



# Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 07:19 PM GMT

PDB ID : 3RKD  
Title : Hepatitis E Virus E2s domain (Genotype I) in complex with a neutralizing antibody  
Authors : Tang, X.H.; Sivaraman, J.  
Deposited on : 2011-04-18  
Resolution : 1.90 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

---

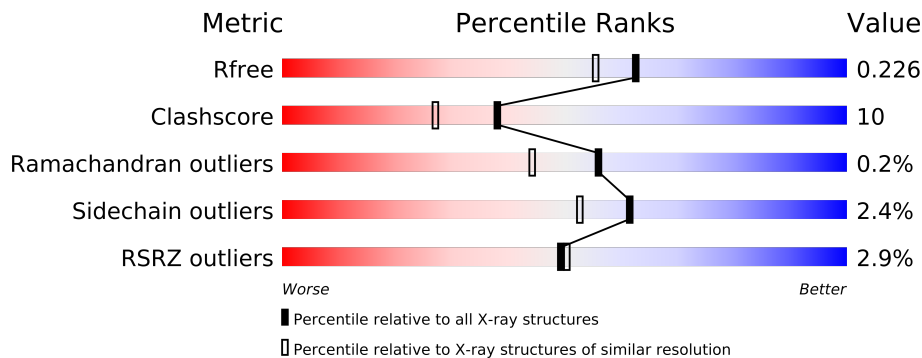
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 1.90 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))
$R_{free}$	66092	3684 (1.90-1.90)
Clashscore	79885	4465 (1.90-1.90)
Ramachandran outliers	78287	4413 (1.90-1.90)
Sidechain outliers	78261	4414 (1.90-1.90)
RSRZ outliers	66119	3686 (1.90-1.90)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	146	
1	B	146	
2	C	214	
2	L	214	
3	D	230	
3	H	230	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9533 atoms, of which 0 are hydrogen and 0 are deuterium.

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	146	Total	C	N	O	0	0	0
			1096	697	185	214			
1	B	145	Total	C	N	O	0	0	0
			1090	694	184	212			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	532	HIS	TYR	ENGINEERED MUTATION	UNP B0VX51
A	604	PRO	-	EXPRESSION TAG	UNP B0VX51
B	532	HIS	TYR	ENGINEERED MUTATION	UNP B0VX51
B	604	PRO	-	EXPRESSION TAG	UNP B0VX51

- Molecule 2 is a protein called Monoclonal Antibody, Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	213	Total	C	N	O	S	0	0	0
			1656	1034	278	338	6			
2	C	213	Total	C	N	O	S	0	0	0
			1656	1034	278	338	6			

- Molecule 3 is a protein called Monoclonal Antibody, Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	218	Total	C	N	O	S	0	0	0
			1637	1044	267	320	6			
3	D	218	Total	C	N	O	S	0	0	0
			1637	1044	267	320	6			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	118	Total 118	O 118	0	0
4	B	107	Total 107	O 107	0	0
4	L	134	Total 134	O 134	0	0
4	H	140	Total 140	O 140	0	0
4	C	133	Total 133	O 133	0	0
4	D	129	Total 129	O 129	0	0

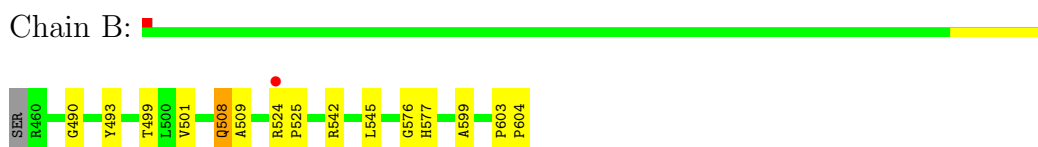
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

