



# Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 07:27 pm BST

PDB ID : 3MCK  
Title : Crystal structure of anti-beta-amyloid antibody C705  
Authors : Teplyakov, A.; Obmolova, G.; Gilliland, G.L.  
Deposited on : 2010-03-29  
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

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

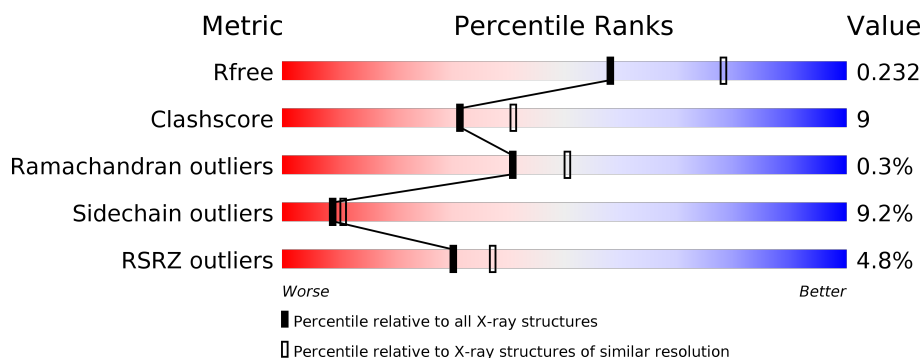
# 1 Overall quality at a glance

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))
$R_{free}$	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (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 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	219	<div> <div>4%</div> <div> <div></div> <div>77%</div> <div>21%</div> <div>.</div> </div> </div>
1	L	219	<div> <div>4%</div> <div> <div></div> <div>80%</div> <div>17%</div> <div>.</div> </div> </div>
2	B	228	<div> <div>6%</div> <div> <div></div> <div>72%</div> <div>20%</div> <div>5%</div> <div>..</div> </div> </div>
2	H	228	<div> <div>5%</div> <div> <div></div> <div>75%</div> <div>18%</div> <div>6%</div> <div>.</div> </div> </div>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 7024 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 C705 MONOCLONAL LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	219	Total	C	N	O	S	0	0	0
			1691	1054	284	343	10			
1	A	219	Total	C	N	O	S	0	0	0
			1691	1054	284	343	10			

- Molecule 2 is a protein called C705 MONOCLONAL HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	226	Total	C	N	O	S	0	0	0
			1692	1069	279	338	6			
2	B	226	Total	C	N	O	S	0	0	0
			1692	1069	279	338	6			

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	H	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0

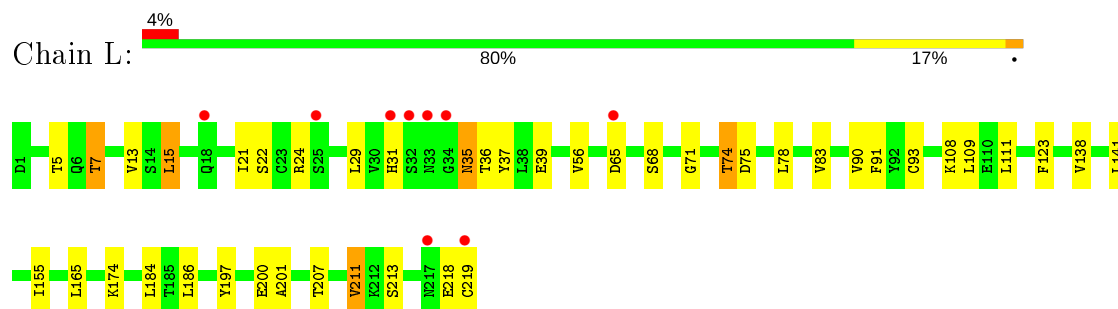
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	L	47	Total O 47 47	0	0
4	H	78	Total O 78 78	0	0
4	A	61	Total O 61 61	0	0
4	B	64	Total O 64 64	0	0

