



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:40 PM GMT

PDB ID : 4PLJ  
Title : Hepatitis E Virus E2s domain (Genotype IV) in complex with a neutralizing antibody 8G12  
Authors : Tang, X.H.; Li, S.W.; Sivaraman, J.  
Deposited on : 2014-05-18  
Resolution : 2.30 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.

---

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

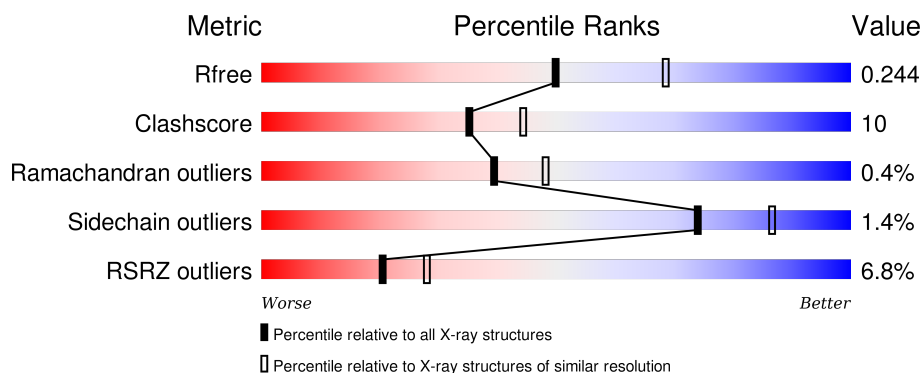
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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	148	<div> <div>4%</div> <div>91%</div> <div>9%</div> </div>
1	B	148	<div> <div>5%</div> <div>89%</div> <div>10%</div> <div>•</div> </div>
2	C	212	<div> <div>17%</div> <div>68%</div> <div>26%</div> <div>5%</div> </div>
2	L	212	<div> <div>3%</div> <div>79%</div> <div>19%</div> <div>•</div> </div>
3	D	229	<div> <div>7%</div> <div>76%</div> <div>17%</div> <div>•</div> <div>6%</div> </div>

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
3	H	229	 A horizontal bar chart showing the quality of chain H. The bar is divided into four segments: a small red segment at the beginning labeled '3%', a large green segment labeled '83%', a yellow segment labeled '12%', and a small grey segment at the end labeled '5%'.

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 9128 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 Capsid protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	148	Total	C	N	O	S	0	0	0
			1129	716	189	222	2			
1	B	147	Total	C	N	O	S	0	0	0
			1123	713	188	220	2			

- Molecule 2 is a protein called 8G12 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	212	Total	C	N	O	S	0	0	0
			1632	1018	274	334	6			
2	C	201	Total	C	N	O	S	0	0	0
			1553	975	255	317	6			

- Molecule 3 is a protein called 8G12 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	218	Total	C	N	O	S	0	0	0
			1669	1064	274	324	7			
3	D	216	Total	C	N	O	S	0	0	0
			1658	1057	272	322	7			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	79	Total	O	0	0
			79	79		
4	B	76	Total	O	0	0
			76	76		
4	L	57	Total	O	0	0
			57	57		
4	H	74	Total	O	0	0
			74	74		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	37	Total	O	0	0
			37	37		
4	D	41	Total	O	0	0
			41	41		

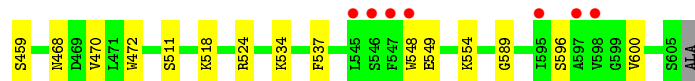
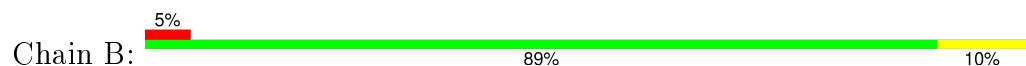
### 3 Residue-property plots [i](#)

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.