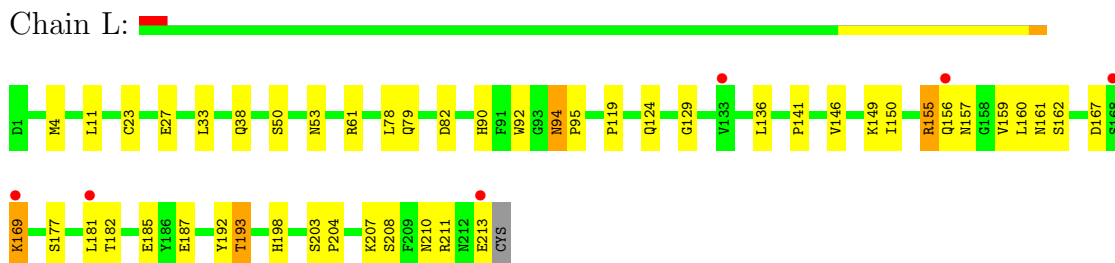
- Molecule 1: Capsid protein



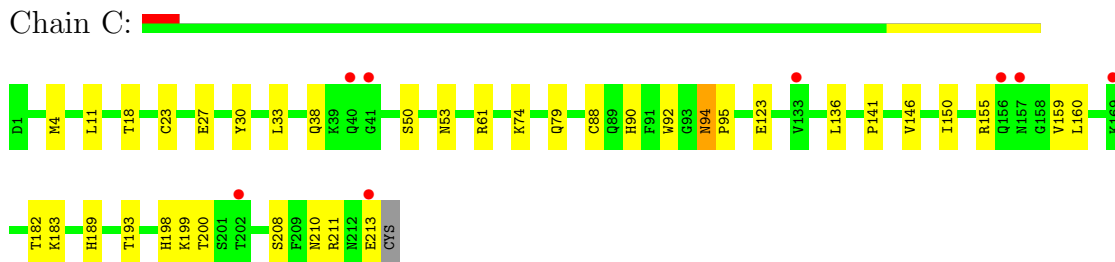
- Molecule 1: Capsid protein



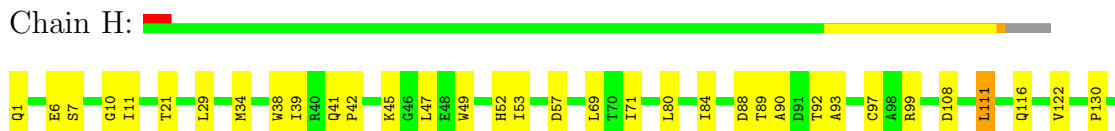
- Molecule 2: Monoclonal Antibody, Light Chain

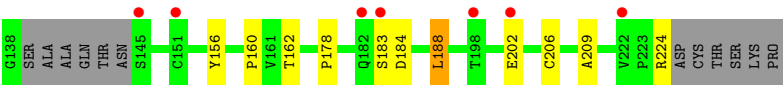


- Molecule 2: Monoclonal Antibody, Light Chain



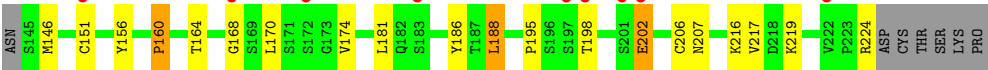
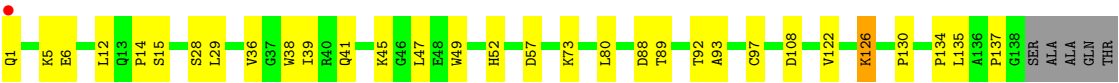
- Molecule 3: Monoclonal Antibody, Heavy Chain





● Molecule 3: Monoclonal Antibody, Heavy Chain

Chain D:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	74.48Å 95.20Å 108.31Å 90.00° 107.31° 90.00°	Depositor
Resolution (Å)	20.00 – 1.90 25.09 – 1.90	Depositor EDS
% Data completeness (in resolution range)	87.9 (20.00-1.90) 96.0 (25.09-1.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.43 (at 1.90Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.189 , 0.217 0.199 , 0.226	Depositor DCC
$R_{free}$ test set	10835 reflections (9.98%)	DCC
Wilson B-factor (Å <sup>2</sup> )	22.4	Xtriage
Anisotropy	0.181	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 39.2	EDS
Estimated twinning fraction	0.017 for h,-k,-h-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 112736 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	9533	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.57% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 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	0.34	0/1122	0.65	1/1540 (0.1%)
1	B	0.33	0/1116	0.65	1/1532 (0.1%)
2	C	0.30	0/1695	0.61	0/2302
2	L	0.31	0/1695	0.62	0/2302
3	D	0.35	1/1680 (0.1%)	0.66	0/2299
3	H	0.36	1/1680 (0.1%)	0.67	1/2299 (0.0%)
All	All	0.33	2/8988 (0.0%)	0.64	3/12274 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	202	GLU	CD-OE2	7.05	1.33	1.25
3	D	202	GLU	CD-OE2	7.05	1.33	1.25

