



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 07:41 PM UTC

PDB ID : 4HZL / pdb_00004hzl
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

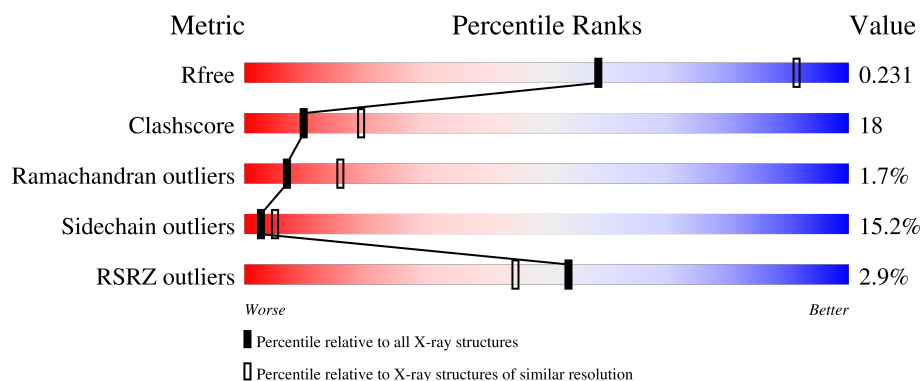
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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_{free}	180053	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	
1	H	222	
2	B	217	
2	L	217	
3	E	17	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	F	17	29% 29% 18% 24%

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		

Continued on next page...

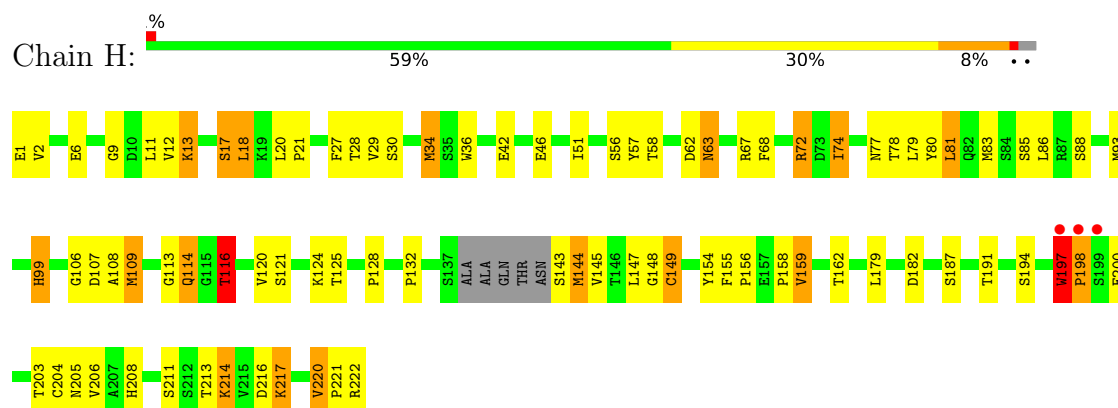
Continued from previous page...

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

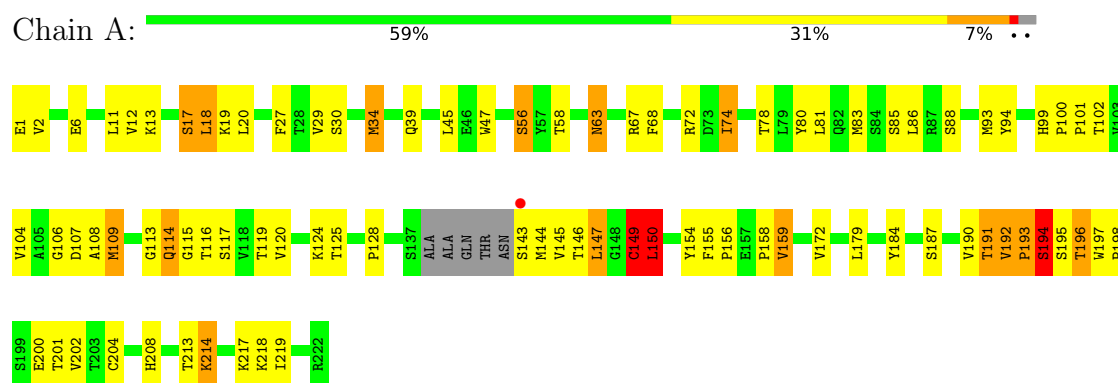
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