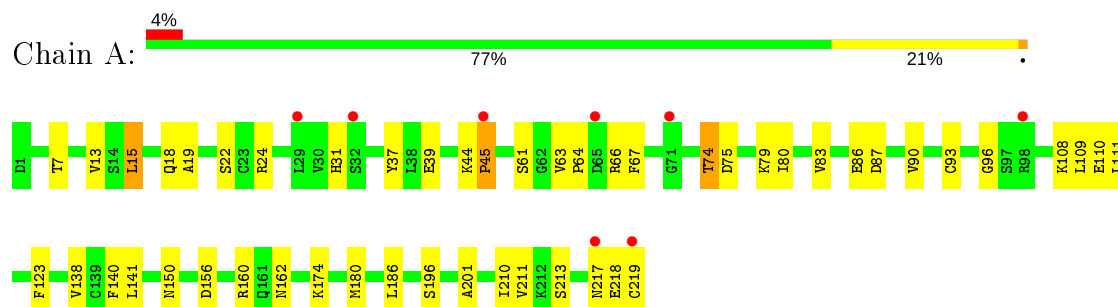
### 3 Residue-property plots [i](#)

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

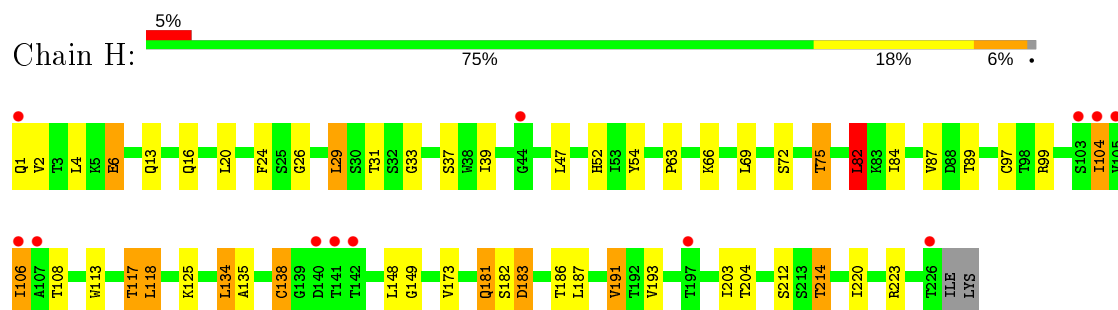
#### • Molecule 1: C705 MONOCLONAL LIGHT CHAIN



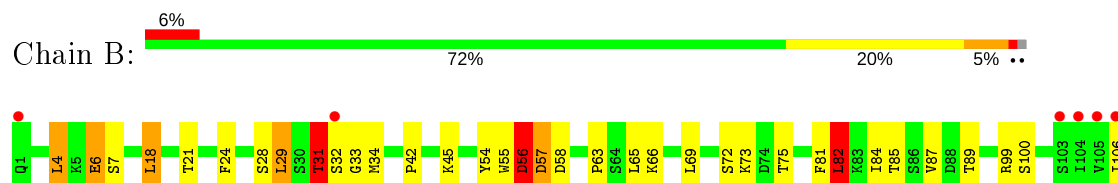
#### • Molecule 1: C705 MONOCLONAL LIGHT CHAIN

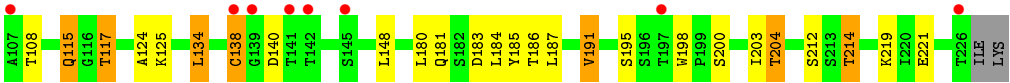


#### • Molecule 2: C705 MONOCLONAL HEAVY CHAIN



#### • Molecule 2: C705 MONOCLONAL HEAVY CHAIN





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	172.25Å 78.25Å 74.63Å 90.00° 95.45° 90.00°	Depositor
Resolution (Å)	15.00 – 2.30 14.98 – 2.30	Depositor EDS
% Data completeness (in resolution range)	93.7 (15.00-2.30) 96.7 (14.98-2.30)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.32 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.203 , 0.254 0.204 , 0.232	Depositor DCC
$R_{free}$ test set	1328 reflections (3.13%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	45.3	Xtriage
Anisotropy	0.115	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 44.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	7024	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.87% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ACT