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	493	TYR	N-CA-C	-5.51	96.13	111.00
1	A	493	TYR	N-CA-C	-5.35	96.56	111.00
3	H	111	LEU	N-CA-C	-5.18	97.02	111.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1096	0	1085	5	0
1	B	1090	0	1080	10	0
2	C	1656	0	1576	30	0
2	L	1656	0	1576	49	0
3	D	1637	0	1630	49	0
3	H	1637	0	1630	40	0
4	A	118	0	0	0	0
4	B	107	0	0	1	0
4	C	133	0	0	2	0
4	D	129	0	0	1	0
4	H	140	0	0	0	0
4	L	134	0	0	0	0
All	All	9533	0	8577	171	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 10.

All (171) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:L:181:LEU:HD21	2:L:185:GLU:HB3	1.23	1.17
3:D:126:LYS:HE2	3:D:126:LYS:H	1.13	1.10
2:L:210:ASN:HB2	2:L:213:GLU:HG3	1.44	0.97
1:B:524:ARG:HE	1:B:604:PRO:HB2	1.31	0.95
2:L:181:LEU:HD21	2:L:185:GLU:CB	1.96	0.94
2:L:90:HIS:HD2	2:L:92:TRP:H	1.19	0.90
3:D:126:LYS:H	3:D:126:LYS:CE	1.88	0.85
2:C:90:HIS:HD2	2:C:92:TRP:H	1.23	0.85
2:L:181:LEU:HD23	2:L:182:THR:N	1.91	0.85
3:D:88:ASP:O	3:D:122:VAL:HG21	1.75	0.85
2:L:181:LEU:CD2	2:L:185:GLU:HB3	2.07	0.84
3:D:126:LYS:HE2	3:D:126:LYS:N	1.91	0.84
3:H:88:ASP:O	3:H:122:VAL:HG21	1.77	0.83
3:H:89:THR:HA	3:H:122:VAL:HG23	1.65	0.79
2:L:181:LEU:HD23	2:L:182:THR:H	1.48	0.79
2:L:38:GLN:HE22	3:H:41:GLN:HE22	1.31	0.78
2:C:94:ASN:HD22	2:C:95:PRO:HA	1.49	0.77
3:D:89:THR:HA	3:D:122:VAL:HG23	1.65	0.77
3:D:130:PRO:HB3	3:D:156:TYR:HB3	1.66	0.77
3:H:89:THR:HA	3:H:122:VAL:CG2	2.17	0.75
2:C:94:ASN:HD22	2:C:95:PRO:CA	1.99	0.74
1:B:524:ARG:NE	1:B:604:PRO:HB2	2.05	0.72
2:C:38:GLN:HE22	3:D:41:GLN:HE22	1.37	0.71
2:L:94:ASN:HD22	2:L:95:PRO:CA	2.02	0.71