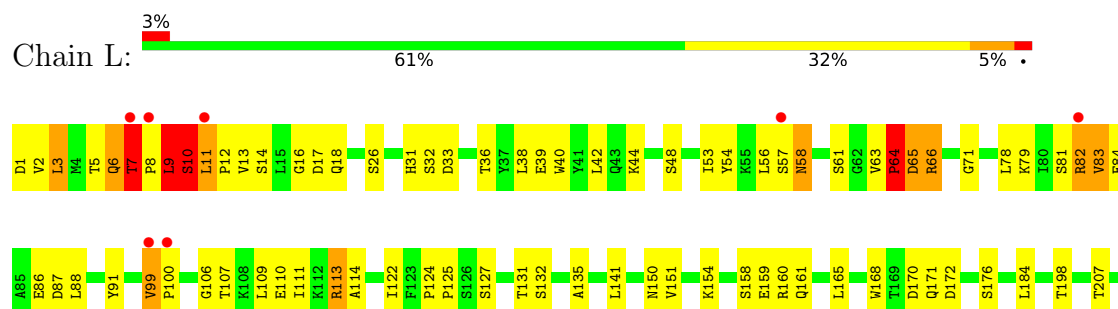
• Molecule 1: Fab heavy chain



• Molecule 1: Fab heavy chain



• Molecule 2: Fab light chain





4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	137.25Å 137.25Å 140.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.85 50.00 – 2.85	Depositor EDS
% Data completeness (in resolution range)	99.8 (50.00-2.85) 99.8 (50.00-2.85)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.45 (at 2.54Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.221 , 0.277 (Not available) , 0.231	Depositor DCC
R_{free} test set	2185 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	25.6	Xtriage
Anisotropy	0.192	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 42.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	0.058 for -h,l,k 0.046 for -l,-k,-h	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	6949	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.92	2/1675 (0.1%)	1.08	7/2290 (0.3%)
1	H	0.98	4/1675 (0.2%)	1.08	7/2290 (0.3%)
2	B	0.85	3/1718 (0.2%)	1.07	7/2333 (0.3%)
2	L	0.83	0/1718	1.07	9/2333 (0.4%)
3	E	0.95	0/102	1.57	3/138 (2.2%)
3	F	0.80	0/102	1.36	2/138 (1.4%)
All	All	0.90	9/6990 (0.1%)	1.09	35/9522 (0.4%)

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 (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	159	VAL	CA-C	12.27	1.67	1.52
1	H	159	VAL	CA-C	12.24	1.67	1.52
1	H	99	HIS	CG-ND1	-7.28	1.30	1.38
1	H	99	HIS	CD2-NE2	-6.38	1.30	1.37
2	B	71	GLY	N-CA	6.01	1.54	1.45
2	B	71	GLY	CA-C	5.95	1.60	1.51
1	A	192	VAL	C-N	5.42	1.40	1.33
2	B	8	PRO	N-CD	5.24	1.55	1.47
1	H	198	PRO	N-CD	5.17	1.55	1.47

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	99	VAL	CA-C-N	-9.96	110.13	120.38
2	L	99	VAL	C-N-CA	-9.96	110.13	120.38
1	A	150	LEU	N-CA-C	9.59	131.23	110.80
2	B	99	VAL	CA-C-N	-9.20	110.91	120.38
2	B	99	VAL	C-N-CA	-9.20	110.91	120.38
3	E	435	THR	N-CA-C	-8.50	97.19	110.36
3	E	437	TRP	N-CA-C	8.44	122.55	111.75
1	H	197	TRP	C-N-CD	8.33	138.92	120.60
3	F	435	THR	N-CA-C	-7.41	100.97	110.53
1	A	149	CYS	CA-C-N	7.39	135.66	121.54
1	A	149	CYS	C-N-CA	7.39	135.66	121.54
2	L	63	VAL	CA-C-N	7.38	129.07	119.84
2	L	63	VAL	C-N-CA	7.38	129.07	119.84
3	F	437	TRP	N-CA-C	7.29	120.09	111.71
1	H	206	VAL	N-CA-C	6.86	117.71	108.11
2	L	66	ARG	N-CA-C	-6.12	105.81	113.28
3	E	431	GLU	N-CA-C	-6.11	104.47	112.41
1	A	192	VAL	CA-C-N	-6.10	113.68	119.90
1	A	192	VAL	C-N-CA	-6.10	113.68	119.90
2	B	72	SER	N-CA-C	6.06	118.33	108.76
2	L	58	ASN	N-CA-C	5.78	118.31	108.02
1	H	116	THR	N-CA-C	-5.67	100.64	109.72
2	L	99	VAL	N-CA-C	5.54	120.85	108.88
2	B	7	THR	CA-C-N	-5.54	112.92	119.84
2	B	7	THR	C-N-CA	-5.54	112.92	119.84
1	H	216	ASP	N-CA-C	-5.52	101.87	110.42
2	B	200	GLU	N-CA-C	5.50	117.37	108.34
2	B	82	ARG	N-CA-C	5.50	122.52	110.80
2	L	7	THR	CA-C-N	-5.42	113.07	119.84
2	L	7	THR	C-N-CA	-5.42	113.07	119.84
1	H	62	ASP	N-CA-C	5.37	118.63	111.75
1	A	18	LEU	N-CA-C	5.28	116.56	108.42
1	H	18	LEU	N-CA-C	5.22	116.46	108.42
1	H	148	GLY	N-CA-C	5.13	120.64	110.83
1	A	149	CYS	N-CA-C	-5.13	99.92	108.34

