



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:20 PM GMT

PDB ID : 4HZL  
Title : Neutralizing antibody mAb#8 in complex with the Epitope II of HCV E2 envelope protein  
Authors : Deng, L.; Zhang, P.  
Deposited on : 2012-11-15  
Resolution : 2.85 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

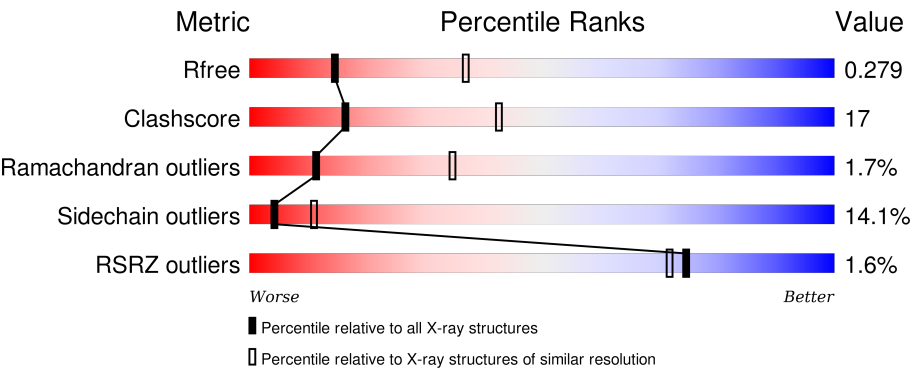
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.85 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 <sub>free</sub>	91344	2228 (2.90-2.82)
Clashscore	102246	2499 (2.90-2.82)
Ramachandran outliers	100387	2439 (2.90-2.82)
Sidechain outliers	100360	2442 (2.90-2.82)
RSRZ outliers	91569	2236 (2.90-2.82)

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	222	<div><div></div><div>61%29%7%..</div></div>
1	H	222	<div><div></div><div>64%27%6%.</div></div>
2	B	217	<div><div>6%</div><div>65%31%..</div></div>
2	L	217	<div><div></div><div>63%31%..</div></div>
3	E	17	<div><div></div><div>41%24%12%24%</div></div>

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Mol	Chain	Length	Quality of chain
3	F	17	 A horizontal bar chart showing the quality of chain F. The bar is divided into four segments: green (29%), yellow (41%), red (6%), and grey (24%). The percentages are labeled below the bar.

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6949 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	217	Total	C	N	O	S	0	0	0
			1632	1034	267	321	10			
1	A	217	Total	C	N	O	S	0	0	0
			1632	1034	267	321	10			

- Molecule 2 is a protein called Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	217	Total	C	N	O	S	0	0	0
			1679	1049	284	340	6			
2	B	217	Total	C	N	O	S	0	0	0
			1679	1049	284	340	6			

- Molecule 3 is a protein called E2 envelop protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	13	Total	C	N	O	0	0	0
			100	65	16	19			
3	F	13	Total	C	N	O	0	0	0
			100	65	16	19			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	45	Total	O	0	0
			45	45		
4	L	31	Total	O	0	0
			31	31		
4	E	8	Total	O	0	0
			8	8		
4	A	30	Total	O	0	0
			30	30		

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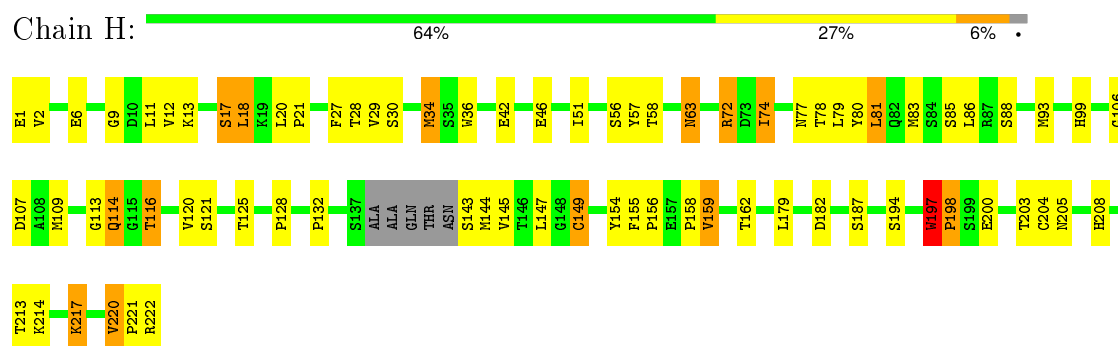
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	11	Total 11	O 11	0	0
4	F	2	Total 2	O 2	0	0