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:H:92:THR:OG1	3:H:122:VAL:HG22	1.91	0.70
2:C:210:ASN:HB2	2:C:213:GLU:HG2	1.73	0.70
2:L:193:THR:HB	2:L:208:SER:HB2	1.73	0.69
2:L:210:ASN:HB2	2:L:213:GLU:CG	2.22	0.69
2:C:50:SER:HB2	2:C:53:ASN:HD22	1.59	0.68
2:L:90:HIS:CD2	2:L:92:TRP:H	2.08	0.67
3:D:36:VAL:CG1	3:D:80:LEU:HD21	2.24	0.67
3:D:45:LYS:HE2	3:D:45:LYS:HA	1.76	0.66
2:L:94:ASN:HD22	2:L:95:PRO:N	1.94	0.66
2:L:150:ILE:HD12	2:L:192:TYR:CD1	2.31	0.66
3:H:69:LEU:HD23	3:H:84:ILE:HG12	1.78	0.64
3:H:162:THR:HG21	3:D:28:SER:HB2	1.80	0.64
2:C:193:THR:HG22	2:C:208:SER:CB	2.27	0.64
2:L:94:ASN:HD22	2:L:95:PRO:HA	1.63	0.63
2:L:50:SER:HB2	2:L:53:ASN:HD22	1.64	0.63
3:D:92:THR:OG1	3:D:122:VAL:HG22	1.99	0.62
1:B:508:GLN:HG3	1:B:509:ALA:N	2.13	0.62
3:H:130:PRO:HB3	3:H:156:TYR:HB3	1.80	0.62
2:C:90:HIS:CD2	2:C:92:TRP:H	2.13	0.62
3:D:134:PRO:HD3	3:D:219:LYS:HG2	1.81	0.62
2:C:61:ARG:CZ	2:C:79:GLN:HG3	2.30	0.61
3:D:89:THR:HA	3:D:122:VAL:CG2	2.29	0.60
3:H:69:LEU:CD2	3:H:84:ILE:HG12	2.31	0.60
2:L:181:LEU:HD21	2:L:185:GLU:CG	2.32	0.60
3:H:10:GLY:C	3:H:11:ILE:HD12	2.22	0.59
2:L:119:PRO:HG2	3:H:224:ARG:NH2	2.16	0.59
3:H:162:THR:CG2	3:H:209:ALA:HB3	2.32	0.59
3:D:1:GLN:OE1	3:D:1:GLN:HA	2.03	0.59
3:H:116:GLN:HE22	3:D:5:LYS:HD2	1.68	0.59
3:D:14:PRO:O	3:D:15:SER:HB2	2.03	0.59
3:H:38:TRP:HE1	3:H:80:LEU:CD2	2.16	0.59
3:D:122:VAL:HG23	3:D:122:VAL:O	2.03	0.58
2:L:136:LEU:HD21	2:L:146:VAL:HG22	1.86	0.57
3:D:216:LYS:C	3:D:216:LYS:HD2	2.25	0.57
2:L:181:LEU:HD22	2:L:182:THR:O	2.05	0.57
2:L:181:LEU:HD11	2:L:185:GLU:HG2	1.86	0.56
2:C:136:LEU:HD21	2:C:146:VAL:HG22	1.87	0.56
2:L:61:ARG:CZ	2:L:79:GLN:HG3	2.36	0.56
2:C:198:HIS:HD2	2:C:200:THR:OG1	1.88	0.56
2:C:193:THR:HG22	2:C:208:SER:HB2	1.89	0.55
3:D:170:LEU:O	3:D:174:VAL:HG23	2.07	0.54
3:H:116:GLN:NE2	3:D:5:LYS:HD2	2.21	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:L:4:MET:HE1	2:L:33:LEU:HD23	1.89	0.54
3:D:6:GLU:HG3	3:D:97:CYS:SG	2.47	0.54
2:C:94:ASN:HD22	2:C:95:PRO:N	2.06	0.54
3:H:41:GLN:HB2	3:H:47:LEU:HD23	1.90	0.53
3:D:188:LEU:C	3:D:188:LEU:HD23	2.28	0.53
2:L:141:PRO:O	2:L:198:HIS:HE1	1.92	0.53
3:D:39:ILE:HD12	3:D:39:ILE:N	2.24	0.53
2:C:33:LEU:HD21	2:C:88:CYS:HB2	1.90	0.53
1:B:542:ARG:NH2	1:B:603:PRO:HD3	2.25	0.52
2:L:159:VAL:C	2:L:160:LEU:HD12	2.28	0.52
2:C:193:THR:HG22	2:C:208:SER:HB3	1.91	0.52
3:H:53:ILE:CG2	3:H:80:LEU:HD11	2.40	0.52
1:A:473:LEU:HD23	1:A:500:LEU:HG	1.90	0.52
3:H:188:LEU:HD23	3:H:188:LEU:C	2.30	0.52
3:H:122:VAL:O	3:H:122:VAL:HG23	2.09	0.52
2:L:162:SER:OG	3:H:178:PRO:HG2	2.10	0.51
2:C:150:ILE:HD12	2:C:155:ARG:HE	1.75	0.51
3:H:183:SER:O	3:H:184:ASP:HB2	2.10	0.51
3:H:1:GLN:HA	3:H:1:GLN:OE1	2.10	0.51
3:D:49:TRP:HE1	3:D:52:HIS:HD2	1.58	0.50
