



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:18 AM GMT

PDB ID : 3AAZ  
Title : Crystal structure of the humanized recombinant Fab fragment of a murine;  
antibody  
Authors : Streltsov, V.A.  
Deposited on : 2009-11-28  
Resolution : 2.20 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

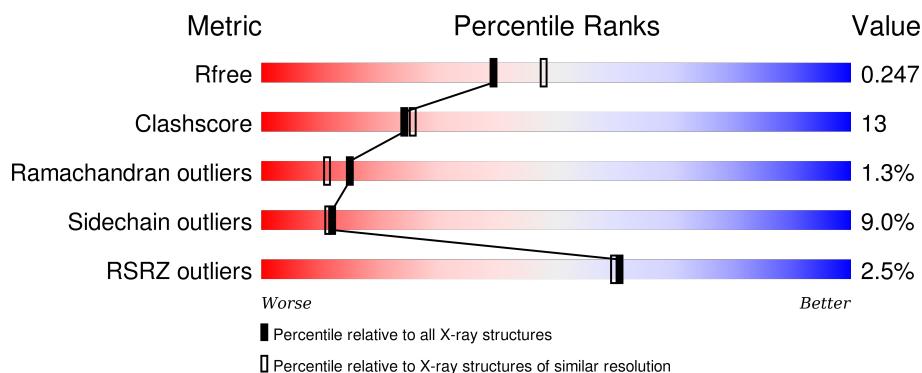
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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	229	<div> <div>5%</div> <div> <div></div> <div>72%</div> <div>21%</div> <div>5%</div> </div> </div>
1	H	229	<div> <div>4%</div> <div> <div></div> <div>62%</div> <div>31%</div> <div>7%</div> </div> </div>
2	B	229	<div> <div>%</div> <div> <div></div> <div>74%</div> <div>22%</div> <div>.</div> </div> </div>
2	L	229	<div> <div></div> <div> <div></div> <div>78%</div> <div>18%</div> <div>.</div> </div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7401 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 Humanized recombinant Fab fragment of a murine; antibody.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	228	Total	C	N	O	S	0	0	0
			1747	1106	296	338	7			
1	H	229	Total	C	N	O	S	0	0	0
			1751	1108	297	339	7			

- Molecule 2 is a protein called Humanized recombinant Fab fragment of a murine; antibody.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	229	Total	C	N	O	S	0	0	0
			1764	1105	295	358	6			
2	L	228	Total	C	N	O	S	0	0	0
			1756	1101	294	355	6			

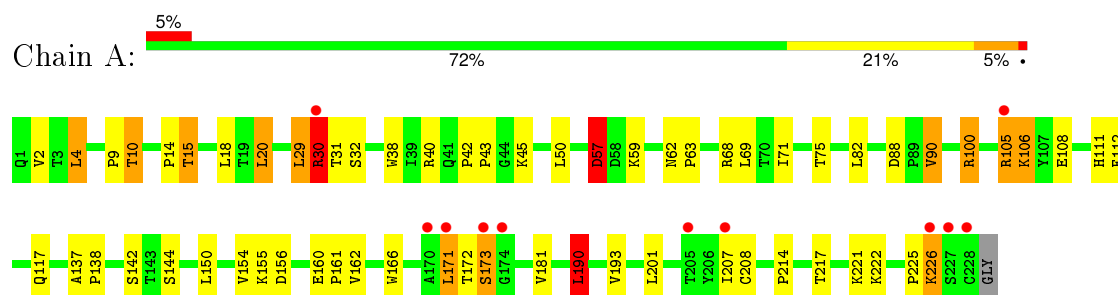
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	105	Total	O	0	0
			105	105		
3	B	77	Total	O	0	0
			77	77		
3	H	125	Total	O	0	0
			125	125		
3	L	76	Total	O	0	0
			76	76		