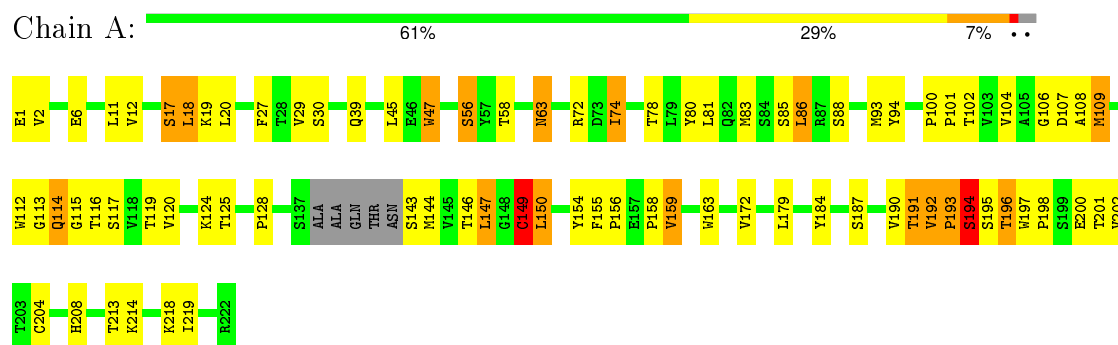
### 3 Residue-property plots

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.

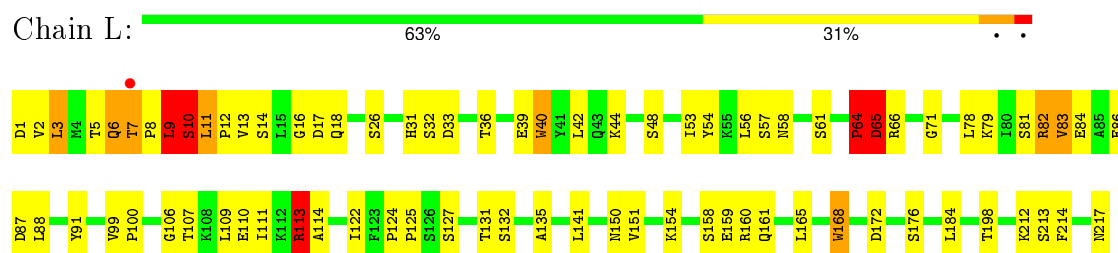
- Molecule 1: Fab heavy chain



- Molecule 1: Fab heavy chain

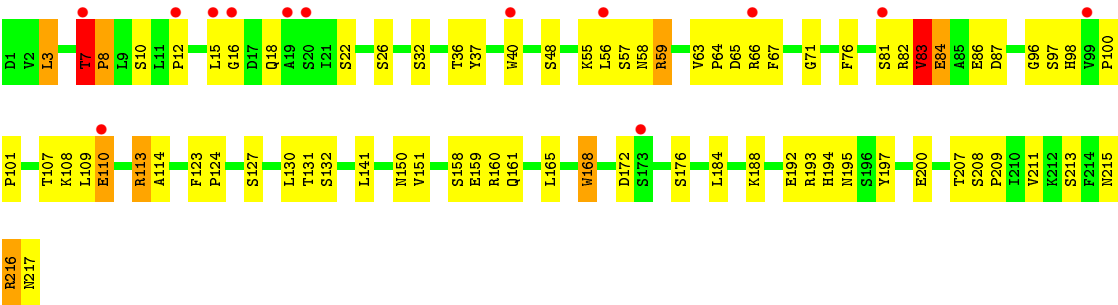


- Molecule 2: Fab light chain

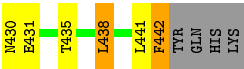


- Molecule 2: Fab light chain

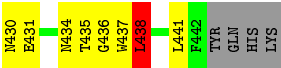
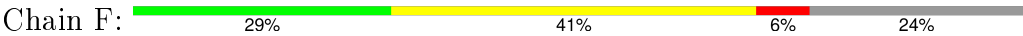




• Molecule 3: E2 envelop protein



• Molecule 3: E2 envelop protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	137.25Å 137.25Å 140.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.85 49.09 – 2.56	Depositor EDS
% Data completeness (in resolution range)	99.8 (50.00-2.85) 99.4 (49.09-2.56)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.45 (at 2.54Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.221 , 0.277 0.224 , 0.279	Depositor DCC
$R_{free}$ test set	1635 reflections (5.40%)	DCC
Wilson B-factor (Å <sup>2</sup> )	25.6	Xtriage
Anisotropy	0.192	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 38.4	EDS
Estimated twinning fraction	0.058 for -h,l,k 0.046 for -l,-k,-h	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.39$ , $\langle L^2 \rangle = 0.22$	Xtriage
Outliers	0 of 43486 reflections	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	6949	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.75% 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	0.69	4/1675 (0.2%)	0.84	6/2290 (0.3%)
1	H	0.73	2/1675 (0.1%)	0.84	2/2290 (0.1%)
2	B	0.69	5/1718 (0.3%)	0.76	1/2333 (0.0%)
2	L	0.64	2/1718 (0.1%)	0.77	1/2333 (0.0%)
3	E	0.92	0/102	1.06	1/138 (0.7%)
3	F	0.84	0/102	0.98	1/138 (0.7%)
All	All	0.69	13/6990 (0.2%)	0.81	12/9522 (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	1
2	B	0	1
2	L	0	3
All	All	0	5

