0/6902	0.78	11/9412 (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
2	D	0	1
2	L	0	1
All	All	0	2

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	65	ARG	NE-CZ-NH1	6.97	123.79	120.30
2	D	171	ASP	CB-CG-OD1	-6.76	112.22	118.30
2	L	65	ARG	NE-CZ-NH1	6.49	123.54	120.30
2	L	144	TYR	C-N-CD	-6.14	107.09	120.60
2	D	144	TYR	C-N-CD	-6.03	107.33	120.60
2	L	145	PRO	CA-N-CD	-5.54	103.75	111.50
2	D	145	PRO	CA-N-CD	-5.52	103.78	111.50
2	L	65	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	H	106	ASN	CB-CA-C	-5.30	99.80	110.40
2	D	65	ARG	NE-CZ-NH2	-5.12	117.74	120.30
2	D	159	ARG	NE-CZ-NH1	5.10	122.85	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	144	TYR	Peptide
2	L	144	TYR	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	C	1687	0	1664	47	0
1	H	1687	0	1664	74	1
2	D	1682	0	1592	66	1
2	L	1682	0	1592	82	0
All	All	6738	0	6512	220	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 17.

All (220) 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:H:106:ASN:ND2	2:L:38:THR:HG23	1.74	1.02
1:C:171:VAL:HG22	1:C:189:VAL:HG22	1.48	0.94
1:H:171:VAL:HG22	1:H:189:VAL:HG22	1.48	0.94
2:L:79:ILE:HD11	2:L:86:ASP:OD2	1.68	0.93
2:D:186:THR:OG1	2:D:188:ASP:OD1	1.90	0.89
1:H:196:TRP:HH2	1:H:218:ILE:O	1.53	0.89
2:D:41:GLN:HB2	2:D:51:LEU:HD11	1.61	0.83
1:H:210:SER:OG	1:H:212:THR:OG1	1.88	0.82
1:C:106:ASN:HB2	2:D:53:TYR:HB3	1.60	0.81
2:L:41:GLN:HB2	2:L:51:LEU:HD11	1.60	0.81
2:L:30:ASP:OD2	2:L:72:GLY:N	2.12	0.81
1:H:164:SER:O	1:C:159:THR:HG21	1.81	0.79
1:H:106:ASN:ND2	2:L:38:THR:CG2	2.45	0.79
1:H:106:ASN:OD1	1:H:107:TYR:N	2.16	0.79
2:D:154:ILE:HD12	2:D:159:ARG:HD3	1.66	0.78
1:H:210:SER:HG	1:H:212:THR:HG1	1.16	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:106:ASN:ND2	2:D:38:THR:OG1	2.19	0.76
1:H:196:TRP:CH2	1:H:218:ILE:O	2.38	0.76
1:C:106:ASN:OD1	1:C:107:TYR:N	2.19	0.76
1:H:59:TYR:OH	2:L:99:PRO:HB3	1.85	0.75
2:L:66:PHE:CZ	2:L:79:ILE:HD12	2.21	0.75
1:C:112:GLY:O	2:D:47:PRO:HB3	1.88	0.74
1:H:107:TYR:HD1	2:L:95:SER:HG	1.36	0.73
2:D:154:ILE:HD11	2:D:183:LEU:HD21	1.71	0.72
2:L:154:ILE:HD11	2:L:183:LEU:HD21	1.71	0.71
