



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 06:50 pm BST

PDB ID : 3GJE
Title : Rational development of high-affinity T-cell receptor-like antibodies
Authors : Stewart-Jones, G.; Wadle, A.; Hombach, A.; Shenderov, E.; Held, G.; Fischer, E.; Kleber, S.; Stenner-Liewen, F.; Bauer, S.; McMichael, A.; Knuth, A.; Abken, H.; Hombach, A.A.; Cerundolo, V.; Jones, E.Y.; Renner, C.
Deposited on : 2009-03-08
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
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

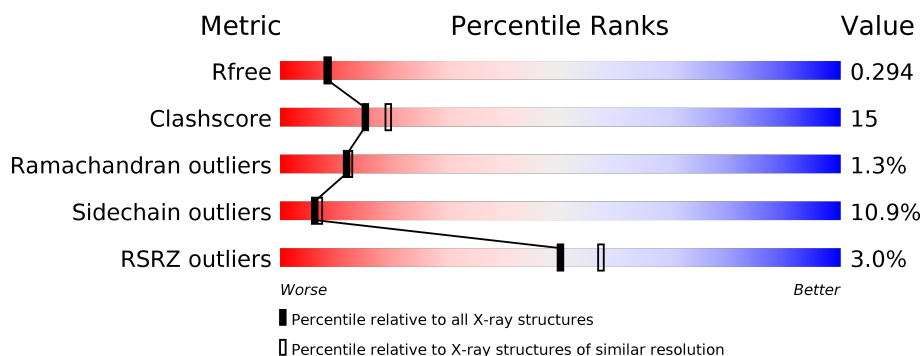
1 Overall quality at a glance

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 ≥ 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	212	<div> <div>%</div> <div> <div></div> <div>73%</div> <div>20%</div> <div>7%</div> </div> </div>
1	L	212	<div> <div>%</div> <div> <div></div> <div>75%</div> <div>21%</div> <div>•</div> </div> </div>
2	B	220	<div> <div>5%</div> <div> <div></div> <div>65%</div> <div>29%</div> <div>5%</div> <div>•</div> </div> </div>
2	H	220	<div> <div>5%</div> <div> <div></div> <div>70%</div> <div>25%</div> <div>•</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6813 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 Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	212	Total	C	N	O	S	0	0	0
			1600	1001	269	326	4			
1	A	212	Total	C	N	O	S	0	0	0
			1600	1001	269	326	4			

- Molecule 2 is a protein called Fab Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	220	Total	C	N	O	S	0	0	0
			1621	1020	269	325	7			
2	B	220	Total	C	N	O	S	0	0	0
			1621	1020	269	325	7			

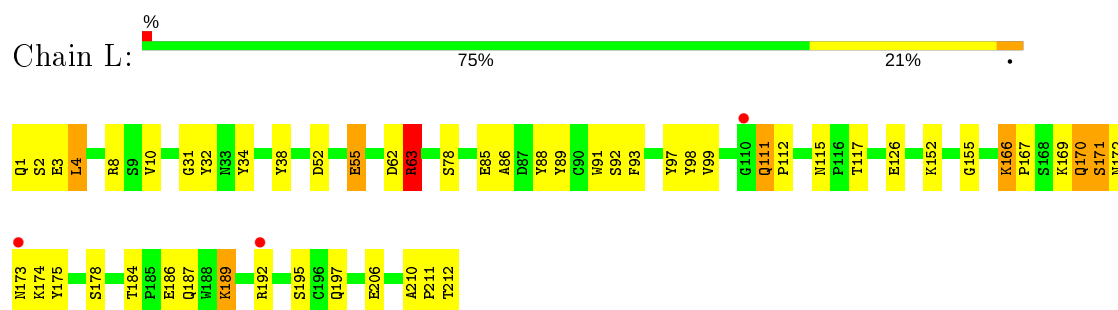
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	L	82	Total	O	0	0
			82	82		
3	H	95	Total	O	0	0
			95	95		
3	A	94	Total	O	0	0
			94	94		
3	B	100	Total	O	0	0
			100	100		