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	168	TRP	CD2-CE2	5.93	1.48	1.41
2	B	168	TRP	CD2-CE2	5.68	1.48	1.41
2	B	40	TRP	CD2-CE2	5.61	1.48	1.41
2	L	40	TRP	CD2-CE2	5.60	1.48	1.41
1	A	159	VAL	CA-C	5.45	1.67	1.52
1	H	159	VAL	CA-C	5.44	1.67	1.52
2	B	71	GLY	N-CA	5.35	1.54	1.46
2	B	71	GLY	CA-C	5.26	1.60	1.51
1	H	198	PRO	N-CD	5.17	1.55	1.47
2	B	8	PRO	N-CD	5.17	1.55	1.47
1	A	47	TRP	CD2-CE2	5.15	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	163	TRP	CD2-CE2	5.10	1.47	1.41
1	A	112	TRP	CD2-CE2	5.09	1.47	1.41

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	150	LEU	N-CA-C	7.49	131.23	111.00
1	A	192	VAL	C-N-CD	5.85	140.68	128.40
2	B	7	THR	C-N-CD	5.66	140.28	128.40
1	A	149	CYS	C-N-CA	5.58	135.66	121.70
2	L	113	ARG	NE-CZ-NH2	5.16	122.88	120.30
1	A	159	VAL	CA-CB-CG1	5.13	118.60	110.90
1	A	86	LEU	CA-CB-CG	5.13	127.09	115.30
3	E	435	THR	N-CA-C	-5.12	97.19	111.00
3	F	438	LEU	CA-CB-CG	5.09	127.01	115.30
1	A	18	LEU	CA-CB-CG	5.04	126.88	115.30
1	H	159	VAL	CA-CB-CG1	5.02	118.43	110.90
1	H	197	TRP	C-N-CD	5.01	138.92	128.40

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	149	CYS	Peptide
2	B	98	HIS	Peptide
2	L	10	SER	Peptide
2	L	6	GLN	Peptide
2	L	64	PRO	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	1632	0	1608	63	0
1	H	1632	0	1608	50	0
2	B	1679	0	1616	52	0
2	L	1679	0	1616	55	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	100	0	92	6	0
3	F	100	0	92	14	0
4	A	30	0	0	5	0
4	B	11	0	0	1	0
4	E	8	0	0	2	0
4	F	2	0	0	4	0
4	H	45	0	0	2	0
4	L	31	0	0	6	0
All	All	6949	0	6632	225	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 17.