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
2	L	6	GLN	Peptide
2	L	64	PRO	Peptide

5.2 Too-close contacts [i](#)

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	66	0
1	H	1632	0	1608	55	0
2	B	1679	0	1616	54	0
2	L	1679	0	1616	57	0
3	E	100	0	92	6	0
3	F	100	0	92	13	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	237	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 18.

All (237) 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	0.87
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:18:LEU:HD23	1:A:83:MET:HE3	1.66	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:H:18:LEU:HD23	1:H:83:MET:HE3	1.69	0.74
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:A:63:ASN:H	1:A:63:ASN:HD22	1.39	0.70
3:E:431:GLU:HG2	4:E:508:HOH:O	1.92	0.69
2:L:7:THR:C	2:L:9:LEU:H	1.99	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:L:88:LEU:O	4:L:313:HOH:O	2.14	0.66
2:B:7:THR:HB	2:B:8:PRO:HD3	1.76	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
1:H:155:PHE:CE1	1:H:156:PRO:HB3	2.32	0.64
1:H:63:ASN:H	1:H:63:ASN:HD22	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: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:143:SER:C	1:A:194:SER:HG	2.10	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:191:THR:C	1:A:192:VAL:HG13	2.28	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
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
2:L:7:THR:C	2:L:9:LEU:N	2.62	0.56
1:A:107:ASP:OD2	3:F:438:LEU:HB2	2.06	0.56
2:B:36:THR:HB	2:B:56:LEU:HD12	1.88	0.55
2:L:213:SER:O	2:L:214:PHE:HB3	2.06	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:A:108:ALA:HA	1:A:109:MET:HE3	1.87	0.55
1:H:21:PRO:HD2	4:H:318:HOH:O	2.07	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
1:A:18:LEU:CD2	1:A:83:MET:CE	2.85	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:193:PRO:C	1:A:196:THR:HG1	2.08	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:108:ALA:HA	1:H:109:MET:HE3	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:193:PRO:C	1:A:195:SER:H	2.18	0.52
2:L:42:LEU:HD13	2:L:91:TYR:CZ	2.45	0.52
2:B:16:GLY:N	2:B:83:VAL:HA	2.18	0.52
2:L:113:ARG:HD3	2:L:114:ALA:O	2.10	0.52
1:A:143:SER:N	1:A:194:SER:OG	2.43	0.52
1:H:116:THR:HG22	4:H:316:HOH:O	2.10	0.52
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:2:VAL:HG13	2:L:26:SER:HB3	1.92	0.51
2:L:3:LEU:N	2:L:26:SER:HB2	2.26	0.51
2:L:16:GLY:C	2:L:82:ARG:O	2.53	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
3:E:438:LEU:HD22	3:E:441:LEU:HD12	1.94	0.50
1:A:78:THR:CG2	1:A:80:TYR:HE1	2.25	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:B:12:PRO:HA	2:B:110:GLU:C	2.35	0.49
1:A:109:MET:HE3	1:A:109:MET:N	2.27	0.49
2:L:71:GLY:HA2	4:L:328:HOH:O	2.12	0.49
1:H:63:ASN:HD22	1:H:63:ASN:N	2.08	0.49
1:A:193:PRO:O	1:A:195:SER:N	2.45	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:2:VAL:HG13	1:A:27:PHE:CD1	2.48	0.49
1:H:57:TYR:HB2	3:E:442:PHE:CD2	2.47	0.49
2:B:3:LEU:N	2:B:26:SER:HB2	2.28	0.49
1:H:109:MET:HE3	1:H:109:MET:N	2.27	0.48
1:H:222:ARG:NH2	2:L:124:PRO:HB2	2.28	0.48
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:A:17:SER:O	1:A:18:LEU:HB3	2.13	0.48
1:A:143:SER:CA	1:A:194:SER:HG	2.25	0.48