3:H:39:ILE:HD11	3:H:111:LEU:HD13	1.93	0.50
3:D:12:LEU:HD21	3:D:122:VAL:HG12	1.94	0.50
3:H:45:LYS:HA	3:H:45:LYS:HE2	1.92	0.50
3:H:88:ASP:OD1	3:H:90:ALA:HB3	2.11	0.49
1:B:501:VAL:HG22	1:B:508:GLN:HB2	1.94	0.49
2:C:94:ASN:ND2	2:C:95:PRO:HA	2.22	0.49
3:D:36:VAL:HG11	3:D:80:LEU:HD21	1.94	0.49
3:D:38:TRP:HE1	3:D:80:LEU:HD13	1.78	0.49
3:H:53:ILE:HG22	3:H:80:LEU:HD11	1.95	0.49
3:H:42:PRO:HB2	3:H:45:LYS:HG3	1.95	0.49
2:L:94:ASN:ND2	2:L:95:PRO:HA	2.27	0.48
3:D:36:VAL:HB	3:D:80:LEU:CD2	2.43	0.48
2:C:136:LEU:HD12	2:C:136:LEU:N	2.28	0.48
2:L:156:GLN:O	2:L:157:ASN:ND2	2.46	0.48
2:L:50:SER:OG	3:H:108:ASP:HA	2.13	0.48
2:L:167:ASP:OD2	2:L:169:LYS:HB3	2.12	0.48
3:D:134:PRO:HB3	3:D:219:LYS:HG3	1.95	0.48
3:H:11:ILE:HD12	3:H:11:ILE:N	2.28	0.48
2:C:18:THR:HG21	2:C:74:LYS:HE2	1.96	0.47
2:L:169:LYS:HE2	2:L:169:LYS:O	2.15	0.47
3:D:41:GLN:HB2	3:D:47:LEU:HD23	1.95	0.47
2:L:94:ASN:C	2:L:94:ASN:HD22	2.15	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:524:ARG:NH1	1:B:525:PRO:O	2.48	0.47
2:C:141:PRO:O	2:C:198:HIS:HE1	1.97	0.46
3:H:7:SER:OG	3:H:21:THR:HB	2.15	0.46
2:L:4:MET:HE3	2:L:23:CYS:SG	2.56	0.46
2:L:124:GLN:HG2	2:L:129:GLY:O	2.15	0.46
3:H:162:THR:HG22	3:H:209:ALA:HB3	1.98	0.46
2:L:155:ARG:HG2	2:L:155:ARG:HH11	1.80	0.46
2:L:159:VAL:O	2:L:160:LEU:HD12	2.16	0.45
3:H:49:TRP:HE1	3:H:52:HIS:HD2	1.62	0.45
3:D:57:ASP:OD2	3:D:73:LYS:HE2	2.17	0.45
2:L:119:PRO:HG2	3:H:224:ARG:CZ	2.46	0.45
1:B:545:LEU:CD1	1:B:599:ALA:HB2	2.47	0.45
3:D:49:TRP:NE1	3:D:52:HIS:HD2	2.15	0.45
2:L:187:GLU:O	2:L:211:ARG:NH2	2.50	0.45
1:A:467:ALA:O	1:A:468:ASN:HB2	2.17	0.45
3:D:164:THR:CG2	3:D:168:GLY:N	2.80	0.45
3:D:73:LYS:HA	3:D:80:LEU:HA	1.98	0.44
3:D:146:MET:HE1	3:D:195:PRO:HA	1.99	0.44
2:C:159:VAL:O	2:C:160:LEU:HD12	2.16	0.44
3:D:216:LYS:HD2	3:D:217:VAL:N	2.33	0.44
1:A:501:VAL:HG22	1:A:508:GLN:HB2	2.00	0.44
2:C:50:SER:OG	3:D:108:ASP:HA	2.18	0.44
3:H:92:THR:O	3:H:93:ALA:HB2	2.18	0.43
2:L:149:LYS:O	2:L:150:ILE:HD13	2.18	0.43
3:H:49:TRP:NE1	3:H:52:HIS:HD2	2.17	0.43
3:H:1:GLN:HB3	3:D:160:PRO:HG3	1.99	0.43
2:C:189:HIS:O	2:C:211:ARG:HD3	2.19	0.43
3:D:130:PRO:CB	3:D:156:TYR:HB3	2.43	0.43
2:L:136:LEU:N	2:L:136:LEU:HD12	2.33	0.43
2:L:203:SER:HA	2:L:204:PRO:HD3	1.92	0.43
3:D:198:THR:O	3:D:202:GLU:N	2.36	0.42
2:L:161:ASN:HD22	2:L:177:SER:HA	1.83	0.42
3:D:12:LEU:CD2	3:D:122:VAL:HG12	2.48	0.42
3:H:71:ILE:HD11	3:H:80:LEU:HD21	2.01	0.42
2:C:18:THR:CG2	2:C:74:LYS:HE2	2.49	0.42
2:L:136:LEU:CD2	2:L:146:VAL:HG22	2.50	0.42
3:H:6:GLU:HG3	3:H:97:CYS:SG	2.60	0.42
2:L:193:THR:HG22	2:L:208:SER:OG	2.19	0.42
2:C:123:GLU:HG3	4:C:313:HOH:O	2.19	0.42
1:A:545:LEU:CD1	1:A:599:ALA:HB2	2.49	0.42
3:D:80:LEU:C	3:D:80:LEU:HD12	2.40	0.42
2:L:4:MET:CE	2:L:23:CYS:SG	3.08	0.42