All (225) 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)
3:F:435:THR:HA	4:F:501:HOH:O	1.34	1.22
2:B:12:PRO:HA	2:B:110:GLU:O	1.62	0.99
1:H:6:GLU:OE1	1:H:114:GLN:NE2	2.02	0.92
2:B:7:THR:HB	2:B:8:PRO:CD	2.00	0.90
2:L:66:ARG:HD2	2:L:82:ARG:HD3	1.56	0.88
1:A:143:SER:C	1:A:194:SER:OG	2.17	0.82
2:L:6:GLN:O	2:L:8:PRO:HD3	1.78	0.82
2:B:16:GLY:H	2:B:83:VAL:HA	1.44	0.82
3:F:430:ASN:N	4:F:502:HOH:O	2.11	0.82
2:B:12:PRO:HB3	2:B:110:GLU:OE2	1.79	0.81
1:A:6:GLU:OE2	1:A:113:GLY:HA3	1.81	0.81
1:H:28:THR:HA	1:H:77:ASN:HD21	1.45	0.81
2:B:197:TYR:O	2:B:213:SER:HB2	1.82	0.79
1:H:182:ASP:HB3	4:B:301:HOH:O	1.82	0.78
2:L:7:THR:O	2:L:9:LEU:HD13	1.82	0.78
3:F:430:ASN:HA	4:F:502:HOH:O	1.85	0.76
2:L:82:ARG:NE	2:L:84:GLU:OE2	2.19	0.75
1:A:143:SER:N	1:A:194:SER:HG	1.84	0.75
1:A:196:THR:O	1:A:200:GLU:HB2	1.88	0.73
2:L:36:THR:HG21	2:L:56:LEU:HD12	1.71	0.72
3:F:430:ASN:CA	4:F:502:HOH:O	2.38	0.72
1:A:193:PRO:O	1:A:196:THR:OG1	2.04	0.72
2:B:15:LEU:HB3	2:B:83:VAL:HG12	1.72	0.72
1:H:18:LEU:HD23	1:H:83:MET:HE3	1.71	0.71
1:A:63:ASN:HD22	1:A:63:ASN:H	1.39	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:LEU:HD23	1:A:83:MET:HE3	1.72	0.69
3:E:431:GLU:HG2	4:E:508:HOH:O	1.92	0.69
2:L:66:ARG:CD	2:L:82:ARG:HD3	2.23	0.68
1:H:9:GLY:H	1:H:116:THR:HG21	1.58	0.68
2:L:6:GLN:O	2:L:8:PRO:CD	2.41	0.68
2:B:7:THR:HB	2:B:8:PRO:HD3	1.76	0.66
2:L:88:LEU:O	4:L:313:HOH:O	2.14	0.66
2:L:3:LEU:H	2:L:26:SER:HB2	1.61	0.65
2:L:65:ASP:HB3	2:L:66:ARG:HG3	1.78	0.65
1:A:18:LEU:HD23	1:A:83:MET:CE	2.26	0.65
1:A:155:PHE:CE1	1:A:156:PRO:HB3	2.31	0.65
2:L:7:THR:C	2:L:9:LEU:H	1.99	0.65
1:H:155:PHE:CE1	1:H:156:PRO:HB3	2.32	0.64
1:H:63:ASN:HD22	1:H:63:ASN:H	1.44	0.63
2:L:99:VAL:O	2:L:99:VAL:HG22	1.97	0.63
2:B:15:LEU:HB3	2:B:83:VAL:CG1	2.30	0.62
2:B:37:TYR:CG	3:F:437:TRP:HB3	2.34	0.62
2:L:1:ASP:HA	2:L:100:PRO:HG2	1.81	0.62
1:H:88:SER:HA	1:H:120:VAL:HB	1.81	0.62
1:A:78:THR:HG22	1:A:80:TYR:CE1	2.35	0.61
1:H:18:LEU:CD2	1:H:83:MET:HE3	2.30	0.61
1:H:143:SER:N	1:H:194:SER:HG	1.98	0.61
1:H:145:VAL:HG23	1:H:194:SER:HB3	1.82	0.61
2:B:141:LEU:HD21	2:B:151:VAL:HG22	1.83	0.61
2:B:8:PRO:O	2:B:107:THR:HG23	2.00	0.60
1:A:19:LYS:CE	4:A:330:HOH:O	2.49	0.60
1:A:197:TRP:CD1	1:A:202:VAL:HG23	2.37	0.59
2:B:37:TYR:HB2	2:B:97:SER:OG	2.02	0.59
2:L:17:ASP:N	2:L:82:ARG:O	2.36	0.59
2:L:7:THR:OG1	2:L:9:LEU:HB3	2.03	0.59
1:A:39:GLN:HB2	1:A:45:LEU:HD23	1.85	0.59
2:B:66:ARG:HA	2:B:81:SER:HB2	1.85	0.58
1:H:17:SER:O	1:H:18:LEU:HB3	2.03	0.58
2:L:81:SER:O	2:L:82:ARG:HB3	2.02	0.58
2:L:66:ARG:NE	4:L:323:HOH:O	2.31	0.58
1:A:197:TRP:CG	1:A:198:PRO:HA	2.38	0.58
1:A:143:SER:CA	1:A:194:SER:OG	2.52	0.57
1:A:19:LYS:HE2	4:A:330:HOH:O	2.04	0.57
2:L:9:LEU:HA	2:L:107:THR:HA	1.87	0.56
1:H:18:LEU:HD23	1:H:83:MET:CE	2.35	0.56
1:A:18:LEU:CD2	1:A:83:MET:HE3	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:168:TRP:CD1	2:L:168:TRP:N	2.73	0.56
1:A:193:PRO:HB2	1:A:196:THR:OG1	2.06	0.56
1:A:107:ASP:OD2	3:F:438:LEU:HB2	2.06	0.56
2:L:213:SER:O	2:L:214:PHE:HB3	2.06	0.55
1:A:143:SER:C	1:A:194:SER:HG	2.10	0.55
2:B:36:THR:HB	2:B:56:LEU:HD12	1.88	0.55
2:L:16:GLY:CA	2:L:82:ARG:O	2.54	0.55
1:A:208:HIS:HB3	1:A:213:THR:HB	1.87	0.55
1:H:18:LEU:CD2	1:H:83:MET:CE	2.85	0.55
1:A:197:TRP:HD1	1:A:202:VAL:HG23	1.71	0.55
1:H:21:PRO:HD2	4:H:318:HOH:O	2.07	0.54