1:A:191:THR:C	1:A:192:VAL:CG1	2.86	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:L:82:ARG:HE	2:L:84:GLU:CD	2.17	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:193:PRO:C	1:A:195:SER:N	2.73	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
2:B:84:GLU:HB3	2:B:86:GLU:CG	2.45	0.47
2:B:127:SER:HA	2:B:130:LEU:HD12	1.97	0.47
2:B:195:ASN:OD1	2:B:215:ASN:HB3	2.15	0.47
3:F:437:TRP:CZ3	3:F:438:LEU:HD23	2.49	0.47
2:L:42:LEU:HD13	2:L:91:TYR:CE1	2.49	0.47
2:B:66:ARG:CZ	2:B:84:GLU:HG3	2.45	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:66:ARG:HH22	2:L:87:ASP:CG	2.23	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
1:H:42:GLU:OE1	2:B:193:ARG:NH2	2.49	0.46
2:L:11:LEU:HD23	2:L:12:PRO:HD2	1.98	0.46
2:B:7:THR:CB	2:B:8:PRO:CD	2.86	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
2:B:63:VAL:O	2:B:64:PRO:C	2.59	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:88:SER:HA	1:A:120:VAL:HB	1.97	0.45
1:A:214:LYS:HE3	1:A:214:LYS:HB2	1.73	0.45
2:B:159:GLU:HG2	2:B:160:ARG:H	1.82	0.45
2:L:8:PRO:C	2:L:10:SER:H	2.21	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
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:B:96:GLY:HA3	3:F:437:TRP:CD2	2.53	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:132:PRO:HD3	1:H:217:LYS:HE2	1.98	0.44
2:L:66:ARG:HB3	2:L:81:SER:O	2.17	0.44
1:H:34:MET:HB2	1:H:34:MET:HE3	1.52	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
1:A:34:MET:HE3	1:A:34:MET:HB2	1.53	0.44
1:H:208:HIS:HB3	1:H:213:THR:HB	2.00	0.44
2:B:83:VAL:O	2:B:87:ASP:OD2	2.35	0.44
1:A:101:PRO:HB2	1:A:104:VAL:HG23	2.00	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
2:B:37:TYR:OH	3:F:436:GLY:HA2	2.18	0.43
2:B:7:THR:OG1	2:B:22:SER:OG	1.96	0.43
1:A:149:CYS:O	1:A:187:SER:HA	2.18	0.43
1:A:193:PRO:HD2	1:A:196:THR:OG1	2.18	0.43
1:H:144:MET:HE3	1:H:191:THR:HG22	2.01	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
1:H:18:LEU:HD21	1:H:83:MET:HE1	2.00	0.42
1:A:172:VAL:HG22	1:A:190:VAL:HG23	2.01	0.42
2:B:168:TRP:CD1	2:B:168:TRP:N	2.87	0.42
1:H:214:LYS:HE3	1:H:214:LYS:HB2	1.70	0.42
2:L:64:PRO:CB	4:L:323:HOH:O	2.67	0.42
2:B:56:LEU:HD23	2:B:57:SER:HB3	2.00	0.42
2:L:40:TRP:CE2	2:L:78:LEU:HB2	2.55	0.42
2:L:57:SER:O	2:L:58:ASN:OD1	2.37	0.42
1:H:9:GLY:H	1:H:116:THR:CG2	2.30	0.42
1:H:220:VAL:HG12	1:H:221:PRO:HD3	2.01	0.42
2:L:44:LYS:HE2	2:L:86:GLU:O	2.19	0.42
2:L:170:ASP:O	2:L:171:GLN:C	2.63	0.42
2:B:83:VAL:C	2:B:84:GLU:HG2	2.45	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
1:H:13:LYS:HA	1:H:121:SER:O	2.20	0.42
1:H:208:HIS:ND1	1:H:211:SER:OG	2.38	0.42
2:B:216:ARG:O	2:B:217:ASN:O	2.38	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:100:PRO:HD2	1:A:108:ALA:O	2.20	0.41
2:B:56:LEU:HD23	2:B:57:SER:CB	2.50	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:A:67:ARG:C	1:A:68:PHE:HD1	2.28	0.41
2:B:123:PHE:HA	2:B:124:PRO:HD3	1.93	0.41
1:H:78:THR:CG2	1:H:80:TYR:CE1	3.04	0.41
1:A:47:TRP:CG	2:B:101:PRO:HG2	2.56	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
1:H:67:ARG:C	1:H:68:PHE:HD1	2.29	0.40
2:L:82:ARG:O	2:L:83:VAL:HB	2.22	0.40
2:B:60:PHE:O	2:B:61:SER:C	2.63	0.40
1:H:78:THR:HG22	1:H:80:TYR:CE1	2.57	0.40
1:A:99:HIS:CE1	1:A:109:MET:HE2	2.56	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
2:B:208:SER:HB2	2:B:209:PRO:HD2	2.04	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	213/222 (96%)	198 (93%)	12 (6%)	3 (1%)	9	19
1	H	213/222 (96%)	198 (93%)	14 (7%)	1 (0%)	24	42