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:D:164:THR:HG23	3:D:168:GLY:N	2.34	0.42
3:H:38:TRP:HE1	3:H:80:LEU:HD22	1.85	0.42
3:D:92:THR:O	3:D:93:ALA:HB2	2.20	0.41
2:L:150:ILE:HD12	2:L:192:TYR:CE1	2.55	0.41
2:L:207:LYS:HA	2:L:207:LYS:HD3	1.83	0.41
2:C:159:VAL:C	2:C:160:LEU:HD12	2.41	0.41
1:B:603:PRO:HG2	4:B:744:HOH:O	2.20	0.41
3:D:135:LEU:HG	3:D:151:CYS:HA	2.02	0.41
2:C:4:MET:HE3	2:C:23:CYS:SG	2.60	0.41
3:H:34:MET:HE3	3:H:99:ARG:HD2	2.01	0.41
1:A:522:ASP:HB2	1:A:604:PRO:HG2	2.02	0.41
3:D:1:GLN:HB2	4:D:471:HOH:O	2.21	0.41
1:B:499:THR:HG21	2:C:30:TYR:CZ	2.56	0.41
2:L:181:LEU:CD2	2:L:182:THR:N	2.74	0.40
3:D:14:PRO:O	3:D:15:SER:CB	2.68	0.40
2:C:182:THR:HG23	4:C:603:HOH:O	2.20	0.40
3:D:181:LEU:HG	3:D:186:TYR:CE2	2.55	0.40
3:D:137:PRO:O	3:D:224:ARG:HD2	2.21	0.40
2:C:136:LEU:CD2	2:C:146:VAL:HG22	2.51	0.40
1:B:576:GLY:O	1:B:577:HIS:C	2.60	0.40
2:L:78:LEU:HG	2:L:82:ASP:HB2	2.04	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	144/146 (99%)	138 (96%)	5 (4%)	1 (1%)	30	15
1	B	143/146 (98%)	137 (96%)	5 (4%)	1 (1%)	30	15
2	C	211/214 (99%)	209 (99%)	2 (1%)	0	100	100
2	L	211/214 (99%)	208 (99%)	3 (1%)	0	100	100
3	D	214/230 (93%)	205 (96%)	9 (4%)	0	100	100
3	H	214/230 (93%)	206 (96%)	8 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1137/1180 (96%)	1103 (97%)	32 (3%)	2 (0%)	56	44