1:A:18:LEU:CD2	1:A:83:MET:CE	2.85	0.54
1:H:155:PHE:CG	1:H:156:PRO:HA	2.42	0.54
2:L:141:LEU:HD21	2:L:151:VAL:HG22	1.88	0.54
3:E:430:ASN:ND2	4:E:508:HOH:O	2.41	0.54
1:A:155:PHE:CG	1:A:156:PRO:HA	2.42	0.54
1:A:191:THR:C	1:A:192:VAL:HG13	2.28	0.54
1:A:146:THR:OG1	1:A:191:THR:HG23	2.09	0.53
1:H:107:ASP:OD2	3:E:438:LEU:HB2	2.08	0.53
2:L:64:PRO:HB3	4:L:323:HOH:O	2.08	0.53
1:H:30:SER:HB3	1:H:74:ILE:HB	1.89	0.53
1:H:149:CYS:O	1:H:187:SER:HA	2.09	0.53
1:H:128:PRO:HB3	1:H:154:TYR:HB3	1.90	0.53
2:B:200:GLU:HB2	2:B:211:VAL:HG22	1.90	0.53
1:H:179:LEU:HD11	1:H:182:ASP:HA	1.91	0.52
1:H:2:VAL:HG13	1:H:27:PHE:CD1	2.45	0.52
2:B:16:GLY:N	2:B:83:VAL:HA	2.18	0.52
2:L:42:LEU:HD13	2:L:91:TYR:CZ	2.45	0.52
1:A:143:SER:N	1:A:194:SER:OG	2.43	0.52
2:L:113:ARG:HD3	2:L:114:ALA:O	2.10	0.52
1:H:116:THR:HG22	4:H:316:HOH:O	2.10	0.52
2:L:7:THR:C	2:L:9:LEU:N	2.62	0.51
1:H:1:GLU:HG2	1:H:2:VAL:H	1.74	0.51
2:B:3:LEU:H	2:B:26:SER:HB2	1.75	0.51
2:L:3:LEU:N	2:L:26:SER:HB2	2.26	0.51
2:L:2:VAL:HG13	2:L:26:SER:HB3	1.92	0.51
2:B:172:ASP:O	2:B:176:SER:HA	2.10	0.51
2:L:39:GLU:HG2	2:L:54:TYR:HA	1.93	0.51
1:H:51:ILE:HD13	1:H:72:ARG:HG2	1.93	0.50
2:L:36:THR:CG2	2:L:56:LEU:HD12	2.41	0.50
1:A:78:THR:CG2	1:A:80:TYR:HE1	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:438:LEU:HD22	3:E:441:LEU:HD12	1.94	0.50
1:H:6:GLU:OE2	1:H:113:GLY:HA3	2.12	0.50
1:H:128:PRO:HD2	1:H:213:THR:HG21	1.92	0.50
1:A:78:THR:CG2	1:A:80:TYR:CE1	2.94	0.50
2:B:64:PRO:O	2:B:67:PHE:HD1	1.94	0.50
2:L:71:GLY:HA2	4:L:328:HOH:O	2.12	0.49
1:A:193:PRO:O	1:A:195:SER:N	2.45	0.49
1:H:63:ASN:HD22	1:H:63:ASN:N	2.08	0.49
2:B:113:ARG:HD3	2:B:114:ALA:O	2.12	0.49
2:B:159:GLU:HG2	2:B:160:ARG:N	2.27	0.49
1:A:193:PRO:C	1:A:196:THR:HG1	2.08	0.49
1:A:2:VAL:HG13	1:A:27:PHE:CD1	2.48	0.49
2:B:3:LEU:N	2:B:26:SER:HB2	2.28	0.49
1:H:57:TYR:HB2	3:E:442:PHE:CD2	2.47	0.49
2:L:44:LYS:HG2	4:L:313:HOH:O	2.14	0.48
2:B:10:SER:HA	2:B:108:LYS:O	2.13	0.48
1:H:222:ARG:NH2	2:L:124:PRO:HB2	2.28	0.48
1:A:143:SER:CA	1:A:194:SER:HG	2.25	0.48
1:A:17:SER:O	1:A:18:LEU:HB3	2.13	0.48
1:A:63:ASN:HD22	1:A:63:ASN:N	2.10	0.48
2:L:125:PRO:HG2	2:L:135:ALA:HB1	1.95	0.48
2:B:36:THR:CB	2:B:56:LEU:HD12	2.45	0.47
1:A:143:SER:O	1:A:194:SER:OG	2.32	0.47
1:A:193:PRO:C	1:A:195:SER:H	2.18	0.47
1:A:30:SER:HB3	1:A:74:ILE:HB	1.96	0.47
1:A:114:GLN:HG2	4:A:311:HOH:O	2.15	0.47
1:A:128:PRO:HB3	1:A:154:TYR:HB3	1.95	0.47
2:B:16:GLY:N	2:B:83:VAL:HG13	2.30	0.47
3:F:437:TRP:CZ3	3:F:438:LEU:HD23	2.49	0.47
2:B:84:GLU:HB3	2:B:86:GLU:CG	2.45	0.47
2:B:195:ASN:OD1	2:B:215:ASN:HB3	2.15	0.47
2:B:127:SER:HA	2:B:130:LEU:HD12	1.97	0.47
2:B:66:ARG:CZ	2:B:84:GLU:HG3	2.45	0.47
2:L:42:LEU:HD13	2:L:91:TYR:CE1	2.49	0.47
2:B:194:HIS:O	2:B:216:ARG:HD3	2.15	0.47
2:B:200:GLU:CB	2:B:211:VAL:HG22	2.46	0.47
2:L:99:VAL:O	2:L:99:VAL:CG2	2.63	0.46
1:H:34:MET:HG2	1:H:79:LEU:HD22	1.98	0.46
2:L:16:GLY:C	2:L:82:ARG:O	2.53	0.46
1:H:28:THR:HA	1:H:77:ASN:ND2	2.24	0.46
1:H:162:THR:OG1	1:H:205:ASN:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:42:GLU:OE1	2:B:193:ARG:NH2	2.49	0.46
2:B:7:THR:CB	2:B:8:PRO:CD	2.86	0.46
2:L:11:LEU:HD23	2:L:12:PRO:HD2	1.98	0.46
2:B:66:ARG:CA	2:B:81:SER:HB2	2.45	0.46
1:H:57:TYR:CB	3:E:442:PHE:CD2	2.99	0.45
1:A:19:LYS:NZ	4:A:314:HOH:O	2.41	0.45
1:A:197:TRP:CD1	1:A:198:PRO:HA	2.51	0.45