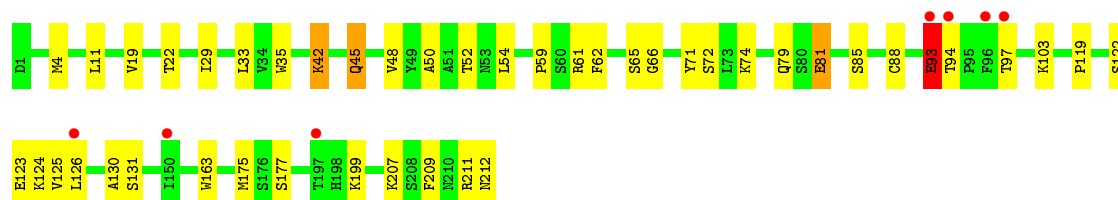
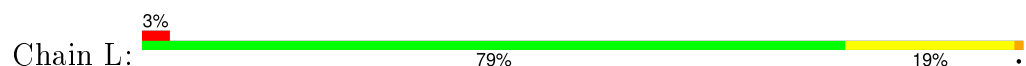
#### • Molecule 1: Capsid protein



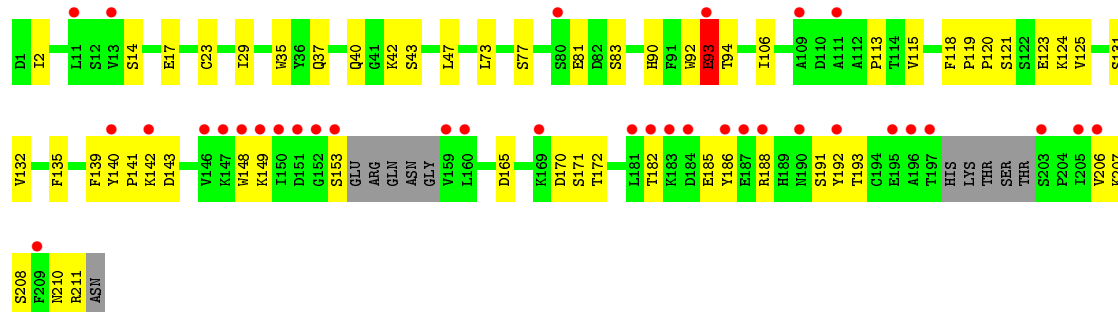
#### • Molecule 1: Capsid protein



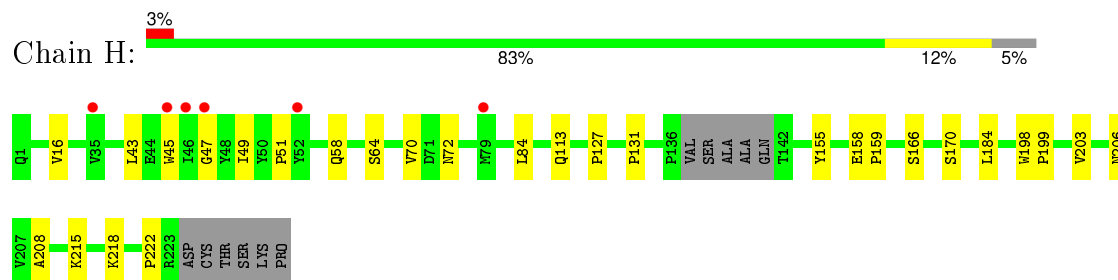
#### • Molecule 2: 8G12 light chain



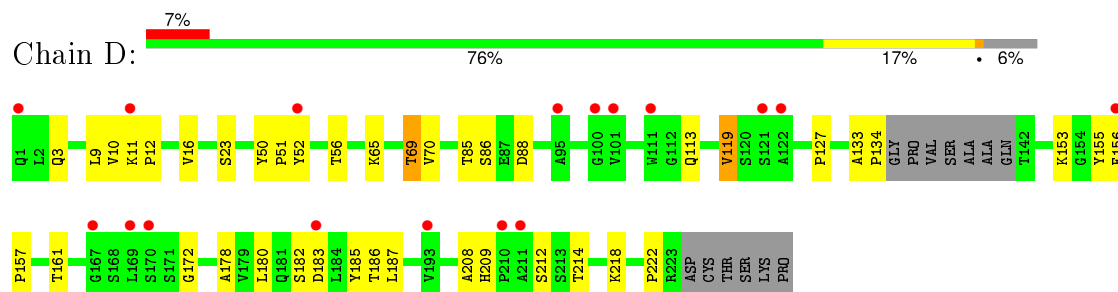
#### • Molecule 2: 8G12 light chain



- Molecule 3: 8G12 heavy chain



- Molecule 3: 8G12 heavy chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	56.77Å 89.46Å 137.64Å 90.00° 95.90° 90.00°	Depositor
Resolution (Å)	29.14 – 2.30 29.14 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (29.14-2.30) 97.3 (29.14-2.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.45 (at 2.29Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, $R_{free}$	0.187 , 0.242 0.192 , 0.244	Depositor DCC
$R_{free}$ test set	1943 reflections (3.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	32.3	Xtriage
Anisotropy	0.642	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 48.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	2 of 61149 reflections (0.003%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	9128	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.25% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.54	1/1157 (0.1%)	0.60	0/1584
1	B	0.54	1/1151 (0.1%)	0.62	1/1577 (0.1%)
2	C	0.49	1/1588 (0.1%)	0.65	3/2156 (0.1%)