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	215/217 (99%)	194 (90%)	16 (7%)	5 (2%)	5	11
2	L	215/217 (99%)	196 (91%)	13 (6%)	6 (3%)	4	9
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%)	7	16

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%)	153 (82%)	34 (18%)	2	2
1	H	187/190 (98%)	155 (83%)	32 (17%)	2	3
2	B	194/194 (100%)	170 (88%)	24 (12%)	4	8
2	L	194/194 (100%)	167 (86%)	27 (14%)	3	6

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	E	10/14 (71%)	9 (90%)	1 (10%)	7	16
3	F	10/14 (71%)	9 (90%)	1 (10%)	7	16
All	All	782/796 (98%)	663 (85%)	119 (15%)	3	5

All (119) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	12	VAL
1	H	13	LYS
1	H	17	SER
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	124	LYS
1	H	125	THR
1	H	144	MET
1	H	147	LEU
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	214	LYS
1	H	217	LYS
1	H	220	VAL
2	L	3	LEU
2	L	5	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	38	LEU
2	L	48	SER
2	L	61	SER
2	L	64	PRO
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	207	THR
3	E	438	LEU
1	A	12	VAL
1	A	13	LYS
1	A	17	SER
1	A	20	LEU
1	A	29	VAL
1	A	34	MET
1	A	56	SER
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	145	VAL
1	A	147	LEU
1	A	150	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
1	A	214	LYS
1	A	217	LYS
2	B	3	LEU
2	B	7	THR
2	B	32	SER
2	B	38	LEU
2	B	48	SER
2	B	59	ARG
2	B	65	ASP
2	B	76	PHE
2	B	77	THR
2	B	82	ARG
2	B	83	VAL
2	B	109	LEU
2	B	110	GLU
2	B	111	ILE
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
2	B	184	LEU
2	B	207	THR
2	B	216	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	F	438	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) 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	31	HIS
2	L	166	ASN
3	E	430	ASN
1	A	63	ASN
1	A	180	GLN
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 oligosaccharides 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, 95th 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 ²)	Q<0.9
1	A	217/222 (97%)	-0.30	1 (0%) 87 85	24, 46, 75, 98	0
1	H	217/222 (97%)	-0.56	3 (1%) 73 67	17, 30, 59, 83	0
2	B	217/217 (100%)	0.38	15 (6%) 23 17	28, 67, 106, 117	0
2	L	217/217 (100%)	-0.26	7 (3%) 50 41	24, 43, 64, 83	0
3	E	13/17 (76%)	-0.58	0 100 100	22, 27, 32, 33	0
3	F	13/17 (76%)	0.42	0 100 100	46, 53, 65, 68	0
All	All	894/912 (98%)	-0.18	26 (2%) 53 45	17, 43, 94, 117	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	99	VAL	5.7
2	B	88	LEU	4.2
2	B	98	HIS	4.0
2	B	100	PRO	3.9
2	B	111	ILE	3.7
2	L	7	THR	3.4
1	H	198	PRO	3.2
2	B	96	GLY	3.2
2	L	8	PRO	3.1
2	B	7	THR	3.1
2	B	97	SER	2.9
2	B	108	LYS	2.8
2	L	11	LEU	2.8
2	B	110	GLU	2.7
1	H	199	SER	2.7
2	B	70	SER	2.5
2	B	71	GLY	2.4
2	B	109	LEU	2.4
2	L	57	SER	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	L	99	VAL	2.2
2	B	20	SER	2.2
1	H	197	TRP	2.2
1	A	143	SER	2.2
2	L	100	PRO	2.1
2	L	82	ARG	2.1
2	B	12	PRO	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 oligosaccharides 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.