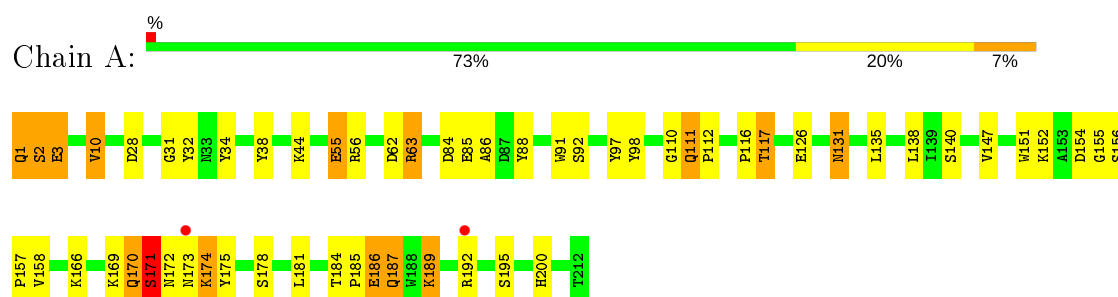
3 Residue-property plots [i](#)

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.

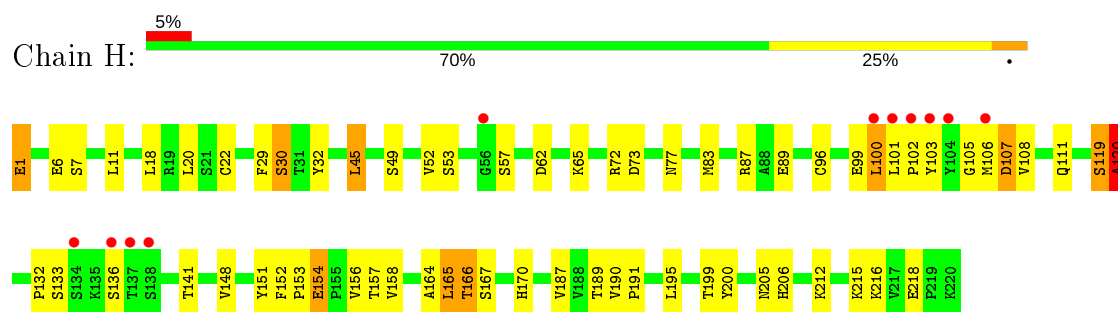
• Molecule 1: Fab Light Chain



• Molecule 1: Fab Light Chain

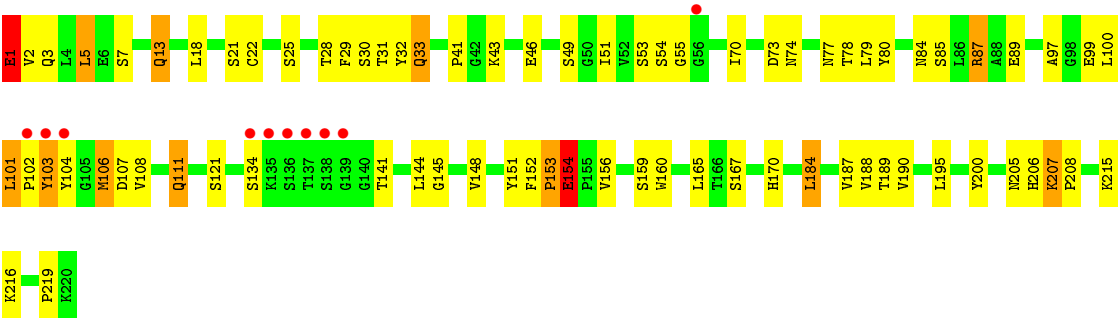


• Molecule 2: Fab Heavy Chain



• Molecule 2: Fab Heavy Chain





4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α , β , γ	117.06 Å 117.06 Å 78.80 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.30 30.02 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.0 (25.00-2.30) 99.0 (30.02-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.85 (at 2.31 Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.222 , 0.302 0.215 , 0.294	Depositor DCC
R_{free} test set	2363 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	45.6	Xtriage
Anisotropy	0.267	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 26.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.488 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6813	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.79% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² 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