2	L	0.44	0/1670	0.59	1/2268 (0.0%)
3	D	0.40	0/1705	0.55	0/2329
3	H	0.46	0/1717	0.56	0/2346
All	All	0.47	3/8988 (0.0%)	0.59	5/12260 (0.0%)

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	C	0	2
2	L	0	1
All	All	0	3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	93	GLU	C-N	8.99	1.54	1.34
1	B	537	PHE	C-N	-6.95	1.18	1.34
1	A	537	PHE	C-N	-5.75	1.20	1.34

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	92	TRP	C-N-CA	-7.04	104.11	121.70
2	C	93	GLU	CA-C-N	-6.22	103.52	117.20
2	L	93	GLU	C-N-CA	5.84	136.29	121.70
1	B	537	PHE	O-C-N	-5.81	113.41	122.70
2	C	29	ILE	N-CA-C	-5.25	96.82	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	93	GLU	Mainchain,Peptide
2	L	93	GLU	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	1129	0	1103	22	0
1	B	1123	0	1097	24	0
2	C	1553	0	1485	49	0
2	L	1632	0	1543	56	0
3	D	1658	0	1614	30	0
3	H	1669	0	1624	17	0
4	A	79	0	0	3	0
4	B	76	0	0	8	0
4	C	37	0	0	4	0
4	D	41	0	0	5	0
4	H	74	0	0	4	0
4	L	57	0	0	5	0
All	All	9128	0	8466	168	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 10.

All (168) 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:B:554:LYS:NZ	2:C:93:GLU:HB3	1.45	1.31
4:B:702:HOH:O	2:C:93:GLU:HB2	1.31	1.28
2:L:93:GLU:HG3	2:L:94:THR:O	1.19	1.25
2:L:93:GLU:HA	2:L:93:GLU:OE1	1.59	1.02
2:L:93:GLU:CG	2:L:94:THR:O	2.10	0.99
1:B:554:LYS:HZ2	2:C:93:GLU:HB3	1.19	0.98
1:B:554:LYS:HZ3	2:C:93:GLU:HB3	1.27	0.98