1:H:106:ASN:HD21	2:L:38:THR:HG23	1.54	0.71
1:C:107:TYR:HD1	2:D:95:SER:HG	1.37	0.71
2:D:71:SER:O	2:D:75:PHE:CZ	2.44	0.71
2:L:29:VAL:CG2	2:L:94:GLN:OE1	2.39	0.70
1:H:106:ASN:HD21	2:L:38:THR:CG2	2.05	0.70
2:L:174:ASP:OD1	2:L:176:THR:HG22	1.92	0.69
1:C:112:GLY:O	2:D:47:PRO:CB	2.43	0.67
2:D:140:LEU:HD11	2:D:150:VAL:HG22	1.76	0.66
2:L:38:THR:HG21	2:L:40:TYR:CZ	2.30	0.66
2:L:29:VAL:CG1	2:L:94:GLN:OE1	2.43	0.66
1:C:210:SER:OG	1:C:212:THR:OG1	1.95	0.65
1:H:171:VAL:HG22	1:H:189:VAL:CG2	2.25	0.65
1:H:102:ILE:O	1:H:104:HIS:N	2.30	0.64
1:C:171:VAL:HG22	1:C:189:VAL:CG2	2.25	0.63
1:C:106:ASN:ND2	2:D:38:THR:HG23	2.13	0.63
2:D:38:THR:HG21	2:D:40:TYR:CZ	2.32	0.63
1:H:196:TRP:CH2	1:H:218:ILE:HG22	2.33	0.63
1:H:102:ILE:C	1:H:104:HIS:H	2.01	0.63
1:H:100:PRO:HD3	1:H:106:ASN:O	1.99	0.63
2:L:30:ASP:OD1	2:L:35:SER:HB2	1.99	0.63
2:L:144:TYR:CD1	2:L:145:PRO:CD	2.81	0.63
1:C:221:ARG:NH2	2:D:124:PRO:O	2.31	0.62
1:C:107:TYR:CD1	2:D:95:SER:OG	2.52	0.62
2:L:65:ARG:O	2:L:79:ILE:HA	1.99	0.62
2:D:144:TYR:CD1	2:D:145:PRO:CD	2.82	0.62
2:D:188:ASP:OD1	2:D:189:GLU:N	2.33	0.61
2:L:65:ARG:NH2	2:L:86:ASP:OD2	2.33	0.61
1:H:106:ASN:HD21	2:L:38:THR:CB	2.13	0.61
1:H:91:THR:HG23	1:H:118:THR:HA	1.80	0.61
1:H:131:PRO:HD3	2:L:127:GLU:OE1	2.01	0.61
1:C:91:THR:HG23	1:C:118:THR:HA	1.83	0.60
2:D:65:ARG:NH2	2:D:86:ASP:OD2	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:106:ASN:HB2	2:L:53:TYR:HB3	1.82	0.60
1:C:100:PRO:HD3	1:C:106:ASN:O	2.02	0.60
2:D:29:VAL:O	2:D:29:VAL:HG12	2.00	0.60
2:L:29:VAL:O	2:L:29:VAL:HG12	2.01	0.59
2:L:143:PHE:N	2:L:176:THR:OG1	2.35	0.59
1:C:162:TRP:CG	1:C:189:VAL:HG21	2.38	0.59
2:L:137:VAL:HG13	2:L:182:THR:HG22	1.85	0.58
1:H:162:TRP:CG	1:H:189:VAL:HG21	2.38	0.58
1:H:106:ASN:ND2	2:L:53:TYR:HB3	2.19	0.58
2:D:85:GLU:N	2:D:85:GLU:OE1	2.35	0.57
2:L:83:GLU:OE2	2:D:65:ARG:HD3	2.05	0.57
1:C:107:TYR:HD1	2:D:95:SER:OG	1.86	0.56
1:C:106:ASN:ND2	2:D:38:THR:CG2	2.69	0.56
2:L:144:TYR:CD1	2:L:145:PRO:HD3	2.40	0.56
2:L:29:VAL:HG21	2:L:94:GLN:OE1	2.05	0.56
1:C:106:ASN:HD21	2:D:38:THR:CB	2.18	0.56
1:H:106:ASN:HD22	2:L:53:TYR:HB3	1.70	0.56