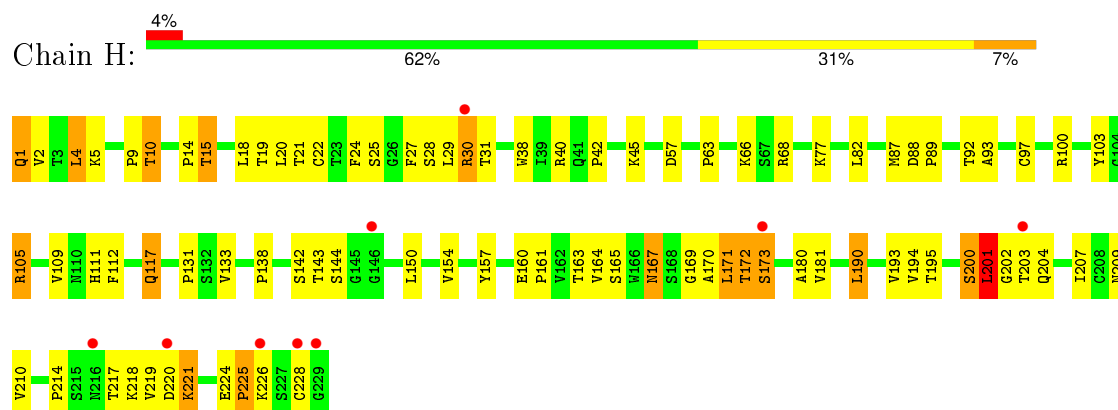
### 3 Residue-property plots

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.

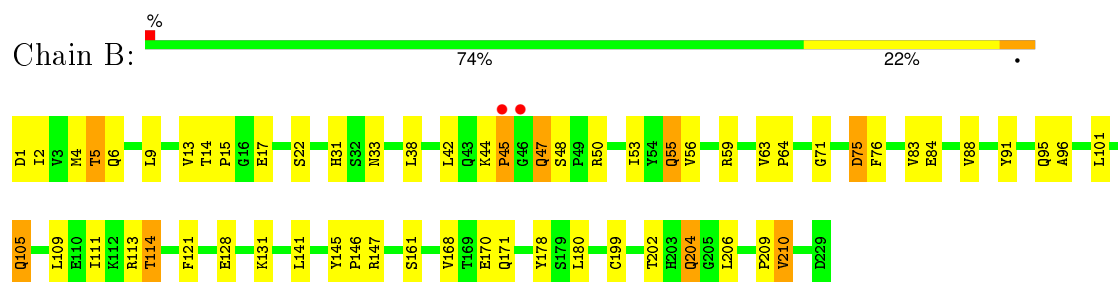
- Molecule 1: Humanized recombinant Fab fragment of a murine; antibody



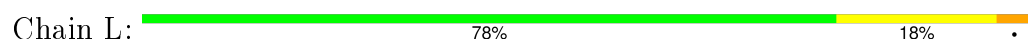
- Molecule 1: Humanized recombinant Fab fragment of a murine; antibody

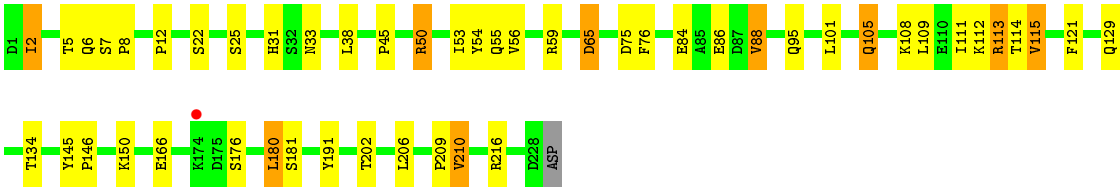


- Molecule 2: Humanized recombinant Fab fragment of a murine; antibody



- Molecule 2: Humanized recombinant Fab fragment of a murine; antibody





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	106.73 Å   106.73 Å   90.87 Å 90.00°   90.00°   120.00°	Depositor
Resolution (Å)	46.03 – 2.20 46.02 – 2.20	Depositor EDS
% Data completeness (in resolution range)	92.5 (46.03-2.20) 92.6 (46.02-2.20)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.57 (at 2.20 Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.209 , 0.271 0.218 , 0.247	Depositor DCC
$R_{free}$ test set	2734 reflections (5.30%)	DCC
Wilson B-factor (Å <sup>2</sup> )	47.0	Xtriage
Anisotropy	0.225	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 14.9	EDS
Estimated twinning fraction	0.033 for -h,-k,l 0.477 for h,-h-k,-l 0.034 for -k,-h,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 54407 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7401	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.27% 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 [i](#)

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

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	0.80	0/1792	0.90	7/2445 (0.3%)
1	H	0.84	1/1796 (0.1%)	0.90	7/2450 (0.3%)
2	B	0.72	1/1803 (0.1%)	0.75	0/2450
2	L	0.72	0/1795	0.76	0/2439
All	All	0.77	2/7186 (0.0%)	0.83	14/9784 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	97	CYS	CB-SG	-7.30	1.69	1.82
2	B	199	CYS	CB-SG	-5.16	1.73	1.81