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:554:LYS:NZ	2:C:93:GLU:CB	2.30	0.95
1:A:554:LYS:HZ2	2:L:93:GLU:CD	1.71	0.93
1:B:554:LYS:HZ2	2:C:93:GLU:CB	1.84	0.89
3:D:88:ASP:OD1	4:D:301:HOH:O	1.91	0.87
3:H:166:SER:H	3:H:206:ASN:HD21	1.21	0.86
2:L:45:GLN:NE2	4:L:302:HOH:O	2.08	0.84
1:A:554:LYS:HZ2	2:L:93:GLU:CG	1.91	0.83
1:A:588:LEU:HA	2:L:93:GLU:OE2	1.80	0.82
2:L:93:GLU:HG3	2:L:94:THR:C	2.00	0.81
3:H:184:LEU:O	4:H:301:HOH:O	2.01	0.78
2:L:93:GLU:CA	2:L:93:GLU:OE1	2.32	0.78
2:L:66:GLY:O	4:L:301:HOH:O	2.01	0.78
2:C:123:GLU:OE2	4:C:301:HOH:O	2.00	0.78
1:A:554:LYS:NZ	2:L:93:GLU:CB	2.49	0.76
2:C:42:LYS:HD2	2:C:43:SER:H	1.51	0.76
1:A:554:LYS:NZ	2:L:93:GLU:CG	2.51	0.74
1:A:468:ASN:HD22	1:B:472:TRP:HH2	1.33	0.73
1:A:588:LEU:CA	2:L:93:GLU:OE2	2.39	0.70
3:D:85:THR:O	3:D:119:VAL:HG11	1.93	0.69
1:A:554:LYS:HZ1	2:L:93:GLU:HB2	1.57	0.68
3:D:182:SER:OG	3:D:183:ASP:N	2.27	0.68
1:A:554:LYS:NZ	2:L:93:GLU:HB2	2.08	0.67
2:C:77:SER:OG	4:C:302:HOH:O	2.10	0.67
1:A:554:LYS:HZ2	2:L:93:GLU:CB	2.08	0.66
2:L:163:TRP:CD1	2:L:175:MET:HG3	2.30	0.66
2:L:124:LYS:HE3	2:L:130:ALA:HA	1.76	0.66
1:A:472:TRP:HH2	1:B:468:ASN:HD22	1.44	0.66
1:B:554:LYS:HZ3	2:C:93:GLU:CB	2.02	0.64
2:C:210:ASN:O	2:C:211:ARG:HG2	1.98	0.64
2:L:123:GLU:OE1	3:H:218:LYS:NZ	2.24	0.64
1:A:588:LEU:C	2:L:93:GLU:OE2	2.37	0.64
2:L:123:GLU:HA	2:L:126:LEU:HD22	1.80	0.63
3:D:3:GLN:OE1	3:D:113:GLN:NE2	2.32	0.62
1:B:459:SER:OG	4:B:701:HOH:O	2.14	0.61
3:H:58:GLN:NE2	4:H:305:HOH:O	2.33	0.61
3:H:208:ALA:HB2	3:H:215:LYS:HD3	1.81	0.61
3:H:166:SER:H	3:H:206:ASN:ND2	1.97	0.60
1:A:469:ASP:HB2	1:A:601:LEU:HD12	1.83	0.60
2:C:142:LYS:HG3	2:C:143:ASP:H	1.66	0.60
1:B:549:GLU:OE1	4:B:702:HOH:O	2.17	0.59
1:B:518:LYS:HE2	4:B:709:HOH:O	2.02	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:211:ARG:O	4:L:303:HOH:O	2.17	0.59
2:C:120:PRO:HD3	2:C:132:VAL:HG22	1.85	0.59
1:B:554:LYS:CE	2:C:93:GLU:HB3	2.32	0.58
2:C:186:TYR:CE1	2:C:192:TYR:HE2	2.21	0.58
1:B:470:VAL:HG22	1:B:600:VAL:HG22	1.86	0.58
2:C:182:THR:HG23	2:C:185:GLU:H	1.68	0.57
1:A:554:LYS:NZ	2:L:93:GLU:CD	2.53	0.57
3:D:178:ALA:HB2	3:D:187:LEU:HD23	1.87	0.56
3:D:161:THR:HG22	3:D:208:ALA:HB3	1.86	0.56
1:A:459:SER:OG	4:A:701:HOH:O	2.12	0.56
3:D:11:LYS:HG3	3:D:12:PRO:HD2	1.87	0.56
2:L:61:ARG:NE	2:L:79:GLN:HE21	2.04	0.55
2:C:42:LYS:CD	2:C:43:SER:H	2.20	0.55
2:L:124:LYS:NZ	2:L:131:SER:H	2.04	0.55
2:C:37:GLN:HB2	2:C:47:LEU:HD11	1.88	0.55