2:L:172:ASP:O	2:L:176:SER:HA	2.16	0.45
1:A:214:LYS:HB2	1:A:214:LYS:HE3	1.73	0.45
1:A:88:SER:HA	1:A:120:VAL:HB	1.97	0.45
2:B:12:PRO:HA	2:B:110:GLU:C	2.35	0.45
2:B:159:GLU:HG2	2:B:160:ARG:H	1.82	0.45
1:A:1:GLU:HG2	1:A:2:VAL:H	1.82	0.45
2:L:154:LYS:HB2	2:L:198:THR:HB	1.99	0.45
2:B:96:GLY:HA3	3:F:437:TRP:CD2	2.53	0.44
1:H:99:HIS:HD2	1:H:107:ASP:O	2.00	0.44
2:B:55:LYS:O	2:B:58:ASN:ND2	2.50	0.44
2:L:66:ARG:HB3	2:L:81:SER:O	2.17	0.44
1:H:132:PRO:HD3	1:H:217:LYS:HE2	1.98	0.44
2:L:8:PRO:O	2:L:10:SER:N	2.39	0.44
1:H:197:TRP:HA	1:H:198:PRO:HA	1.67	0.44
2:B:83:VAL:O	2:B:87:ASP:OD2	2.35	0.44
1:H:208:HIS:HB3	1:H:213:THR:HB	2.00	0.44
2:B:37:TYR:OH	3:F:436:GLY:HA2	2.18	0.43
1:A:179:LEU:HD13	1:A:184:TYR:CZ	2.53	0.43
1:A:201:THR:HG21	1:A:218:LYS:NZ	2.33	0.43
1:A:101:PRO:HB2	1:A:104:VAL:HG23	2.00	0.43
2:B:7:THR:OG1	2:B:22:SER:OG	1.96	0.43
1:A:193:PRO:HD2	1:A:196:THR:OG1	2.18	0.43
1:A:149:CYS:O	1:A:187:SER:HA	2.18	0.43
1:A:191:THR:C	1:A:192:VAL:CG1	2.86	0.43
1:H:11:LEU:HD22	1:H:155:PHE:HE1	1.83	0.43
1:A:74:ILE:N	4:A:321:HOH:O	2.50	0.43
1:A:102:THR:OG1	3:F:434:ASN:HA	2.19	0.43
2:L:159:GLU:HG2	2:L:160:ARG:N	2.34	0.43
1:A:47:TRP:CD2	2:B:101:PRO:HG2	2.54	0.43
2:L:82:ARG:HE	2:L:84:GLU:CD	2.17	0.42
1:A:193:PRO:C	1:A:195:SER:N	2.73	0.42
2:B:168:TRP:CD1	2:B:168:TRP:N	2.87	0.42
1:A:172:VAL:HG22	1:A:190:VAL:HG23	2.01	0.42
2:L:64:PRO:CB	4:L:323:HOH:O	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:56:LEU:HD23	2:B:57:SER:HB3	2.00	0.42
1:H:214:LYS:HE3	1:H:214:LYS:HB2	1.70	0.42
2:L:57:SER:O	2:L:58:ASN:OD1	2.37	0.42
2:L:40:TRP:CE2	2:L:78:LEU:HB2	2.55	0.42
1:H:9:GLY:H	1:H:116:THR:CG2	2.30	0.42
2:L:44:LYS:HE2	2:L:86:GLU:O	2.19	0.42
1:H:220:VAL:HG12	1:H:221:PRO:HD3	2.01	0.42
2:L:91:TYR:O	2:L:106:GLY:HA2	2.20	0.42
2:L:53:ILE:HG21	2:L:56:LEU:O	2.19	0.42
2:B:37:TYR:CD2	3:F:437:TRP:HB3	2.55	0.42
1:A:147:LEU:HG	1:A:219:ILE:HG21	2.02	0.42
2:B:216:ARG:O	2:B:217:ASN:O	2.38	0.42
1:H:13:LYS:HA	1:H:121:SER:O	2.20	0.42
2:L:66:ARG:HH22	2:L:87:ASP:CG	2.23	0.41
2:L:56:LEU:HD23	2:L:57:SER:HB3	2.02	0.41
3:F:438:LEU:HD22	3:F:441:LEU:HD12	2.02	0.41
1:A:109:MET:HE1	3:F:437:TRP:HZ2	1.86	0.41
2:B:56:LEU:HD23	2:B:57:SER:CB	2.50	0.41
1:A:100:PRO:HD2	1:A:108:ALA:O	2.20	0.41
2:L:31:HIS:HD2	2:L:33:ASP:H	1.69	0.41
2:L:122:ILE:HG22	2:L:212:LYS:HB3	2.02	0.41
1:H:203:THR:HG23	1:H:217:LYS:H	1.86	0.41
2:B:188:LYS:O	2:B:192:GLU:HG3	2.21	0.41
1:A:56:SER:OG	3:F:431:GLU:OE1	2.32	0.41
1:H:34:MET:HB2	1:H:34:MET:HE3	1.80	0.41
2:B:123:PHE:HA	2:B:124:PRO:HD3	1.93	0.41
2:B:63:VAL:O	2:B:64:PRO:C	2.59	0.41
1:A:47:TRP:CG	2:B:101:PRO:HG2	2.56	0.41
1:H:78:THR:CG2	1:H:80:TYR:CE1	3.04	0.41
1:A:94:TYR:O	1:A:115:GLY:HA2	2.21	0.41
1:H:6:GLU:H	1:H:114:GLN:NE2	2.19	0.40
2:L:82:ARG:O	2:L:83:VAL:HB	2.22	0.40
1:H:78:THR:HG22	1:H:80:TYR:CE1	2.57	0.40
2:B:208:SER:HB2	2:B:209:PRO:HD2	2.04	0.40
1:H:36:TRP:CE2	1:H:81:LEU:HB2	2.56	0.40
1:A:11:LEU:HD12	1:A:119:THR:O	2.21	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	213/222 (96%)	198 (93%)	12 (6%)	3 (1%)	14	40
1	H	213/222 (96%)	198 (93%)	14 (7%)	1 (0%)	34	67
2	B	215/217 (99%)	194 (90%)	16 (7%)	5 (2%)	8	26
2	L	215/217 (99%)	196 (91%)	13 (6%)	6 (3%)	6	21
3	E	11/17 (65%)	11 (100%)	0	0	100	100
3	F	11/17 (65%)	10 (91%)	1 (9%)	0	100	100
All	All	878/912 (96%)	807 (92%)	56 (6%)	15 (2%)	11	35