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	0.97	1/1641 (0.1%)	0.96	3/2240 (0.1%)
1	L	0.97	1/1641 (0.1%)	0.90	1/2240 (0.0%)
2	B	1.04	2/1658 (0.1%)	0.93	4/2257 (0.2%)
2	H	1.08	5/1658 (0.3%)	1.05	7/2257 (0.3%)
All	All	1.02	9/6598 (0.1%)	0.96	15/8994 (0.2%)

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
1	L	0	1
2	B	0	2
2	H	0	5
All	All	0	9

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	96	CYS	CB-SG	-9.50	1.66	1.82
2	H	1	GLU	CD-OE2	9.32	1.35	1.25
2	B	1	GLU	CD-OE2	8.79	1.35	1.25
2	H	120	ALA	N-CA	6.05	1.58	1.46
1	L	10	VAL	CA-CB	5.61	1.66	1.54
2	B	46	GLU	CG-CD	5.38	1.60	1.51
1	A	10	VAL	CA-CB	5.28	1.65	1.54
2	H	154	GLU	CD-OE1	5.21	1.31	1.25
2	H	22	CYS	CB-SG	-5.16	1.73	1.81

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	120	ALA	N-CA-C	-12.88	76.22	111.00
1	A	63	ARG	NE-CZ-NH2	-10.62	114.99	120.30
1	A	63	ARG	NE-CZ-NH1	7.54	124.07	120.30
2	H	119	SER	C-N-CA	6.56	138.09	121.70
2	B	152	PHE	N-CA-CB	-6.28	99.29	110.60
2	H	152	PHE	N-CA-CB	-6.08	99.66	110.60
2	B	154	GLU	N-CA-C	6.08	127.41	111.00
1	L	63	ARG	NE-CZ-NH2	-5.82	117.39	120.30
2	H	120	ALA	C-N-CA	5.75	136.06	121.70
1	A	3	GLU	N-CA-C	5.48	125.80	111.00
2	B	18	LEU	CA-CB-CG	5.42	127.76	115.30
2	H	154	GLU	N-CA-C	5.16	124.92	111.00
2	B	184	LEU	CA-CB-CG	5.16	127.16	115.30
2	H	18	LEU	CA-CB-CG	5.15	127.14	115.30
2	H	96	CYS	CA-CB-SG	-5.01	104.97	114.00

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	2	SER	Peptide
2	B	151	TYR	Peptide
2	B	153	PRO	Peptide
2	H	107	ASP	Peptide
2	H	119	SER	Peptide
2	H	151	TYR	Peptide
2	H	153	PRO	Peptide
2	H	72	ARG	Peptide
1	L	155	GLY	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	1600	0	1534	46	0
1	L	1600	0	1534	49	0
2	B	1621	0	1592	60	0
2	H	1621	0	1592	49	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	94	0	0	7	0
3	B	100	0	0	12	0
3	H	95	0	0	6	0
3	L	82	0	0	3	0
All	All	6813	0	6252	190	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 15.