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	40	ARG	NE-CZ-NH2	-8.83	115.88	120.30
1	H	201	LEU	CA-CB-CG	6.67	130.65	115.30
1	A	4	LEU	CA-CB-CG	6.55	130.37	115.30
1	H	4	LEU	CA-CB-CG	6.10	129.33	115.30
1	H	29	LEU	CA-CB-CG	5.88	128.83	115.30
1	H	68	ARG	NE-CZ-NH2	-5.83	117.38	120.30
1	H	201	LEU	N-CA-C	-5.83	95.26	111.00
1	A	190	LEU	CA-CB-CG	5.62	128.24	115.30
1	H	68	ARG	NE-CZ-NH1	5.59	123.10	120.30
1	A	29	LEU	CA-CB-CG	5.52	128.00	115.30
1	A	100	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	A	171	LEU	CA-CB-CG	-5.25	103.22	115.30
1	A	106	LYS	N-CA-C	-5.09	97.26	111.00
1	A	40	ARG	NE-CZ-NH2	-5.06	117.77	120.30

There are no chirality outliers.

There are no planarity outliers.

## 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	1747	0	1735	44	0
1	H	1751	0	1739	54	0
2	B	1764	0	1707	44	0
2	L	1756	0	1704	41	0
3	A	105	0	0	6	0
3	B	77	0	0	5	0
3	H	125	0	0	8	0
3	L	76	0	0	7	0
All	All	7401	0	6885	181	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 13.