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	0.44	0/1728	0.60	0/2341
1	L	0.44	0/1728	0.61	0/2341
2	B	0.46	0/1734	0.74	5/2373 (0.2%)
2	H	0.48	0/1734	0.73	5/2373 (0.2%)
All	All	0.46	0/6924	0.67	10/9428 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	106	ILE	CB-CA-C	-7.22	97.16	111.60
2	H	47	LEU	CA-CB-CG	6.68	130.66	115.30
2	H	82	LEU	CA-CB-CG	6.38	129.98	115.30
2	B	82	LEU	CA-CB-CG	5.93	128.94	115.30
2	B	57	ASP	CB-CG-OD2	5.29	123.06	118.30
2	B	56	ASP	CB-CG-OD2	5.26	123.03	118.30
2	B	58	ASP	CB-CG-OD2	5.25	123.03	118.30
2	H	183	ASP	CB-CG-OD2	5.09	122.88	118.30
2	B	4	LEU	CA-CB-CG	5.06	126.93	115.30
2	H	187	LEU	CA-CB-CG	5.01	126.82	115.30

There are no chirality outliers.



All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	31	THR	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	1691	0	1629	27	0
1	L	1691	0	1629	23	0
2	B	1692	0	1674	46	0
2	H	1692	0	1674	35	0
3	B	4	0	3	0	0
3	H	4	0	3	0	0
4	A	61	0	0	0	0
4	B	64	0	0	1	0
4	H	78	0	0	1	0
4	L	47	0	0	0	0
All	All	7024	0	6612	121	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 9.