All (190) 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:A:126:GLU:HB2	3:A:351:HOH:O	1.41	1.20
1:L:63:ARG:HH11	1:L:63:ARG:HG2	1.12	1.10
1:L:63:ARG:HD3	1:L:78:SER:O	1.51	1.06
1:L:211:PRO:O	1:L:212:THR:HG23	1.59	1.02
2:H:20:LEU:HG	2:H:83:MET:HE2	1.45	0.95
1:L:169:LYS:HG3	1:L:173:ASN:HA	1.47	0.94
1:L:166:LYS:HD2	1:L:167:PRO:HD2	1.50	0.92
1:L:63:ARG:NH1	1:L:63:ARG:HG2	1.83	0.91
2:B:32:TYR:CE1	2:B:100:LEU:HD13	2.06	0.90
1:A:169:LYS:CG	1:A:173:ASN:HA	2.01	0.90
2:B:87:ARG:HG3	2:B:89:GLU:OE1	1.73	0.88
2:H:99:GLU:HB2	2:H:105:GLY:O	1.76	0.86
2:H:191:PRO:HD3	2:B:5:LEU:HD12	1.60	0.83
2:B:32:TYR:CD1	2:B:100:LEU:CD1	2.62	0.83
1:L:169:LYS:CG	1:L:173:ASN:HA	2.08	0.82
2:B:30:SER:HB3	2:B:74:ASN:HB3	1.62	0.81
1:L:2:SER:HB2	1:L:97:TYR:OH	1.80	0.81
2:B:32:TYR:CD1	2:B:100:LEU:HD12	2.17	0.80
1:A:63:ARG:NH2	1:A:84:ASP:OD2	2.14	0.80
1:A:170:GLN:O	1:A:171:SER:C	2.21	0.79
1:L:3:GLU:O	1:L:4:LEU:HB2	1.83	0.78
1:L:63:ARG:HH11	1:L:63:ARG:CG	1.95	0.78
1:A:31:GLY:O	1:A:32:TYR:CG	2.37	0.77
1:L:172:ASN:OD1	1:L:174:LYS:HB2	1.86	0.75
1:A:63:ARG:HH22	1:A:84:ASP:CG	1.91	0.73
2:B:102:PRO:O	3:B:362:HOH:O	2.06	0.73
1:A:1:GLN:HB3	1:A:97:TYR:CZ	2.24	0.72
2:B:32:TYR:CD1	2:B:100:LEU:HD13	2.24	0.72
1:L:166:LYS:HD2	1:L:167:PRO:CD	2.18	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:152:LYS:HB2	1:L:195:SER:HB2	1.73	0.70
1:A:169:LYS:HG3	1:A:173:ASN:HA	1.74	0.69
2:B:99:GLU:HA	3:B:263:HOH:O	1.91	0.68
1:L:34:TYR:CG	2:H:103:TYR:HB3	2.28	0.68
1:L:170:GLN:HG3	1:L:174:LYS:O	1.93	0.68
2:B:87:ARG:CG	2:B:89:GLU:OE1	2.44	0.66
2:B:28:THR:HB	3:B:253:HOH:O	1.96	0.66
1:L:211:PRO:O	1:L:212:THR:CG2	2.39	0.66
2:B:13:GLN:HE21	2:B:13:GLN:H	1.44	0.65
2:H:99:GLU:HG3	2:H:99:GLU:O	1.95	0.65
1:A:185:PRO:O	1:A:189:LYS:HD3	1.96	0.65
1:L:1:GLN:N	1:L:2:SER:HA	2.12	0.65
1:L:31:GLY:O	1:L:32:TYR:CG	2.50	0.65
2:H:62:ASP:OD1	2:H:65:LYS:HE3	1.97	0.65
2:H:29:PHE:HB3	2:H:77:ASN:HD22	1.61	0.64
1:L:63:ARG:NH1	1:L:63:ARG:CG	2.55	0.64
1:L:169:LYS:HE2	1:L:173:ASN:HB3	1.80	0.64
2:H:1:GLU:OE1	1:A:117:THR:HG22	1.98	0.64
2:H:32:TYR:CD1	2:H:100:LEU:HD12	2.32	0.64
2:H:20:LEU:HG	2:H:83:MET:CE	2.26	0.63
2:H:107:ASP:HB3	3:H:289:HOH:O	1.99	0.62
2:H:30:SER:O	2:H:53:SER:HB2	1.99	0.62
2:H:165:LEU:HD23	2:H:166:THR:N	2.15	0.61
1:L:170:GLN:O	1:L:171:SER:C	2.36	0.61
1:L:169:LYS:HD3	3:L:222:HOH:O	2.01	0.60
1:A:169:LYS:HG2	1:A:173:ASN:HA	1.84	0.60
2:H:32:TYR:CE1	2:H:100:LEU:HD12	2.37	0.60
1:A:34:TYR:CG	2:B:103:TYR:HB3	2.36	0.60
2:H:165:LEU:HD23	2:H:166:THR:H	1.66	0.59
2:B:145:GLY:HA2	2:B:160:TRP:CH2	2.38	0.59
1:L:169:LYS:HD2	1:L:175:TYR:CZ	2.38	0.58
2:H:32:TYR:CE1	2:H:100:LEU:CD1	2.87	0.58
2:H:87:ARG:HD2	2:H:89:GLU:OE1	2.04	0.58
1:L:52:ASP:HB2	1:L:55:GLU:HG3	1.86	0.57
1:A:34:TYR:CD2	2:B:103:TYR:HB3	2.40	0.57
2:H:158:VAL:O	3:H:329:HOH:O	2.18	0.57