3:H:127:PRO:HB3	3:H:155:TYR:HB3	1.89	0.54
3:H:72:ASN:ND2	4:H:303:HOH:O	2.23	0.54
1:B:554:LYS:NZ	2:C:93:GLU:CG	2.70	0.53
1:B:554:LYS:HZ2	2:C:93:GLU:CG	2.20	0.53
2:L:212:ASN:HA	4:L:303:HOH:O	2.08	0.53
2:C:148:TRP:O	2:C:149:LYS:HD2	2.09	0.53
3:H:16:VAL:HG12	3:H:84:LEU:HD11	1.91	0.53
2:L:42:LYS:HE2	3:H:113:GLN:O	2.09	0.53
3:D:9:LEU:HB2	3:D:157:PRO:HG3	1.89	0.53
3:D:127:PRO:HB3	3:D:155:TYR:HB3	1.91	0.52
1:A:554:LYS:HD3	2:L:93:GLU:OE1	2.08	0.52
2:L:124:LYS:HE3	2:L:131:SER:H	1.74	0.52
2:L:61:ARG:CZ	2:L:79:GLN:HE21	2.22	0.52
1:B:511:SER:HB3	4:B:735:HOH:O	2.09	0.52
1:B:524:ARG:HB3	1:B:524:ARG:HH21	1.75	0.51
2:L:124:LYS:CE	2:L:131:SER:H	2.24	0.51
2:L:122:SER:O	2:L:126:LEU:HD13	2.11	0.50
2:L:175:MET:HE1	2:L:177:SER:HB2	1.94	0.50
2:L:74:LYS:HE3	4:L:305:HOH:O	2.10	0.50
2:C:186:TYR:O	2:C:192:TYR:OH	2.29	0.50
2:C:193:THR:HG23	2:C:208:SER:HB3	1.94	0.50
1:A:554:LYS:CD	2:L:93:GLU:OE1	2.61	0.49
3:D:178:ALA:HA	3:D:187:LEU:HB3	1.92	0.49
3:D:153:LYS:HA	3:D:186:THR:HG22	1.92	0.49
2:C:113:PRO:HB3	2:C:139:PHE:HB3	1.94	0.49
2:L:124:LYS:HZ1	2:L:131:SER:H	1.59	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:142:LYS:HG3	2:C:143:ASP:N	2.26	0.49
2:C:35:TRP:CD2	2:C:73:LEU:HB2	2.48	0.49
3:D:212:SER:HB3	3:D:214:THR:HG23	1.95	0.49
3:D:10:VAL:HG21	3:D:16:VAL:HB	1.95	0.48
3:H:64:SER:N	4:H:302:HOH:O	2.16	0.48
2:C:149:LYS:HG3	2:C:153:SER:C	2.33	0.48
2:C:186:TYR:HE1	2:C:192:TYR:HE2	1.61	0.48
2:L:4:MET:HG2	2:L:97:THR:HG22	1.96	0.48
2:L:85:SER:OG	2:L:103:LYS:HD3	2.14	0.48
2:L:22:THR:HG22	2:L:72:SER:OG	2.13	0.48
3:D:172:GLY:O	4:D:302:HOH:O	2.20	0.47
4:B:702:HOH:O	2:C:93:GLU:CB	2.14	0.47
3:D:161:THR:CG2	3:D:208:ALA:HB3	2.44	0.47
2:C:140:TYR:CG	2:C:141:PRO:HA	2.49	0.47
2:C:93:GLU:CG	2:C:94:THR:O	2.63	0.47
2:L:59:PRO:HG2	2:L:62:PHE:CE2	2.50	0.47
3:D:86:SER:HA	3:D:119:VAL:HG13	1.96	0.46
3:H:45:TRP:CH2	3:H:47:GLY:HA2	2.51	0.46
2:L:124:LYS:HB3	2:L:124:LYS:HE2	1.54	0.46
2:C:2:ILE:HD12	2:C:90:HIS:CE1	2.50	0.46
2:C:93:GLU:HG3	2:C:94:THR:C	2.36	0.46
2:L:52:THR:HG22	2:L:65:SER:HA	1.97	0.46
1:B:589:GLY:N	2:C:93:GLU:OE1	2.50	0.45
2:C:124:LYS:HE3	2:C:131:SER:OG	2.16	0.45
3:D:23:SER:N	4:D:303:HOH:O	2.48	0.45
2:L:35:TRP:CZ3	2:L:88:CYS:HB3	2.51	0.45
2:C:206:VAL:O	2:C:207:LYS:HG2	2.17	0.45
2:C:170:ASP:OD1	2:C:172:THR:HG22	2.17	0.45
3:D:157:PRO:O	3:D:209:HIS:HE1	1.99	0.45
3:D:209:HIS:HD2	3:D:212:SER:CB	2.30	0.45
3:H:199:PRO:CB	3:H:222:PRO:HG3	2.46	0.45