All (181) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:105:ARG:HG3	1:H:105:ARG:HH21	1.00	1.10
1:A:105:ARG:HG3	1:A:105:ARG:HH21	1.10	1.09
1:A:29:LEU:O	1:A:30:ARG:HB2	1.52	1.07
2:B:105:GLN:NE2	2:B:105:GLN:H	1.64	0.96
2:L:31:HIS:HD2	2:L:33:ASN:H	1.18	0.90
1:H:105:ARG:HG3	1:H:105:ARG:NH2	1.82	0.89
2:B:105:GLN:HE21	2:B:105:GLN:H	0.93	0.89
1:A:14:PRO:O	1:A:15:THR:HB	1.70	0.89
1:A:105:ARG:NH2	1:A:105:ARG:HG3	1.85	0.88
3:A:235:HOH:O	1:H:15:THR:HG21	1.75	0.86
1:H:209:ASN:HA	3:H:303:HOH:O	1.74	0.86
1:H:105:ARG:HH21	1:H:105:ARG:CG	1.85	0.85
2:B:31:HIS:HD2	2:B:33:ASN:H	1.24	0.83
2:B:31:HIS:CD2	2:B:33:ASN:H	1.99	0.80
1:A:59:LYS:HE3	1:A:71:ILE:O	1.81	0.80
1:A:208:CYS:HA	3:A:286:HOH:O	1.82	0.78
2:L:113:ARG:HD3	2:L:114:THR:O	1.84	0.77
1:A:15:THR:HG21	3:H:266:HOH:O	1.85	0.77
1:H:14:PRO:O	1:H:15:THR:HB	1.84	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:31:HIS:CD2	2:L:33:ASN:H	2.03	0.76
2:B:105:GLN:N	2:B:105:GLN:HE21	1.78	0.76
1:A:30:ARG:HG2	1:A:75:THR:HB	1.68	0.74
2:B:1:ASP:HB2	3:B:293:HOH:O	1.88	0.73
2:L:105:GLN:H	2:L:105:GLN:HE21	1.35	0.73
1:A:154:VAL:HB	1:A:190:LEU:HD22	1.71	0.73
1:H:160:GLU:HG3	1:H:161:PRO:HA	1.70	0.72
2:L:2:ILE:HG22	3:L:240:HOH:O	1.90	0.71
1:H:167:ASN:HB2	1:H:171:LEU:HG	1.71	0.71
1:A:88:ASP:OD1	1:A:90:VAL:HG12	1.89	0.71
1:A:138:PRO:HB2	1:A:201:LEU:HD11	1.73	0.71
1:H:103:TYR:HB2	1:H:109:VAL:HG22	1.72	0.70
2:B:45:PRO:HB3	2:B:170:GLU:HG3	1.73	0.70
2:L:105:GLN:H	2:L:105:GLN:NE2	1.90	0.70
1:A:166:TRP:CE3	3:A:286:HOH:O	2.44	0.69
1:A:105:ARG:CG	1:A:105:ARG:HH21	1.99	0.67
2:L:6:GLN:H	2:L:105:GLN:HE22	1.42	0.67
1:A:111:HIS:HE1	3:B:230:HOH:O	1.78	0.67
1:H:88:ASP:OD2	1:H:89:PRO:HD2	1.95	0.67
1:H:172:THR:OG1	1:H:173:SER:N	2.26	0.67
1:A:111:HIS:HD2	1:A:112:PHE:O	1.78	0.66
1:A:105:ARG:HD3	1:A:106:LYS:NZ	2.11	0.66
1:H:133:VAL:HG21	1:H:210:VAL:HG21	1.78	0.65
1:A:43:PRO:HD2	3:A:231:HOH:O	1.96	0.64
1:H:111:HIS:HD2	1:H:112:PHE:O	1.81	0.62
1:H:10:THR:HG21	1:H:214:PRO:HG3	1.81	0.62
2:L:55:GLN:O	2:L:56:VAL:HB	2.00	0.62
1:H:103:TYR:HB2	1:H:109:VAL:CG2	2.30	0.61
2:L:112:LYS:HD2	2:L:145:TYR:OH	2.00	0.61
1:H:200:SER:O	1:H:201:LEU:HG	2.02	0.60
2:B:38:LEU:HD22	2:B:76:PHE:CG	2.38	0.59
2:L:6:GLN:H	2:L:105:GLN:NE2	1.99	0.59
2:L:88:VAL:HG22	2:L:109:LEU:O	2.02	0.59
2:L:101:LEU:HD23	2:L:101:LEU:N	2.16	0.58
2:B:53:ILE:HD13	2:B:59:ARG:HA	1.85	0.58
2:B:202:THR:HG22	2:B:209:PRO:HG3	1.84	0.58
1:A:30:ARG:HG2	1:A:75:THR:CB	2.34	0.58
2:B:6:GLN:H	2:B:105:GLN:NE2	2.02	0.57
2:B:42:LEU:HD13	2:B:91:TYR:CZ	2.39	0.57
2:L:150:LYS:HB3	2:L:202:THR:OG1	2.03	0.57
1:H:24:PHE:CD2	1:H:27:PHE:CZ	2.92	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:206:LEU:HD13	2:L:210:VAL:HG12	1.87	0.56