2:D:150:VAL:HG21	2:D:179:MET:HE2	1.88	0.56
1:C:188:SER:HB3	2:D:139:PHE:CE1	2.41	0.55
1:C:106:ASN:CB	2:D:53:TYR:HB3	2.34	0.55
1:C:106:ASN:HD22	2:D:53:TYR:HB3	1.71	0.55
2:D:143:PHE:O	2:D:176:THR:HG22	2.07	0.55
2:D:137:VAL:HG13	2:D:182:THR:HG22	1.89	0.55
2:L:186:THR:OG1	2:L:189:GLU:HG2	2.07	0.54
2:D:144:TYR:CD1	2:D:145:PRO:HD3	2.42	0.54
2:D:51:LEU:O	2:D:62:ILE:HD13	2.06	0.54
1:H:141:ASN:O	1:H:193:SER:OG	2.14	0.54
1:H:215:ASP:OD2	1:C:213:LYS:NZ	2.40	0.54
1:H:40:THR:HG23	1:H:41:PRO:HD2	1.90	0.54
1:C:161:THR:HB	1:C:204:ASN:HB2	1.88	0.54
2:L:32:ASP:C	2:L:34:ASP:H	2.12	0.53
1:H:106:ASN:CB	2:L:53:TYR:HB3	2.39	0.53
1:C:106:ASN:HD22	2:D:53:TYR:CB	2.22	0.52
2:L:30:ASP:OD1	2:L:35:SER:CB	2.57	0.52
2:L:29:VAL:HG13	2:L:94:GLN:NE2	2.24	0.52
2:D:73:THR:HG22	2:D:74:ASP:OD1	2.09	0.52
2:L:79:ILE:CD1	2:L:86:ASP:OD2	2.52	0.52
2:D:51:LEU:O	2:D:62:ILE:CD1	2.57	0.52
1:H:196:TRP:HH2	1:H:218:ILE:C	2.12	0.52
1:H:9:GLY:HA3	1:H:115:THR:HG22	1.92	0.52
1:C:40:THR:OG1	1:C:42:GLU:OE2	2.27	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:2:ILE:HD13	2:L:94:GLN:NE2	2.25	0.51
2:D:190:TYR:CZ	2:D:215:ARG:HG3	2.45	0.51
1:H:150:VAL:CG2	1:H:185:LEU:HG	2.40	0.51
1:H:40:THR:CG2	1:H:41:PRO:HD2	2.40	0.51
2:D:84:GLU:O	2:D:110:ILE:CD1	2.58	0.51
2:L:154:ILE:HD12	2:L:159:ARG:HD2	1.92	0.51
2:D:43:LYS:O	2:D:46:GLN:HB2	2.11	0.51
1:H:159:THR:HG21	1:C:164:SER:O	2.11	0.51
2:L:84:GLU:O	2:L:110:ILE:CD1	2.59	0.51
2:D:186:THR:OG1	2:D:189:GLU:HG2	2.11	0.50
1:C:20:LEU:HG	1:C:83:MET:HE2	1.94	0.50
1:C:196:TRP:O	1:C:197:PRO:C	2.49	0.50
1:H:35:SER:OG	1:H:97:THR:OG1	2.05	0.50
1:H:196:TRP:O	1:H:197:PRO:C	2.47	0.50
2:L:119:VAL:HA	2:L:139:PHE:O	2.12	0.49
2:L:29:VAL:HG11	2:L:94:GLN:OE1	2.11	0.49
1:H:221:ARG:NH2	2:L:124:PRO:O	2.45	0.49
1:C:161:THR:HG22	1:C:162:TRP:N	2.27	0.49
2:D:154:ILE:HD12	2:D:159:ARG:CD	2.40	0.49
2:L:32:ASP:O	2:L:34:ASP:N	2.45	0.49
2:D:84:GLU:O	2:D:110:ILE:HD11	2.13	0.49
2:L:31:TYR:HD2	2:L:31:TYR:O	1.96	0.49
2:D:119:VAL:HA	2:D:139:PHE:O	2.13	0.48
2:L:214:ASN:HB3	2:L:216:ASN:OD1	2.13	0.48
1:H:106:ASN:HB2	2:L:50:LEU:CD1	2.43	0.48
1:H:1:ASP:OD2	2:D:112:ARG:NH1	2.46	0.48