1:L:34:TYR:CD2	2:H:103:TYR:HB3	2.40	0.57
1:L:32:TYR:HB2	3:L:373:HOH:O	2.04	0.56
1:A:55:GLU:OE2	3:A:244:HOH:O	2.17	0.56
2:H:11:LEU:HD21	2:H:120:ALA:HB1	1.88	0.56
2:B:101:LEU:HD12	3:B:372:HOH:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:174:LYS:NZ	2:B:1:GLU:OE2	2.40	0.54
1:A:186:GLU:HG2	3:A:245:HOH:O	2.07	0.54
1:A:56:ARG:NH1	3:A:219:HOH:O	2.41	0.54
2:B:190:VAL:HG11	2:B:200:TYR:CE1	2.43	0.54
3:L:254:HOH:O	2:H:102:PRO:HA	2.07	0.54
1:A:169:LYS:HD2	3:A:231:HOH:O	2.08	0.53
2:H:99:GLU:CB	2:H:105:GLY:O	2.53	0.53
1:L:1:GLN:H3	1:L:2:SER:HA	1.72	0.53
1:A:56:ARG:HE	1:A:62:ASP:HA	1.73	0.53
2:H:62:ASP:HA	2:H:65:LYS:HE3	1.90	0.53
2:B:41:PRO:O	2:B:43:LYS:HG2	2.09	0.52
2:B:33:GLN:NE2	2:B:53:SER:H	2.07	0.52
2:H:164:ALA:CB	2:B:205:ASN:HD22	2.23	0.52
1:A:172:ASN:C	1:A:174:LYS:H	2.13	0.52
2:B:219:PRO:HD2	3:B:297:HOH:O	2.09	0.52
2:B:101:LEU:CD1	3:B:372:HOH:O	2.57	0.52
2:B:28:THR:CG2	2:B:31:THR:HG23	2.39	0.52
1:A:31:GLY:O	1:A:32:TYR:CD1	2.62	0.51
2:B:111:GLN:H	2:B:111:GLN:NE2	2.08	0.51
2:H:99:GLU:CG	2:H:99:GLU:O	2.58	0.51
1:L:169:LYS:HE3	1:L:173:ASN:O	2.11	0.51
2:B:13:GLN:H	2:B:13:GLN:NE2	2.07	0.51
1:L:89:TYR:CD2	2:H:45:LEU:HD22	2.46	0.51
2:B:87:ARG:CD	2:B:89:GLU:OE1	2.59	0.51
1:L:91:TRP:CZ2	1:L:98:TYR:CD1	2.99	0.51
2:B:51:ILE:HD11	2:B:55:GLY:HA2	1.93	0.51
1:A:31:GLY:O	1:A:32:TYR:CD2	2.65	0.50
2:B:99:GLU:OE2	2:B:102:PRO:HA	2.11	0.50
1:L:31:GLY:O	1:L:32:TYR:CD2	2.65	0.50
2:H:20:LEU:CG	2:H:83:MET:HE2	2.32	0.50
1:A:169:LYS:CD	1:A:173:ASN:HA	2.42	0.49
2:H:216:LYS:CD	2:H:218:GLU:OE2	2.59	0.49
2:B:148:VAL:HG11	2:B:156:VAL:HG11	1.94	0.49
1:A:91:TRP:CZ2	1:A:98:TYR:CD1	3.00	0.49
2:B:144:LEU:HD12	2:B:188:VAL:HG12	1.95	0.49
2:H:156:VAL:HG22	2:H:206:HIS:HB2	1.95	0.49
2:B:97:ALA:HA	2:B:108:VAL:O	2.13	0.49
1:L:126:GLU:OE1	2:H:215:LYS:NZ	2.35	0.49
2:B:144:LEU:CD1	2:B:188:VAL:CG1	2.91	0.49
2:B:145:GLY:HA2	2:B:160:TRP:HH2	1.76	0.48
2:B:32:TYR:HA	2:B:100:LEU:HA	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:184:THR:OG1	1:L:187:GLN:HG2	2.12	0.48
1:A:34:TYR:O	1:A:92:SER:HA	2.13	0.48
2:H:190:VAL:HG11	2:H:200:TYR:CE1	2.48	0.48
1:A:184:THR:OG1	1:A:187:GLN:HG3	2.13	0.48
2:B:32:TYR:HD1	2:B:100:LEU:HD12	1.70	0.48
2:B:156:VAL:HG22	2:B:206:HIS:HB2	1.96	0.48
1:A:138:LEU:CD1	2:B:187:VAL:HG11	2.44	0.48
2:H:132:PRO:O	3:H:260:HOH:O	2.20	0.48
1:L:1:GLN:N	1:L:2:SER:CA	2.76	0.48
2:H:205:ASN:HD22	2:H:212:LYS:NZ	2.12	0.47
1:L:34:TYR:O	1:L:92:SER:HA	2.14	0.47
1:L:38:TYR:O	1:L:88:TYR:HA	2.15	0.47
1:A:186:GLU:CG	3:A:245:HOH:O	2.62	0.46
2:H:164:ALA:HB1	2:B:205:ASN:HD22	1.80	0.46
1:A:31:GLY:C	1:A:32:TYR:CG	2.89	0.46
2:H:212:LYS:HE2	3:B:324:HOH:O	2.15	0.46
2:H:216:LYS:HD3	2:H:218:GLU:OE2	2.16	0.46
2:B:219:PRO:HB3	3:B:322:HOH:O	2.16	0.46
2:B:30:SER:O	2:B:53:SER:HB2	2.16	0.46
2:B:78:THR:HG22	2:B:80:TYR:CZ	2.51	0.46