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	490	GLY
1	A	490	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	A	119/119 (100%)	118 (99%)	1 (1%)	89	89
1	B	118/119 (99%)	117 (99%)	1 (1%)	89	89
2	C	188/189 (100%)	183 (97%)	5 (3%)	57	47
2	L	188/189 (100%)	182 (97%)	6 (3%)	51	39
3	D	189/199 (95%)	183 (97%)	6 (3%)	51	39
3	H	189/199 (95%)	184 (97%)	5 (3%)	59	49
All	All	991/1014 (98%)	967 (98%)	24 (2%)	61	53

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	508	GLN
1	B	508	GLN
2	L	11	LEU
2	L	27	GLU
2	L	94	ASN
2	L	155	ARG
2	L	169	LYS
2	L	193	THR
3	H	29	LEU
3	H	57	ASP
3	H	160	PRO
3	H	188	LEU

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type
3	H	206	CYS
2	C	11	LEU
2	C	27	GLU
2	C	94	ASN
2	C	183	LYS
2	C	199	LYS
3	D	29	LEU
3	D	126	LYS
3	D	160	PRO
3	D	188	LEU
3	D	206	CYS
3	D	207	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	532	HIS
1	A	560	ASN
1	B	508	GLN
2	L	3	GLN
2	L	38	GLN
2	L	53	ASN
2	L	90	HIS
2	L	94	ASN
2	L	138	ASN
2	L	157	ASN
2	L	161	ASN
2	L	198	HIS
2	L	210	ASN
3	H	52	HIS
3	H	116	GLN
2	C	3	GLN
2	C	38	GLN
2	C	45	GLN
2	C	53	ASN
2	C	76	ASN
2	C	90	HIS
2	C	94	ASN
2	C	157	ASN
2	C	161	ASN
2	C	198	HIS
2	C	210	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
3	D	52	HIS
3	D	116	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

### 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	146/146 (100%)	-0.22	1 (0%) 84 87	14, 19, 27, 40	0
1	B	145/146 (99%)	-0.11	1 (0%) 84 87	14, 21, 32, 45	0
2	C	213/214 (99%)	0.09	8 (3%) 38 40	15, 26, 39, 49	0
2	L	213/214 (99%)	0.15	6 (2%) 50 51	15, 24, 39, 57	0
3	D	218/230 (94%)	0.18	10 (4%) 31 31	17, 27, 45, 54	0
3	H	218/230 (94%)	0.10	7 (3%) 45 46	15, 25, 43, 50	0
All	All	1153/1180 (97%)	0.06	33 (2%) 49 50	14, 24, 40, 57	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	183	SER	3.6
3	D	202	GLU	3.5
1	B	524	ARG	3.2
3	D	1	GLN	3.0
2	L	213	GLU	3.0
3	H	183	SER	2.9
2	C	41	GLY	2.9
3	D	201	SER	2.8
2	C	169	LYS	2.7
2	L	169	LYS	2.6
2	L	156	GLN	2.6
2	C	133	VAL	2.6
2	C	40	GLN	2.6
2	C	202	THR	2.5
2	L	181	LEU	2.4
2	C	213	GLU	2.3
1	A	459	SER	2.3
3	D	151	CYS	2.3
3	H	202	GLU	2.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
3	D	168	GLY	2.3
3	H	151	CYS	2.3
3	D	172	SER	2.2
3	H	182	GLN	2.2
3	H	222	VAL	2.2
3	D	198	THR	2.2
3	H	145	SER	2.2
3	H	198	THR	2.2
2	C	157	ASN	2.2
2	L	133	VAL	2.1
3	D	197	SER	2.1
2	L	168	SER	2.0
2	C	156	GLN	2.0
3	D	222	VAL	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.