All (121) 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)
2:H:181:GLN:HG2	2:H:181:GLN:O	1.45	1.14
2:H:29:LEU:HB3	2:H:75:THR:HG22	1.59	0.84
2:B:4:LEU:HD13	2:B:24:PHE:HB3	1.66	0.76
2:B:212:SER:OG	2:B:214:THR:HG23	1.87	0.74
1:A:123:PHE:HB2	1:A:138:VAL:HG13	1.70	0.72
1:L:35:ASN:H	1:L:35:ASN:HD22	1.38	0.72
2:B:28:SER:O	2:B:31:THR:HG22	1.88	0.71
2:H:63:PRO:HA	2:H:66:LYS:HD2	1.73	0.70
1:L:123:PHE:HB2	1:L:138:VAL:HG13	1.73	0.70
2:H:54:TYR:HE2	2:H:106:ILE:HB	1.58	0.69
1:L:13:VAL:HG11	1:L:83:VAL:HG11	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:181:GLN:HG2	2:B:184:LEU:O	1.93	0.67
2:H:182:SER:O	2:H:183:ASP:HB2	1.93	0.67
2:H:4:LEU:HD13	2:H:24:PHE:HB3	1.77	0.66
2:H:181:GLN:NE2	2:H:186:THR:OG1	2.29	0.66
2:H:54:TYR:CE2	2:H:106:ILE:HB	2.31	0.65
2:B:82:LEU:HD13	2:B:84:ILE:HG13	1.80	0.63
2:H:181:GLN:O	2:H:181:GLN:CG	2.32	0.63
2:H:173:VAL:HG22	2:H:191:VAL:HG13	1.80	0.63
2:B:54:TYR:CE2	2:B:106:ILE:HB	2.34	0.62
2:B:63:PRO:HA	2:B:66:LYS:HG3	1.84	0.60
1:A:90:VAL:HG22	1:A:108:LYS:HD3	1.85	0.58
1:L:56:VAL:HG11	1:L:71:GLY:O	2.04	0.58
2:B:55:TRP:HZ3	2:B:106:ILE:HD13	1.68	0.58
1:A:24:ARG:HA	1:A:74:THR:O	2.05	0.57
2:B:31:THR:HG23	2:B:34:MET:HG2	1.85	0.57
2:B:28:SER:O	2:B:31:THR:CG2	2.51	0.57
2:B:54:TYR:HE2	2:B:106:ILE:HB	1.69	0.56
1:A:37:TYR:HB3	2:B:108:THR:HG21	1.86	0.56
1:A:19:ALA:O	1:A:79:LYS:HA	2.06	0.56
1:A:96:GLY:HA3	2:B:108:THR:HG23	1.87	0.56
1:A:108:LYS:HG3	1:A:110:GLU:HG3	1.88	0.56
2:H:6:GLU:OE1	2:H:97:CYS:N	2.39	0.55
1:L:7:THR:HG23	1:L:22:SER:HB2	1.88	0.55
2:H:212:SER:OG	2:H:214:THR:HG23	2.07	0.55
2:H:69:LEU:HD23	2:H:84:ILE:HG12	1.88	0.55
2:B:69:LEU:HD23	2:B:84:ILE:HG12	1.87	0.54
2:B:6:GLU:OE2	2:B:6:GLU:N	2.36	0.54
1:L:90:VAL:HG22	1:L:108:LYS:HD2	1.90	0.54
1:L:91:PHE:CE1	1:L:109:LEU:HG	2.42	0.54
1:A:15:LEU:HD13	1:A:111:LEU:HD21	1.90	0.54
2:H:4:LEU:HD13	2:H:24:PHE:CB	2.38	0.53
1:L:24:ARG:HA	1:L:74:THR:O	2.09	0.53
2:B:33:GLY:HA2	2:B:55:TRP:CZ3	2.44	0.53
1:A:24:ARG:HD3	1:A:74:THR:HG23	1.90	0.52
2:B:18:LEU:HD21	2:B:84:ILE:HD12	1.91	0.52
1:A:64:PRO:HD2	1:A:67:PHE:HD1	1.75	0.51
2:H:82:LEU:HD13	2:H:84:ILE:HG13	1.93	0.51
2:B:6:GLU:HA	2:B:21:THR:O	2.11	0.50
2:H:37:SER:OG	2:H:52:HIS:HD2	1.93	0.50
1:A:156:ASP:HA	1:A:196:SER:HB3	1.94	0.50
2:B:18:LEU:HD23	2:B:84:ILE:HB	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:124:ALA:HB2	2:B:183:ASP:HB3	1.93	0.50
2:B:72:SER:HB2	2:B:81:PHE:HB2	1.94	0.50
1:A:138:VAL:HG11	2:B:134:LEU:HD21	1.92	0.49
2:H:6:GLU:HB2	2:H:117:THR:OG1	2.12	0.49
2:B:18:LEU:CD2	2:B:84:ILE:HB	2.42	0.49
1:L:197:TYR:O	1:L:213:SER:HA	2.13	0.49
2:H:20:LEU:HD12	2:H:82:LEU:HD11	1.95	0.49
2:H:193:VAL:HG21	2:H:203:ILE:HD11	1.95	0.48
1:A:7:THR:HG22	1:A:22:SER:HB2	1.94	0.48
2:B:54:TYR:C	2:B:56:ASP:H	2.17	0.48
1:L:35:ASN:ND2	1:L:35:ASN:H	2.09	0.48