1:H:150:VAL:HG23	1:H:150:VAL:O	2.13	0.48
2:L:43:LYS:O	2:L:46:GLN:HB2	2.13	0.48
2:D:12:ALA:HA	2:D:109:GLU:O	2.13	0.48
1:H:162:TRP:CD2	1:H:189:VAL:HG21	2.49	0.48
2:D:174:ASP:CG	2:D:176:THR:HG1	2.16	0.48
1:H:103:TYR:C	1:H:104:HIS:O	2.50	0.47
1:H:161:THR:HG22	1:H:162:TRP:N	2.29	0.47
2:L:31:TYR:C	2:L:31:TYR:CD2	2.87	0.47
1:C:106:ASN:ND2	2:D:53:TYR:CB	2.78	0.47
2:L:12:ALA:HA	2:L:109:GLU:O	2.14	0.47
2:L:84:GLU:O	2:L:110:ILE:HD11	2.14	0.47
2:L:204:THR:HG22	2:L:204:THR:O	2.14	0.47
2:L:185:LEU:N	2:L:185:LEU:HD12	2.29	0.47
1:H:139:GLN:NE2	1:H:141:ASN:HD22	2.12	0.47
2:D:188:ASP:OD1	2:D:189:GLU:HG2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:107:TYR:HD1	2:L:95:SER:CB	2.28	0.47
2:L:29:VAL:HG22	2:L:94:GLN:OE1	2.15	0.47
1:H:102:ILE:C	1:H:104:HIS:N	2.68	0.46
1:H:139:GLN:HE21	1:H:141:ASN:HD22	1.62	0.46
2:L:190:TYR:CE2	2:L:215:ARG:HD2	2.51	0.46
2:D:59:GLU:HB3	2:D:62:ILE:HD11	1.98	0.46
2:L:56:SER:HB2	2:L:68:GLY:O	2.15	0.46
1:C:106:ASN:ND2	2:D:38:THR:CB	2.79	0.45
1:C:162:TRP:CD2	1:C:189:VAL:HG21	2.51	0.45
2:D:56:SER:HB2	2:D:68:GLY:O	2.16	0.45
2:D:150:VAL:HG21	2:D:179:MET:CE	2.46	0.45
1:H:106:ASN:HB2	2:L:50:LEU:HD11	1.98	0.45
2:L:149:ASN:OD1	2:L:150:VAL:N	2.49	0.45
1:H:106:ASN:CB	2:L:50:LEU:HD13	2.47	0.45
2:D:149:ASN:OD1	2:D:150:VAL:N	2.49	0.45
2:D:51:LEU:HA	2:D:62:ILE:HD13	1.99	0.45
2:L:190:TYR:CZ	2:L:215:ARG:HG3	2.52	0.45
2:L:150:VAL:HG11	2:L:179:MET:HE2	1.99	0.45
2:L:66:PHE:CE1	2:L:79:ILE:HD12	2.53	0.44
1:H:139:GLN:HE21	1:H:141:ASN:ND2	2.16	0.44
1:C:106:ASN:ND2	2:D:53:TYR:HB3	2.32	0.44
1:H:20:LEU:HG	1:H:83:MET:HE2	1.98	0.44
2:L:144:TYR:CE1	2:L:145:PRO:HD3	2.53	0.44
1:H:9:GLY:H	1:H:115:THR:HG21	1.82	0.44
2:D:171:ASP:OD1	2:D:173:LYS:N	2.51	0.44
1:H:33:TYR:HB3	1:H:99:HIS:CG	2.53	0.43
1:C:143:MET:HE3	1:C:190:THR:HG22	1.98	0.43
1:C:196:TRP:O	1:C:196:TRP:CD1	2.71	0.43
1:H:107:TYR:HD1	2:L:95:SER:OG	1.98	0.43
1:C:191:VAL:HG13	1:C:192:PRO:HD2	2.01	0.43
1:H:106:ASN:HB3	2:L:50:LEU:HD22	2.00	0.43
1:H:107:TYR:HD1	2:L:95:SER:HB2	1.84	0.43
2:L:142:ASN:HA	2:L:176:THR:HG21	2.01	0.43
2:D:143:PHE:C	2:D:176:THR:HG22	2.39	0.43