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	L	7	THR
2	L	9	LEU
2	L	64	PRO
2	B	7	THR
2	B	83	VAL
2	L	65	ASP
1	A	106	GLY
1	A	150	LEU
2	L	82	ARG
2	B	84	GLU
1	H	106	GLY
2	L	83	VAL
1	A	194	SER
2	B	59	ARG
2	B	100	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	A	187/190 (98%)	159 (85%)	28 (15%)	3	9
1	H	187/190 (98%)	157 (84%)	30 (16%)	3	7
2	B	194/194 (100%)	172 (89%)	22 (11%)	7	19
2	L	194/194 (100%)	167 (86%)	27 (14%)	4	11
3	E	10/14 (71%)	8 (80%)	2 (20%)	1	4
3	F	10/14 (71%)	9 (90%)	1 (10%)	9	26
All	All	782/796 (98%)	672 (86%)	110 (14%)	4	11

All (110) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	12	VAL
1	H	17	SER
1	H	18	LEU
1	H	20	LEU
1	H	29	VAL
1	H	34	MET
1	H	46	GLU
1	H	56	SER
1	H	58	THR
1	H	63	ASN
1	H	72	ARG
1	H	74	ILE
1	H	81	LEU
1	H	85	SER
1	H	86	LEU
1	H	93	MET
1	H	109	MET
1	H	114	GLN
1	H	116	THR
1	H	125	THR
1	H	144	MET
1	H	147	LEU