2:B:82:LEU:CD1	2:B:84:ILE:HG13	2.44	0.48
1:L:219:CYS:HB2	2:H:138:CYS:O	2.14	0.47
1:A:138:VAL:HG11	2:B:134:LEU:CD2	2.45	0.47
1:L:15:LEU:HD13	1:L:111:LEU:HD21	1.95	0.47
1:A:141:LEU:HD13	1:A:180:MET:HG2	1.96	0.47
2:B:180:LEU:HD13	2:B:185:TYR:CE1	2.50	0.47
2:B:204:THR:HB	2:B:219:LYS:HA	1.96	0.47
1:A:66:ARG:O	1:A:80:ILE:HA	2.14	0.47
2:B:106:ILE:HG22	2:B:106:ILE:O	2.13	0.47
1:A:150:ASN:O	1:A:201:ALA:HA	2.14	0.47
1:A:64:PRO:HD2	1:A:67:PHE:CD1	2.50	0.47
1:A:39:GLU:O	1:A:93:CYS:HA	2.15	0.47
2:B:198:TRP:HB2	2:B:203:ILE:HD12	1.96	0.46
2:B:42:PRO:HB2	2:B:45:LYS:HD3	1.97	0.46
2:H:33:GLY:O	2:H:106:ILE:HD11	2.16	0.46
2:H:16:GLN:O	2:H:87:VAL:HG22	2.16	0.46
1:L:138:VAL:HG11	2:H:134:LEU:HD21	1.98	0.46
2:B:56:ASP:O	2:B:57:ASP:CB	2.63	0.46
2:H:118:LEU:HD12	4:H:274:HOH:O	2.15	0.46
1:A:160:ARG:HE	1:A:162:ASN:HB2	1.82	0.45
2:H:54:TYR:HD2	2:H:106:ILE:HD12	1.81	0.45
2:H:148:LEU:HG	2:H:220:ILE:HG21	1.98	0.45
1:A:63:VAL:HA	1:A:64:PRO:HD3	1.83	0.45
2:H:134:LEU:HB2	2:H:149:GLY:C	2.37	0.45
2:H:54:TYR:CD2	2:H:106:ILE:HD12	2.52	0.45
1:L:21:ILE:HD12	1:L:78:LEU:HD23	1.99	0.45
2:B:115:GLN:H	2:B:115:GLN:HG3	1.49	0.45
2:B:33:GLY:HA2	2:B:55:TRP:CE3	2.51	0.45
2:H:39:ILE:HD12	2:H:113:TRP:CH2	2.52	0.45
2:B:7:SER:HA	2:B:117:THR:HG21	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:181:GLN:OE1	2:B:186:THR:OG1	2.35	0.45
2:H:33:GLY:C	2:H:106:ILE:HD11	2.37	0.44
1:L:39:GLU:O	1:L:93:CYS:HA	2.16	0.44
1:L:138:VAL:HG11	2:H:134:LEU:CD2	2.48	0.44
1:A:83:VAL:HG13	1:A:87:ASP:HB2	1.99	0.44
2:B:18:LEU:HD23	2:B:87:VAL:CG1	2.48	0.43
2:B:100:SER:OG	2:B:106:ILE:HG23	2.18	0.43
1:A:44:LYS:HE3	1:A:86:GLU:O	2.20	0.42
2:H:2:VAL:HA	2:H:26:GLY:HA3	2.02	0.42
1:L:141:LEU:HD23	1:L:201:ALA:HB2	2.02	0.42
2:B:82:LEU:C	2:B:82:LEU:HD12	2.40	0.42
1:L:155:ILE:HD11	1:L:184:LEU:HD21	2.02	0.42
1:L:37:TYR:HB3	2:H:108:THR:HG21	2.02	0.42
2:B:54:TYR:C	2:B:56:ASP:N	2.73	0.42
2:H:135:ALA:HB3	2:H:223:ARG:HG3	2.02	0.42
1:L:200:GLU:HG2	1:L:211:VAL:HG12	2.02	0.41
1:L:200:GLU:HG2	1:L:211:VAL:CG1	2.51	0.41
2:B:33:GLY:O	2:B:106:ILE:HG12	2.20	0.41
1:A:18:GLN:NE2	1:A:79:LYS:HB3	2.36	0.41
2:B:82:LEU:O	2:B:82:LEU:HD12	2.20	0.41
1:L:29:LEU:HB2	1:L:36:THR:HG23	2.02	0.41
2:B:85:THR:HG23	4:B:238:HOH:O	2.20	0.41
1:A:44:LYS:HB3	1:A:45:PRO:HD2	2.03	0.41
1:A:123:PHE:HE1	1:A:140:PHE:HD2	1.69	0.41
2:B:148:LEU:HB2	2:B:191:VAL:HG23	2.03	0.40
2:B:29:LEU:HD13	2:B:73:LYS:HD2	2.02	0.40
1:L:39:GLU:OE2	2:H:108:THR:HB	2.21	0.40
1:A:219:CYS:HB2	2:B:138:CYS:HB2	1.86	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	217/219 (99%)	208 (96%)	8 (4%)	1 (0%)	29	35
1	L	217/219 (99%)	208 (96%)	9 (4%)	0	100	100
2	B	224/228 (98%)	210 (94%)	14 (6%)	0	100	100
2	H	224/228 (98%)	211 (94%)	11 (5%)	2 (1%)	17	20
All	All	882/894 (99%)	837 (95%)	42 (5%)	3 (0%)	41	50