1:A:110:GLY:O	1:A:111:GLN:O	2.34	0.45
1:L:184:THR:HG23	1:L:187:GLN:OE1	2.16	0.45
1:A:152:LYS:HB2	1:A:195:SER:HB2	1.98	0.45
1:A:38:TYR:O	1:A:88:TYR:HA	2.17	0.45
2:B:29:PHE:HB3	2:B:77:ASN:ND2	2.31	0.45
2:H:148:VAL:HG11	2:H:156:VAL:HG11	1.98	0.45
2:B:13:GLN:CG	3:B:221:HOH:O	2.65	0.45
2:B:1:GLU:CG	2:B:2:VAL:H	2.30	0.44
2:H:62:ASP:OD1	2:H:65:LYS:CE	2.65	0.44
1:A:38:TYR:OH	2:B:106:MET:HG2	2.18	0.44
2:B:73:ASP:HB2	3:B:268:HOH:O	2.18	0.44
1:A:111:GLN:HA	1:A:112:PRO:HD3	1.90	0.44
2:B:28:THR:HG22	2:B:31:THR:HG23	1.98	0.44
2:B:30:SER:HB3	2:B:74:ASN:CB	2.41	0.44
1:A:169:LYS:NZ	1:A:173:ASN:HB3	2.33	0.44
2:B:32:TYR:HE1	2:B:100:LEU:HD13	1.72	0.44
2:B:106:MET:HE1	3:B:251:HOH:O	2.18	0.44
2:B:33:GLN:HG2	2:B:99:GLU:O	2.17	0.44
1:A:169:LYS:HE2	1:A:175:TYR:CZ	2.53	0.43
2:B:153:PRO:HD2	2:B:208:PRO:HG2	2.00	0.43
1:A:172:ASN:OD1	1:A:174:LYS:HB2	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:205:ASN:HD22	2:H:212:LYS:HZ2	1.66	0.43
2:B:84:ASN:O	2:B:85:SER:C	2.55	0.43
1:L:4:LEU:HD22	1:L:99:VAL:HG13	2.00	0.43
1:A:172:ASN:O	1:A:174:LYS:N	2.51	0.43
1:L:34:TYR:CD1	2:H:103:TYR:HB3	2.53	0.43
2:H:73:ASP:HA	3:H:233:HOH:O	2.17	0.43
1:A:3:GLU:HG3	3:A:253:HOH:O	2.18	0.43
2:H:216:LYS:HD2	2:H:218:GLU:OE2	2.19	0.43
1:L:189:LYS:HA	1:L:189:LYS:HD2	1.88	0.43
1:L:111:GLN:HA	1:L:112:PRO:HD3	1.88	0.43
1:A:152:LYS:HD3	1:A:157:PRO:HA	2.01	0.42
2:B:99:GLU:O	2:B:99:GLU:HG2	2.18	0.42
2:H:32:TYR:HA	2:H:100:LEU:HA	2.02	0.42
2:H:32:TYR:CE1	2:H:100:LEU:HD13	2.55	0.42
1:L:93:PHE:HD1	1:L:98:TYR:CE1	2.37	0.42
1:L:192:ARG:O	1:L:210:ALA:HB1	2.20	0.42
1:A:170:GLN:O	1:A:172:ASN:N	2.52	0.42
2:B:13:GLN:HB3	3:B:221:HOH:O	2.20	0.42
2:H:99:GLU:HA	3:H:257:HOH:O	2.19	0.42
1:A:116:PRO:HA	1:A:140:SER:O	2.20	0.41
1:A:151:TRP:O	1:A:152:LYS:HD3	2.20	0.41
2:B:70:ILE:O	2:B:70:ILE:HG23	2.20	0.41
1:L:169:LYS:HG2	1:L:173:ASN:HA	1.93	0.41
2:H:52:VAL:HG22	2:H:57:SER:HB3	2.01	0.41
1:L:169:LYS:HG3	1:L:173:ASN:CA	2.34	0.41
2:H:32:TYR:CE1	2:H:100:LEU:HB2	2.55	0.41
1:A:85:GLU:O	1:A:86:ALA:HB2	2.20	0.41
2:B:207:LYS:HB3	2:B:208:PRO:HD3	2.01	0.41
2:H:157:THR:HG22	3:H:232:HOH:O	2.20	0.41
1:A:135:LEU:HB2	1:A:181:LEU:HB3	2.02	0.41
2:B:22:CYS:HB3	2:B:79:LEU:HB3	2.03	0.41
1:A:131:ASN:HA	1:A:185:PRO:HG2	2.03	0.41
1:A:147:VAL:HG12	1:A:200:HIS:HB2	2.03	0.41
1:L:85:GLU:O	1:L:86:ALA:HB2	2.21	0.40
2:H:187:VAL:HG23	2:H:187:VAL:O	2.21	0.40
2:B:101:LEU:O	2:B:104:TYR:HB3	2.22	0.40
1:L:211:PRO:O	1:L:212:THR:CB	2.69	0.40
1:L:197:GLN:HB2	1:L:206:GLU:OE2	2.21	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	210/212 (99%)	188 (90%)	17 (8%)	5 (2%)	6	4
1	L	210/212 (99%)	187 (89%)	21 (10%)	2 (1%)	15	17
2	B	218/220 (99%)	194 (89%)	23 (11%)	1 (0%)	29	35
2	H	218/220 (99%)	203 (93%)	12 (6%)	3 (1%)	11	11
All	All	856/864 (99%)	772 (90%)	73 (8%)	11 (1%)	12	12