1:A:106:LYS:O	1:A:108:GLU:OE2	2.24	0.56
2:L:53:ILE:HD13	2:L:59:ARG:HA	1.87	0.56
2:L:166:GLU:HA	2:L:181:SER:O	2.06	0.56
2:B:180:LEU:C	2:B:180:LEU:HD23	2.26	0.56
1:H:5:LYS:HA	1:H:117:GLN:HE22	1.71	0.56
1:H:221:LYS:HD2	3:H:231:HOH:O	2.06	0.55
1:H:42:PRO:HB2	1:H:45:LYS:HG3	1.88	0.55
1:H:160:GLU:HG3	1:H:161:PRO:CA	2.37	0.55
2:B:171:GLN:HG3	2:B:178:TYR:CZ	2.42	0.55
1:A:160:GLU:HG3	1:A:161:PRO:HA	1.88	0.54
1:A:10:THR:HG21	1:A:214:PRO:HG3	1.89	0.54
1:H:117:GLN:NE2	1:H:117:GLN:H	2.06	0.54
1:H:24:PHE:CD2	1:H:27:PHE:HZ	2.26	0.54
2:B:204:GLN:HG2	2:B:204:GLN:O	2.07	0.54
1:H:142:SER:C	2:L:121:PHE:HD1	2.11	0.53
1:A:42:PRO:HD2	1:A:45:LYS:HB2	1.90	0.53
1:H:14:PRO:O	1:H:15:THR:CB	2.56	0.53
1:H:154:VAL:HB	1:H:190:LEU:HD23	1.90	0.53
2:B:147:ARG:CZ	2:B:168:VAL:HG21	2.39	0.53
2:L:84:GLU:HG2	3:L:285:HOH:O	2.08	0.53
1:A:201:LEU:C	1:A:201:LEU:HD23	2.29	0.52
2:B:1:ASP:CB	3:B:293:HOH:O	2.54	0.52
1:H:221:LYS:HB2	3:H:231:HOH:O	2.10	0.52
2:B:147:ARG:NH2	2:B:168:VAL:HG21	2.25	0.52
2:L:6:GLN:HA	2:L:22:SER:O	2.10	0.52
2:L:180:LEU:C	2:L:180:LEU:HD23	2.31	0.52
2:L:2:ILE:HD11	2:L:25:SER:HB2	1.91	0.51
2:B:128:GLU:O	2:B:131:LYS:HB3	2.10	0.51
2:L:54:TYR:HD1	2:L:55:GLN:HG2	1.76	0.51
1:A:117:GLN:HG2	3:A:236:HOH:O	2.10	0.51
1:A:105:ARG:HD3	1:A:106:LYS:HZ2	1.75	0.51
1:A:105:ARG:HD3	1:A:106:LYS:HZ3	1.76	0.51
2:L:113:ARG:CD	2:L:114:THR:O	2.55	0.51
1:A:138:PRO:HG2	1:A:225:PRO:HB3	1.93	0.51
2:B:6:GLN:H	2:B:105:GLN:HE22	1.59	0.50
2:B:6:GLN:HA	2:B:22:SER:O	2.12	0.50
1:H:138:PRO:HD3	1:H:150:LEU:CB	2.41	0.50
1:H:220:ASP:HA	3:H:303:HOH:O	2.12	0.50
2:L:65:ASP:OD2	2:L:65:ASP:N	2.38	0.49
2:B:206:LEU:HD13	2:B:210:VAL:CG1	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:13:VAL:HG11	2:B:83:VAL:HG21	1.94	0.49
2:B:50:ARG:HB3	2:B:50:ARG:HH21	1.76	0.49
1:A:172:THR:HG23	1:A:173:SER:H	1.76	0.49
1:H:170:ALA:HA	1:H:172:THR:HG22	1.95	0.49
1:H:154:VAL:HB	1:H:190:LEU:CD2	2.43	0.49
1:A:190:LEU:C	1:A:190:LEU:HD23	2.33	0.49
2:B:145:TYR:CD1	2:B:146:PRO:HA	2.48	0.49
1:H:202:GLY:H	1:H:204:GLN:HE21	1.61	0.49
1:H:38:TRP:CD1	1:H:82:LEU:HB2	2.48	0.48
1:H:63:PRO:HB2	3:H:251:HOH:O	2.14	0.48
2:B:202:THR:HG23	3:B:295:HOH:O	2.13	0.48
1:A:31:THR:CG2	1:A:31:THR:O	2.61	0.48
1:A:207:ILE:HG22	1:A:222:LYS:HA	1.96	0.48
1:A:155:LYS:HE3	1:A:156:ASP:OD1	2.14	0.48
2:B:14:THR:O	2:B:17:GLU:HB2	2.14	0.48
2:L:129:GLN:HB2	3:L:295:HOH:O	2.14	0.48
2:L:38:LEU:HD22	2:L:76:PHE:CG	2.49	0.47
1:A:142:SER:C	2:B:121:PHE:HD1	2.17	0.47
1:H:171:LEU:N	3:H:334:HOH:O	2.39	0.47
1:H:138:PRO:HD3	1:H:150:LEU:HB3	1.96	0.47
2:L:191:TYR:CZ	2:L:216:ARG:HG3	2.48	0.47
1:H:31:THR:O	1:H:31:THR:HG22	2.13	0.47
1:H:217:THR:HG22	1:H:219:VAL:HG23	1.96	0.47