2:D:4:LEU:HD23	2:D:92:CYS:SG	2.59	0.43
1:C:192:PRO:O	1:C:195:THR:HB	2.19	0.43
2:L:29:VAL:HG13	2:L:94:GLN:CD	2.39	0.43
1:C:196:TRP:N	1:C:197:PRO:HD2	2.34	0.43
2:L:112:ARG:NH1	1:C:1:ASP:OD2	2.35	0.43
2:L:32:ASP:C	2:L:34:ASP:N	2.72	0.42
2:D:29:VAL:O	2:D:29:VAL:CG1	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:192:PRO:O	1:H:195:THR:HB	2.19	0.42
2:L:30:ASP:OD2	2:L:71:SER:HA	2.19	0.42
1:H:106:ASN:C	1:H:106:ASN:OD1	2.57	0.42
1:H:161:THR:HB	1:H:204:ASN:HB2	2.01	0.42
2:D:168:THR:HG21	2:D:178:SER:HB2	2.00	0.42
1:H:127:PRO:HB3	1:H:153:TYR:HB3	2.02	0.42
1:C:158:VAL:CG1	1:C:159:THR:N	2.83	0.42
1:H:196:TRP:O	1:H:196:TRP:CE3	2.72	0.42
1:C:127:PRO:HB3	1:C:153:TYR:HB3	2.01	0.42
1:H:196:TRP:N	1:H:197:PRO:HD2	2.35	0.42
1:H:106:ASN:CB	2:L:50:LEU:CD1	2.97	0.42
1:H:106:ASN:ND2	2:L:53:TYR:CB	2.83	0.42
1:H:196:TRP:CZ2	1:H:218:ILE:HG22	2.54	0.42
1:C:42:GLU:H	1:C:42:GLU:HG3	1.60	0.41
1:H:191:VAL:HG13	1:H:192:PRO:HD2	2.02	0.41
1:C:196:TRP:O	1:C:197:PRO:O	2.38	0.41
1:C:30:SER:O	1:C:53:HIS:HB2	2.20	0.41
2:D:185:LEU:N	2:D:185:LEU:HD12	2.35	0.41
2:D:119:VAL:HG13	2:D:140:LEU:CD2	2.50	0.41
2:D:70:GLY:HA3	2:D:75:PHE:CD2	2.55	0.41
1:H:101:LEU:HB3	1:H:102:ILE:HG13	2.02	0.41
1:C:144:VAL:HG23	1:C:193:SER:HA	2.02	0.41
2:L:150:VAL:O	2:L:150:VAL:HG23	2.21	0.41
2:L:168:THR:HG21	2:L:178:SER:HB2	2.01	0.41
2:D:204:THR:O	2:D:204:THR:HG22	2.20	0.41
1:H:188:SER:HB3	2:L:139:PHE:CE1	2.56	0.41
2:L:142:ASN:HA	2:L:176:THR:CG2	2.50	0.41
2:D:18:ARG:HD3	2:D:78:ASN:OD1	2.20	0.41
1:H:112:GLY:O	2:L:47:PRO:HB3	2.21	0.41
1:H:30:SER:O	1:H:53:HIS:HB2	2.21	0.41
2:D:54:VAL:HG12	2:D:54:VAL:O	2.21	0.41
2:L:29:VAL:HG13	2:L:94:GLN:OE1	2.18	0.41
1:H:196:TRP:O	1:H:197:PRO:O	2.40	0.40
1:C:58:THR:HG21	1:C:60:TYR:OH	2.22	0.40
2:L:29:VAL:HG13	2:L:94:GLN:HE22	1.86	0.40
1:H:156:GLU:OE2	1:H:157:PRO:HA	2.22	0.40
1:H:38:ARG:HD3	1:H:48:VAL:HG11	2.04	0.40
1:H:107:TYR:CD1	2:L:95:SER:HB2	2.56	0.40
2:D:144:TYR:CG	2:D:145:PRO:N	2.89	0.40
2:L:151:LYS:HB2	2:L:199:GLU:HB2	2.02	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:103:TYR:OH	2:D:163:VAL:O[2_645]	1.85	0.35