2:L:122:SER:HA	2:L:125:VAL:HG22	1.99	0.44
2:C:81:GLU:OE1	2:C:81:GLU:N	2.47	0.44
3:D:65:LYS:N	4:D:311:HOH:O	2.46	0.44
1:A:460:ARG:O	4:A:702:HOH:O	2.21	0.44
3:D:69:THR:HB	4:D:318:HOH:O	2.18	0.44
1:B:524:ARG:NH2	1:B:524:ARG:HB3	2.32	0.44
2:L:11:LEU:HD13	2:L:19:VAL:HG23	1.99	0.44
2:C:118:PHE:HA	2:C:119:PRO:HD3	1.88	0.44
2:C:171:SER:HA	4:C:310:HOH:O	2.17	0.44
3:H:49:ILE:O	3:H:51:PRO:HD3	2.18	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:10:VAL:O	3:D:119:VAL:HA	2.18	0.43
3:D:209:HIS:HB3	3:D:214:THR:OG1	2.18	0.43
1:B:468:ASN:O	4:B:703:HOH:O	2.20	0.43
1:B:468:ASN:HA	1:B:600:VAL:HG13	2.01	0.43
2:L:33:LEU:O	2:L:50:ALA:O	2.37	0.43
2:C:188:ARG:HA	2:C:188:ARG:HD2	1.91	0.43
1:B:534:LYS:HE2	4:B:714:HOH:O	2.19	0.43
2:C:115:VAL:HA	2:C:135:PHE:O	2.18	0.43
2:L:119:PRO:HB3	2:L:209:PHE:CE2	2.54	0.43
3:D:218:LYS:HD3	3:D:218:LYS:HA	1.87	0.43
1:A:461:PRO:HG2	1:A:464:VAL:HG12	2.01	0.42
2:C:93:GLU:HG3	2:C:94:THR:O	2.18	0.42
2:L:74:LYS:HE2	2:L:74:LYS:HB3	1.85	0.42
2:L:11:LEU:HD13	2:L:19:VAL:CG2	2.49	0.42
2:L:81:GLU:CD	2:L:81:GLU:H	2.22	0.42
2:L:42:LYS:HD3	2:L:42:LYS:HA	1.67	0.42
2:L:48:VAL:HG22	2:L:54:LEU:HD12	2.02	0.42
3:H:131:PRO:HD3	3:H:218:LYS:HE2	2.02	0.42
3:D:50:TYR:CZ	3:D:52:TYR:HB3	2.55	0.42
1:A:549:GLU:OE1	2:L:93:GLU:OE1	2.38	0.41
2:C:172:THR:HG23	4:C:312:HOH:O	2.19	0.41
3:D:209:HIS:HD2	3:D:212:SER:OG	2.03	0.41
2:C:35:TRP:CE2	2:C:73:LEU:HB2	2.55	0.41
1:A:534:LYS:HE2	4:A:710:HOH:O	2.20	0.41
2:C:83:SER:HB2	2:C:106:ILE:HG12	2.03	0.41
1:A:554:LYS:HZ1	2:L:93:GLU:CB	2.23	0.41
2:C:14:SER:N	2:C:17:GLU:OE1	2.48	0.41
1:B:554:LYS:NZ	2:C:93:GLU:CD	2.74	0.41
3:D:51:PRO:HB3	3:D:70:VAL:HG21	2.02	0.41
3:D:133:ALA:HA	3:D:134:PRO:HD3	1.93	0.41
2:L:29:ILE:HD11	2:L:71:TYR:CE2	2.56	0.41
2:C:121:SER:O	2:C:125:VAL:HG22	2.21	0.40
2:L:207:LYS:HA	2:L:207:LYS:HD3	1.64	0.40
3:D:156:PHE:HA	3:D:157:PRO:HA	1.89	0.40
1:B:548:TRP:CE2	1:B:596:SER:HB2	2.56	0.40
3:H:198:TRP:HD1	3:H:203:VAL:HG23	1.86	0.40
3:D:180:LEU:HD13	3:D:185:TYR:CE1	2.57	0.40
3:H:158:GLU:HA	3:H:159:PRO:HA	1.89	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	A	146/148 (99%)	140 (96%)	6 (4%)	0	100	100
1	B	145/148 (98%)	140 (97%)	5 (3%)	0	100	100
2	C	195/212 (92%)	183 (94%)	11 (6%)	1 (0%)	34	41
2	L	210/212 (99%)	200 (95%)	8 (4%)	2 (1%)	19	21
3	D	212/229 (93%)	201 (95%)	10 (5%)	1 (0%)	34	41
3	H	214/229 (93%)	209 (98%)	5 (2%)	0	100	100
All	All	1122/1178 (95%)	1073 (96%)	45 (4%)	4 (0%)	39	48