2:B:113:ARG:HD3	2:B:114:THR:O	2.14	0.47
1:H:167:ASN:HB2	1:H:171:LEU:CG	2.40	0.47
1:A:57:ASP:OD1	1:A:59:LYS:NZ	2.48	0.47
2:B:44:LYS:HA	2:B:45:PRO:HD2	1.50	0.47
1:H:9:PRO:HG2	3:H:269:HOH:O	2.15	0.47
2:B:141:LEU:N	2:B:141:LEU:HD12	2.30	0.47
1:A:29:LEU:O	1:A:30:ARG:CB	2.38	0.47
2:L:202:THR:HG22	2:L:209:PRO:HG3	1.98	0.46
1:H:100:ARG:HA	1:H:112:PHE:HA	1.96	0.46
2:B:15:PRO:HG3	2:B:111:ILE:HG23	1.97	0.46
2:B:55:GLN:O	2:B:56:VAL:HB	2.16	0.46
1:H:42:PRO:HD2	1:H:45:LYS:HB2	1.98	0.46
2:B:71:GLY:HA3	2:B:75:ASP:O	2.14	0.46
2:L:12:PRO:HB2	2:L:112:LYS:HD3	1.97	0.46
2:B:96:ALA:HA	2:B:101:LEU:HD22	1.98	0.46
2:L:145:TYR:CD1	2:L:146:PRO:HA	2.51	0.45
2:L:2:ILE:HD12	2:L:95:GLN:HG2	1.99	0.45
1:H:180:ALA:HA	1:H:190:LEU:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:GLU:HG3	1:A:161:PRO:CA	2.47	0.45
1:H:143:THR:HG22	1:H:144:SER:N	2.31	0.45
2:B:6:GLN:N	2:B:105:GLN:HE22	2.14	0.45
1:H:1:GLN:H3	1:H:1:GLN:HE21	1.64	0.45
1:A:10:THR:HG21	1:A:214:PRO:HB3	1.98	0.44
2:B:5:THR:HA	2:B:105:GLN:HE22	1.81	0.44
1:A:9:PRO:HG2	3:A:333:HOH:O	2.16	0.44
2:L:50:ARG:HB3	2:L:50:ARG:HH21	1.82	0.44
2:B:2:ILE:O	2:B:2:ILE:HG13	2.16	0.44
1:A:18:LEU:HD11	1:A:20:LEU:HD13	1.99	0.44
2:B:105:GLN:N	2:B:105:GLN:NE2	2.48	0.43
1:A:100:ARG:HA	1:A:112:PHE:HA	1.98	0.43
2:B:63:VAL:HA	2:B:64:PRO:HD3	1.82	0.43
2:B:59:ARG:HD3	2:B:63:VAL:O	2.19	0.43
1:A:62:ASN:HA	1:A:63:PRO:HD2	1.89	0.43
2:L:2:ILE:HD11	2:L:25:SER:CB	2.49	0.43
2:L:113:ARG:O	3:L:279:HOH:O	2.22	0.43
1:H:164:VAL:HA	1:H:209:ASN:O	2.18	0.42
1:H:111:HIS:HE1	3:L:273:HOH:O	2.01	0.42
2:B:4:MET:CE	2:B:95:GLN:HB3	2.48	0.42
1:H:92:THR:O	1:H:93:ALA:HB2	2.20	0.42
1:H:165:SER:HB2	1:H:169:GLY:HA2	2.00	0.42
1:H:131:PRO:HB3	1:H:157:TYR:HB3	2.02	0.42
1:H:21:THR:HG22	1:H:22:CYS:N	2.33	0.42
2:L:86:GLU:HB2	3:L:248:HOH:O	2.19	0.42
1:H:18:LEU:HD22	1:H:87:MET:CE	2.50	0.42
2:L:115:VAL:HG13	3:L:278:HOH:O	2.19	0.42
1:H:150:LEU:O	1:H:194:VAL:HG12	2.20	0.41
1:A:137:ALA:HA	1:A:138:PRO:HD2	1.88	0.41
2:L:112:LYS:HA	2:L:145:TYR:OH	2.21	0.41
2:B:47:GLN:HG3	2:B:48:SER:N	2.35	0.41
1:A:69:LEU:HD22	1:A:82:LEU:HD11	2.03	0.41
2:L:7:SER:HA	2:L:8:PRO:HA	1.75	0.41
3:B:293:HOH:O	2:L:8:PRO:HB2	2.21	0.41
2:B:88:VAL:HG23	2:B:109:LEU:O	2.21	0.40
1:H:224:GLU:HB3	1:H:225:PRO:CD	2.51	0.40
2:L:50:ARG:HB3	2:L:50:ARG:NH2	2.37	0.40
1:A:38:TRP:O	1:A:50:LEU:HB2	2.22	0.40
2:L:111:ILE:HG21	2:L:176:SER:OG	2.20	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	226/229 (99%)	208 (92%)	14 (6%)	4 (2%)	11	7
1	H	227/229 (99%)	209 (92%)	12 (5%)	6 (3%)	7	3
2	B	227/229 (99%)	214 (94%)	12 (5%)	1 (0%)	39	42
2	L	226/229 (99%)	219 (97%)	6 (3%)	1 (0%)	39	42
All	All	906/916 (99%)	850 (94%)	44 (5%)	12 (1%)	15	11