## 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	C	219/221 (99%)	202 (92%)	14 (6%)	3 (1%)	12	17
1	H	219/221 (99%)	203 (93%)	11 (5%)	5 (2%)	7	7
2	D	216/218 (99%)	203 (94%)	11 (5%)	2 (1%)	19	27
2	L	216/218 (99%)	202 (94%)	12 (6%)	2 (1%)	19	27
All	All	870/878 (99%)	810 (93%)	48 (6%)	12 (1%)	12	17

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	103	TYR
1	H	105	GLY
1	H	181	ASP
2	L	145	PRO
1	C	181	ASP
2	D	145	PRO
1	C	107	TYR
2	D	217	GLU
1	H	107	TYR
2	L	72	GLY
1	C	197	PRO
1	H	197	PRO

### 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	C	192/192 (100%)	182 (95%)	10 (5%)	25	41
1	H	192/192 (100%)	186 (97%)	6 (3%)	43	64
2	D	191/191 (100%)	181 (95%)	10 (5%)	25	41
2	L	191/191 (100%)	181 (95%)	10 (5%)	25	41
All	All	766/766 (100%)	730 (95%)	36 (5%)	29	45

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	1	ASP
1	H	33	TYR
1	H	104	HIS
1	H	107	TYR
1	H	142	SER
1	H	181	ASP
2	L	20	THR
2	L	28	SER
2	L	35	SER
2	L	65	ARG
2	L	89	THR
2	L	101	THR
2	L	107	LYS
2	L	127	GLU
2	L	185	LEU
2	L	218	CYS
1	C	1	ASP
1	C	13	ASN
1	C	33	TYR
1	C	42	GLU
1	C	57	ARG
1	C	58	THR
1	C	71	SER
1	C	142	SER

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Mol	Chain	Res	Type
1	C	181	ASP
1	C	211	SER
2	D	1	ASP
2	D	4	LEU
2	D	20	THR
2	D	28	SER
2	D	65	ARG
2	D	127	GLU
2	D	157	SER
2	D	176	THR
2	D	185	LEU
2	D	215	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	77	ASN
1	H	139	GLN
1	H	179	GLN
2	L	57	ASN
1	C	77	ASN
1	C	106	ASN
1	C	179	GLN
2	D	42	GLN
2	D	57	ASN

### 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 ⓘ

There are no carbohydrates in this entry.



## 5.6 Ligand geometry

There are no ligands in this entry.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	C	221/221 (100%)	0.23	11 (4%) 29 27	32, 41, 50, 56	0
1	H	221/221 (100%)	0.08	7 (3%) 47 46	31, 38, 49, 52	0
2	D	218/218 (100%)	0.14	9 (4%) 37 36	32, 39, 55, 62	0
2	L	218/218 (100%)	0.06	9 (4%) 37 36	30, 37, 49, 69	0
All	All	878/878 (100%)	0.13	36 (4%) 37 36	30, 39, 51, 69	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	137	ALA	5.6
1	C	104	HIS	5.4
1	C	102	ILE	5.2
1	C	106	ASN	4.7
1	H	138	ALA	4.6
1	C	136	SER	4.0
1	H	139	GLN	3.8
1	H	106	ASN	3.7
2	L	218	CYS	3.6
2	L	31	TYR	3.6
1	H	103	TYR	3.4
2	D	29	VAL	3.2
1	C	138	ALA	3.2
2	D	217	GLU	3.1
2	L	94	GLN	3.1
1	C	105	GLY	2.9
2	D	33	GLY	2.9
1	C	139	GLN	2.7
1	C	107	TYR	2.7
2	L	29	VAL	2.7
2	D	31	TYR	2.7

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Mol	Chain	Res	Type	RSRZ
2	L	217	GLU	2.6
1	H	179	GLN	2.6
2	L	159	ARG	2.5
2	D	216	ASN	2.5
2	D	7	SER	2.5
1	C	179	GLN	2.4
2	D	36	TYR	2.4
1	C	197	PRO	2.3
1	H	197	PRO	2.2
2	L	213	PHE	2.2
2	D	161	ASN	2.1
2	L	32	ASP	2.1
1	H	33	TYR	2.0
2	L	27	GLN	2.0
2	D	69	SER	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.