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	120	ALA
1	A	2	SER
1	A	111	GLN
1	A	156	SER
1	L	4	LEU
2	H	30	SER
1	L	111	GLN
2	B	154	GLU
2	H	154	GLU
1	A	155	GLY
1	A	171	SER

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	179/179 (100%)	161 (90%)	18 (10%)	7	9
1	L	179/179 (100%)	167 (93%)	12 (7%)	16	21
2	B	182/182 (100%)	152 (84%)	30 (16%)	2	2
2	H	182/182 (100%)	163 (90%)	19 (10%)	7	8
All	All	722/722 (100%)	643 (89%)	79 (11%)	6	7

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	8	ARG
1	L	55	GLU
1	L	62	ASP
1	L	63	ARG
1	L	115	ASN
1	L	117	THR
1	L	166	LYS
1	L	170	GLN
1	L	171	SER
1	L	178	SER
1	L	186	GLU
1	L	189	LYS
2	H	6	GLU
2	H	7	SER
2	H	45	LEU
2	H	49	SER
2	H	100	LEU
2	H	101	LEU
2	H	106	MET
2	H	108	VAL
2	H	111	GLN
2	H	133	SER
2	H	136	SER
2	H	141	THR
2	H	165	LEU
2	H	166	THR
2	H	167	SER
2	H	170	HIS
2	H	189	THR
2	H	195	LEU
2	H	199	THR
1	A	1	GLN
1	A	10	VAL