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	173	SER
1	H	201	LEU
1	A	30	ARG
1	H	66	LYS
1	H	173	SER
1	H	225	PRO
1	H	228	CYS
1	A	57	ASP
2	B	45	PRO
1	A	226	LYS
1	H	30	ARG
2	L	45	PRO

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	202/202 (100%)	181 (90%)	21 (10%)	9	8
1	H	202/202 (100%)	174 (86%)	28 (14%)	4	3
2	B	202/202 (100%)	191 (95%)	11 (5%)	27	31
2	L	201/202 (100%)	188 (94%)	13 (6%)	21	23
All	All	807/808 (100%)	734 (91%)	73 (9%)	12	11

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	VAL
1	A	4	LEU
1	A	10	THR
1	A	15	THR
1	A	20	LEU
1	A	30	ARG
1	A	32	SER
1	A	57	ASP
1	A	68	ARG
1	A	90	VAL
1	A	105	ARG
1	A	144	SER
1	A	150	LEU
1	A	162	VAL
1	A	171	LEU
1	A	181	VAL
1	A	190	LEU
1	A	193	VAL
1	A	217	THR
1	A	221	LYS
1	A	226	LYS
2	B	5	THR
2	B	9	LEU
2	B	47	GLN
2	B	55	GLN
2	B	75	ASP
2	B	84	GLU
2	B	105	GLN
2	B	114	THR
2	B	161	SER
2	B	204	GLN
2	B	210	VAL
1	H	1	GLN

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Mol	Chain	Res	Type
1	H	2	VAL
1	H	4	LEU
1	H	10	THR
1	H	15	THR
1	H	19	THR
1	H	20	LEU
1	H	25	SER
1	H	28	SER
1	H	30	ARG
1	H	57	ASP
1	H	77	LYS
1	H	105	ARG
1	H	117	GLN
1	H	163	THR
1	H	167	ASN
1	H	171	LEU
1	H	172	THR
1	H	181	VAL
1	H	190	LEU
1	H	193	VAL
1	H	195	THR
1	H	200	SER
1	H	203	THR
1	H	207	ILE
1	H	218	LYS
1	H	221	LYS
1	H	226	LYS
2	L	2	ILE
2	L	5	THR
2	L	50	ARG
2	L	65	ASP
2	L	75	ASP
2	L	88	VAL
2	L	105	GLN
2	L	108	LYS
2	L	113	ARG
2	L	115	VAL
2	L	134	THR
2	L	180	LEU
2	L	210	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	79	GLN
1	A	111	HIS
1	A	204	GLN
2	B	31	HIS
2	B	35	HIS
2	B	105	GLN
2	B	204	GLN
1	H	1	GLN
1	H	79	GLN
1	H	111	HIS
1	H	117	GLN
1	H	167	ASN
1	H	204	GLN
2	L	31	HIS
2	L	105	GLN
2	L	142	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

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	228/229 (99%)	0.01	11 (4%) 34 34	17, 27, 37, 44	0
1	H	229/229 (100%)	-0.02	9 (3%) 43 42	16, 25, 36, 45	0
2	B	229/229 (100%)	-0.15	2 (0%) 85 85	13, 30, 36, 42	0
2	L	228/229 (99%)	-0.14	1 (0%) 93 93	14, 29, 38, 43	0
All	All	914/916 (99%)	-0.08	23 (2%) 61 60	13, 28, 37, 45	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	171	LEU	5.6
2	B	46	GLY	5.0
1	A	170	ALA	4.8
1	A	173	SER	4.8
1	H	228	CYS	4.3
1	A	227	SER	3.9
1	A	228	CYS	3.9
1	A	105	ARG	3.0
1	H	229	GLY	2.9
1	A	207	ILE	2.9
1	A	174	GLY	2.8
1	A	205	THR	2.7
1	H	203	THR	2.7
2	B	45	PRO	2.6
1	H	173	SER	2.5
1	A	226	LYS	2.4
1	H	216	ASN	2.2
1	H	220	ASP	2.2
1	A	30	ARG	2.2
1	H	30	ARG	2.1
1	H	146	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
1	H	226	LYS	2.0
2	L	174	LYS	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.