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	138	CYS
1	A	45	PRO
2	H	104	ILE

### 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	196/196 (100%)	182 (93%)	14 (7%)	14	19
1	L	196/196 (100%)	181 (92%)	15 (8%)	13	16
2	B	197/199 (99%)	173 (88%)	24 (12%)	5	5
2	H	197/199 (99%)	178 (90%)	19 (10%)	8	10
All	All	786/790 (100%)	714 (91%)	72 (9%)	9	11

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	5	THR
1	L	7	THR
1	L	15	LEU
1	L	31	HIS
1	L	35	ASN
1	L	65	ASP
1	L	68	SER
1	L	74	THR

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Mol	Chain	Res	Type
1	L	75	ASP
1	L	165	LEU
1	L	174	LYS
1	L	186	LEU
1	L	207	THR
1	L	211	VAL
1	L	218	GLU
2	H	1	GLN
2	H	6	GLU
2	H	13	GLN
2	H	29	LEU
2	H	31	THR
2	H	72	SER
2	H	75	THR
2	H	82	LEU
2	H	89	THR
2	H	99	ARG
2	H	104	ILE
2	H	117	THR
2	H	118	LEU
2	H	125	LYS
2	H	134	LEU
2	H	181	GLN
2	H	191	VAL
2	H	204	THR
2	H	214	THR
1	A	13	VAL
1	A	15	LEU
1	A	31	HIS
1	A	61	SER
1	A	74	THR
1	A	75	ASP
1	A	109	LEU
1	A	174	LYS
1	A	186	LEU
1	A	210	ILE
1	A	211	VAL
1	A	213	SER
1	A	217	ASN
1	A	218	GLU
2	B	6	GLU
2	B	18	LEU

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Mol	Chain	Res	Type
2	B	29	LEU
2	B	31	THR
2	B	32	SER
2	B	56	ASP
2	B	65	LEU
2	B	75	THR
2	B	82	LEU
2	B	89	THR
2	B	99	ARG
2	B	115	GLN
2	B	117	THR
2	B	125	LYS
2	B	134	LEU
2	B	138	CYS
2	B	140	ASP
2	B	187	LEU
2	B	191	VAL
2	B	195	SER
2	B	200	SER
2	B	204	THR
2	B	214	THR
2	B	221	GLU

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

Mol	Chain	Res	Type
1	L	35	ASN
2	H	13	GLN
2	H	52	HIS
2	H	78	ASN
2	H	181	GLN
2	H	201	GLN
1	A	18	GLN
2	B	52	HIS
2	B	78	ASN

### 5.3.3 RNA ⓘ

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](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	ACT	H	1001	-	1,3,3	1.79	0	0,3,3	0.00	-
3	ACT	B	1002	-	1,3,3	1.72	0	0,3,3	0.00	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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	219/219 (100%)	0.03	8 (3%) 41 48	29, 50, 80, 98	0
1	L	219/219 (100%)	0.04	9 (4%) 37 44	29, 49, 83, 100	0
2	B	226/228 (99%)	0.19	14 (6%) 20 26	28, 46, 82, 113	0
2	H	226/228 (99%)	0.11	12 (5%) 26 33	30, 45, 80, 117	0
All	All	890/894 (99%)	0.09	43 (4%) 30 37	28, 47, 83, 117	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	105	VAL	7.9
2	H	105	VAL	7.6
2	H	142	THR	6.9
2	B	103	SER	5.9
2	H	106	ILE	5.7
2	H	103	SER	5.7
1	A	219	CYS	5.2
2	B	106	ILE	5.1
2	B	104	ILE	4.5
1	L	34	GLY	4.4
2	B	107	ALA	4.0
1	L	219	CYS	4.0
2	H	140	ASP	4.0
1	A	29	LEU	3.9
2	H	141	THR	3.9
2	B	138	CYS	3.8
1	L	217	ASN	3.7
2	H	104	ILE	3.5
2	B	141	THR	3.3
1	L	32	SER	3.3
2	B	139	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
2	B	145	SER	3.2
2	B	142	THR	3.2
2	H	107	ALA	3.1
2	B	32	SER	2.9
1	A	71	GLY	2.9
2	B	226	THR	2.8
2	B	1	GLN	2.8
2	H	1	GLN	2.8
1	A	32	SER	2.7
1	A	217	ASN	2.6
2	B	197	THR	2.6
2	H	226	THR	2.6
1	A	65	ASP	2.6
2	H	197	THR	2.5
1	A	45	PRO	2.4
1	L	25	SER	2.3
1	L	65	ASP	2.2
2	H	44	GLY	2.1
1	L	18	GLN	2.1
1	L	31	HIS	2.0
1	A	98	ARG	2.0
1	L	33	ASN	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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	ACT	B	1002	4/4	0.82	0.26	45,47,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	ACT	H	1001	4/4	0.86	0.25	34,43,44,45	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.