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Mol	Chain	Res	Type
1	H	149	CYS
1	H	158	PRO
1	H	159	VAL
1	H	197	TRP
1	H	200	GLU
1	H	204	CYS
1	H	217	LYS
1	H	220	VAL
2	L	3	LEU
2	L	5	THR
2	L	9	LEU
2	L	10	SER
2	L	11	LEU
2	L	13	VAL
2	L	14	SER
2	L	18	GLN
2	L	32	SER
2	L	48	SER
2	L	61	SER
2	L	64	PRO
2	L	65	ASP
2	L	79	LYS
2	L	109	LEU
2	L	110	GLU
2	L	111	ILE
2	L	113	ARG
2	L	127	SER
2	L	131	THR
2	L	132	SER
2	L	150	ASN
2	L	158	SER
2	L	161	GLN
2	L	165	LEU
2	L	184	LEU
2	L	217	ASN
3	E	438	LEU
3	E	442	PHE
1	A	12	VAL
1	A	17	SER
1	A	20	LEU
1	A	29	VAL
1	A	56	SER

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Mol	Chain	Res	Type
1	A	58	THR
1	A	63	ASN
1	A	72	ARG
1	A	74	ILE
1	A	81	LEU
1	A	85	SER
1	A	86	LEU
1	A	93	MET
1	A	109	MET
1	A	114	GLN
1	A	116	THR
1	A	117	SER
1	A	124	LYS
1	A	125	THR
1	A	144	MET
1	A	147	LEU
1	A	158	PRO
1	A	159	VAL
1	A	191	THR
1	A	193	PRO
1	A	194	SER
1	A	196	THR
1	A	204	CYS
2	B	3	LEU
2	B	7	THR
2	B	18	GLN
2	B	32	SER
2	B	48	SER
2	B	59	ARG
2	B	65	ASP
2	B	76	PHE
2	B	82	ARG
2	B	83	VAL
2	B	109	LEU
2	B	110	GLU
2	B	113	ARG
2	B	131	THR
2	B	132	SER
2	B	150	ASN
2	B	158	SER
2	B	161	GLN
2	B	165	LEU

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Mol	Chain	Res	Type
2	B	184	LEU
2	B	207	THR
2	B	216	ARG
3	F	438	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	63	ASN
1	H	77	ASN
1	H	99	HIS
1	H	114	GLN
1	H	164	ASN
2	L	18	GLN
2	L	31	HIS
2	L	35	ASN
2	L	47	GLN
2	L	150	ASN
3	E	430	ASN
1	A	63	ASN
2	B	31	HIS
2	B	58	ASN
2	B	150	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 [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	217/222 (97%)	-0.64	0 100 100	24, 46, 75, 98	0
1	H	217/222 (97%)	-0.75	0 100 100	17, 30, 59, 83	0
2	B	217/217 (100%)	0.04	13 (5%) 25 18	28, 67, 106, 117	0
2	L	217/217 (100%)	-0.50	1 (0%) 91 90	24, 43, 65, 83	0
3	E	13/17 (76%)	-0.79	0 100 100	22, 27, 32, 33	0
3	F	13/17 (76%)	-0.37	0 100 100	46, 53, 65, 68	0
All	All	894/912 (98%)	-0.46	14 (1%) 74 72	17, 43, 94, 117	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	12	PRO	4.6
2	B	99	VAL	4.4
2	B	110	GLU	3.3
2	B	19	ALA	3.0
2	B	7	THR	2.7
2	B	66	ARG	2.7
2	L	7	THR	2.5
2	B	81	SER	2.3
2	B	20	SER	2.3
2	B	56	LEU	2.2
2	B	40	TRP	2.2
2	B	15	LEU	2.1
2	B	173	SER	2.1
2	B	16	GLY	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 [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.