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	L	93	GLU
2	L	199	LYS
2	C	40	GLN
3	D	222	PRO

### 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	125/125 (100%)	124 (99%)	1 (1%)	86	94
1	B	125/125 (100%)	125 (100%)	0	100	100
2	C	179/190 (94%)	176 (98%)	3 (2%)	68	83

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	L	185/190 (97%)	181 (98%)	4 (2%)	60	77
3	D	189/199 (95%)	186 (98%)	3 (2%)	70	84
3	H	190/199 (96%)	187 (98%)	3 (2%)	70	84
All	All	993/1028 (97%)	979 (99%)	14 (1%)	74	86

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

Mol	Chain	Res	Type
1	A	528	THR
2	L	42	LYS
2	L	45	GLN
2	L	81	GLU
2	L	93	GLU
3	H	43	LEU
3	H	70	VAL
3	H	170	SER
2	C	23	CYS
2	C	165	ASP
2	C	191	SER
3	D	56	THR
3	D	69	THR
3	D	119	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	468	ASN
1	B	468	ASN
2	L	32	ASN
2	L	70	GLN
2	L	79	GLN
3	H	58	GLN
3	H	60	GLN
3	H	143	ASN
3	H	181	GLN
3	H	206	ASN
3	D	209	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	537:PHE	C	538:VAL	N	1.18

## 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	A	148/148 (100%)	0.09	6 (4%) 41 50	29, 42, 60, 78	0
1	B	147/148 (99%)	0.20	7 (4%) 34 43	27, 40, 55, 72	0
2	C	201/212 (94%)	0.89	35 (17%) 2 3	34, 72, 107, 125	0
2	L	212/212 (100%)	0.26	7 (3%) 50 59	27, 55, 75, 88	0
3	D	216/229 (94%)	0.58	17 (7%) 15 22	38, 62, 84, 105	0
3	H	218/229 (95%)	0.06	6 (2%) 56 66	28, 44, 64, 91	0
All	All	1142/1178 (96%)	0.36	78 (6%) 20 28	27, 52, 91, 125	0

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	93	GLU	5.9
2	C	188	ARG	5.8
2	C	197	THR	5.7
2	C	150	ILE	4.9
2	C	196	ALA	4.7
2	C	146	VAL	4.6
2	C	153	SER	4.6
2	C	93	GLU	4.4
2	C	109	ALA	4.3
2	C	206	VAL	4.2
3	D	167	GLY	4.0
2	C	142	LYS	3.8
2	C	186	TYR	3.7
2	C	160	LEU	3.7
2	C	152	GLY	3.6
2	C	111	ALA	3.6
1	B	598	VAL	3.5
2	C	13	VAL	3.5
3	H	45	TRP	3.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	C	184	ASP	3.4
1	B	546	SER	3.3
2	C	147	LYS	3.3
3	D	52	TYR	3.3
2	C	190	ASN	3.3
1	B	597	ALA	3.1
3	D	183	ASP	3.1
2	C	80	SER	3.1
2	C	192	TYR	3.1
2	C	187	GLU	3.0
2	C	182	THR	3.0
3	D	211	ALA	2.9
3	D	95	ALA	2.9
2	C	148	TRP	2.9
2	C	181	LEU	2.9
1	B	547	PHE	2.8
2	C	209	PHE	2.8
3	D	210	PRO	2.8
2	C	203	SER	2.8
3	D	193	VAL	2.8
2	C	151	ASP	2.8
1	A	606	ALA	2.7
3	D	170	SER	2.7
1	B	545	LEU	2.6
2	C	205	ILE	2.6
3	D	156	PHE	2.6
2	C	183	LYS	2.6
2	C	195	GLU	2.5
3	H	46	ILE	2.5
3	D	122	ALA	2.5
1	B	548	TRP	2.5
3	H	52	TYR	2.4
2	L	150	ILE	2.4
2	C	159	VAL	2.4
3	H	47	GLY	2.4
2	L	126	LEU	2.4
3	D	101	VAL	2.4
1	A	597	ALA	2.4
2	C	11	LEU	2.4
3	H	79	MET	2.4
3	D	1	GLN	2.4
3	H	35	VAL	2.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
3	D	111	TRP	2.3
3	D	121	SER	2.3
2	L	197	THR	2.3
1	B	595	ILE	2.3
3	D	100	GLY	2.2
2	L	97	THR	2.2
2	C	149	LYS	2.2
2	C	169	LYS	2.1
2	L	96	PHE	2.1
2	L	94	THR	2.1
1	A	598	VAL	2.1
3	D	169	LEU	2.1
1	A	555	ALA	2.1
1	A	593	VAL	2.1
1	A	546	SER	2.0
3	D	11	LYS	2.0
2	C	140	TYR	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.