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Mol	Chain	Res	Type
1	A	28	ASP
1	A	44	LYS
1	A	55	GLU
1	A	117	THR
1	A	131	ASN
1	A	154	ASP
1	A	158	VAL
1	A	166	LYS
1	A	170	GLN
1	A	171	SER
1	A	174	LYS
1	A	178	SER
1	A	186	GLU
1	A	187	GLN
1	A	189	LYS
1	A	192	ARG
2	B	1	GLU
2	B	3	GLN
2	B	5	LEU
2	B	7	SER
2	B	13	GLN
2	B	21	SER
2	B	25	SER
2	B	33	GLN
2	B	49	SER
2	B	54	SER
2	B	87	ARG
2	B	101	LEU
2	B	103	TYR
2	B	106	MET
2	B	107	ASP
2	B	111	GLN
2	B	121	SER
2	B	134	SER
2	B	141	THR
2	B	154	GLU
2	B	159	SER
2	B	165	LEU
2	B	167	SER
2	B	170	HIS
2	B	184	LEU
2	B	189	THR

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Mol	Chain	Res	Type
2	B	195	LEU
2	B	207	LYS
2	B	215	LYS
2	B	216	LYS

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

Mol	Chain	Res	Type
1	L	71	ASN
1	L	115	ASN
1	L	173	ASN
1	L	200	HIS
1	L	203	ASN
2	H	77	ASN
2	H	205	ASN
1	A	71	ASN
1	A	131	ASN
1	A	173	ASN
1	A	203	ASN
2	B	13	GLN
2	B	33	GLN
2	B	77	ASN
2	B	111	GLN

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, 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	212/212 (100%)	-0.03	2 (0%) 84 88	24, 43, 66, 75	0
1	L	212/212 (100%)	-0.06	3 (1%) 75 80	23, 44, 66, 75	0
2	B	220/220 (100%)	0.05	10 (4%) 33 40	27, 41, 66, 81	0
2	H	220/220 (100%)	0.09	11 (5%) 28 35	28, 41, 66, 81	0
All	All	864/864 (100%)	0.01	26 (3%) 50 57	23, 42, 66, 81	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	138	SER	7.0
2	B	56	GLY	6.4
2	H	136	SER	6.0
2	H	56	GLY	5.9
2	B	137	THR	5.2
2	H	137	THR	4.6
2	H	134	SER	4.4
2	B	136	SER	4.0
2	H	102	PRO	3.7
2	B	138	SER	3.5
2	B	134	SER	3.5
1	L	110	GLY	3.4
2	H	103	TYR	3.1
1	L	173	ASN	3.1
2	H	104	TYR	2.8
2	B	102	PRO	2.7
1	A	192	ARG	2.6
2	B	104	TYR	2.5
2	H	106	MET	2.4
1	L	192	ARG	2.4
2	B	139	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
2	H	100	LEU	2.3
2	B	103	TYR	2.3
2	B	135	LYS	2.3
1	A	173	ASN	2.1
2	H	101	LEU	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.