



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 06:47 AM EDT

PDB ID : 2GJZ / pdb_00002gjz
Title : Structure of Catalytic Elimination Antibody 13G5 from a crystal in space group P2(1)
Authors : Debler, E.W.; Wilson, I.A.
Deposited on : 2006-03-31
Resolution : 2.65 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

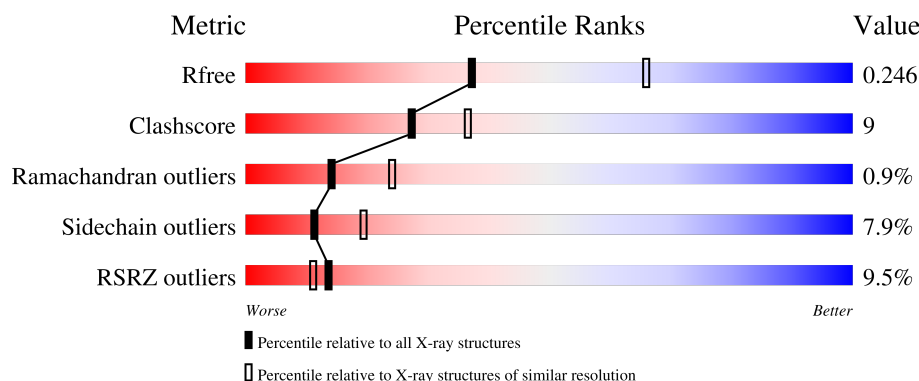
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

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	217	10% 83% 13% .
1	L	217	3% 76% 20% .
2	B	221	8% 74% 23% .
2	H	221	17% 71% 25% .

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6706 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 Catalytic elimination antibody 13G5 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	217	Total	C	N	O	S	0	0	0
			1684	1053	286	339	6			
1	A	217	Total	C	N	O	S	0	0	0
			1684	1053	286	339	6			

- Molecule 2 is a protein called Catalytic elimination antibody 13G5 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	221	Total	C	N	O	S	0	0	0
			1650	1043	270	328	9			
2	B	221	Total	C	N	O	S	0	0	0
			1650	1043	270	328	9			

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	L	5	Total	Zn	0	0
			5	5		
3	H	2	Total	Zn	0	0
			2	2		
3	A	1	Total	Zn	0	0
			1	1		
3	B	3	Total	Zn	0	0
			3	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	L	6	Total	O	0	0
			6	6		
4	H	3	Total	O	0	0
			3	3		

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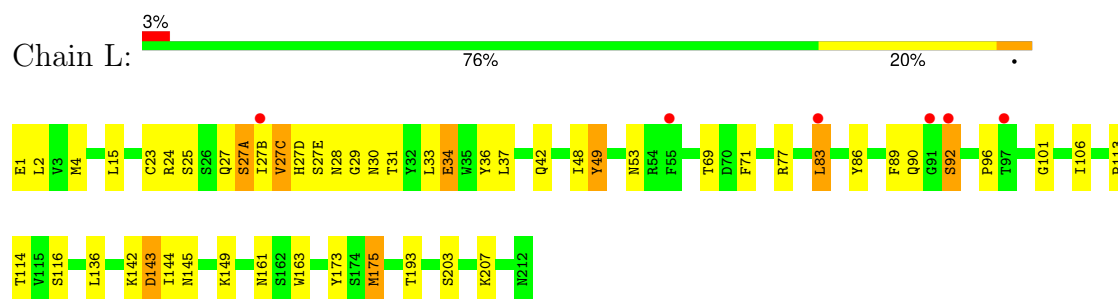
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	9	Total	O	0	0
			9	9		
4	B	9	Total	O	0	0
			9	9		

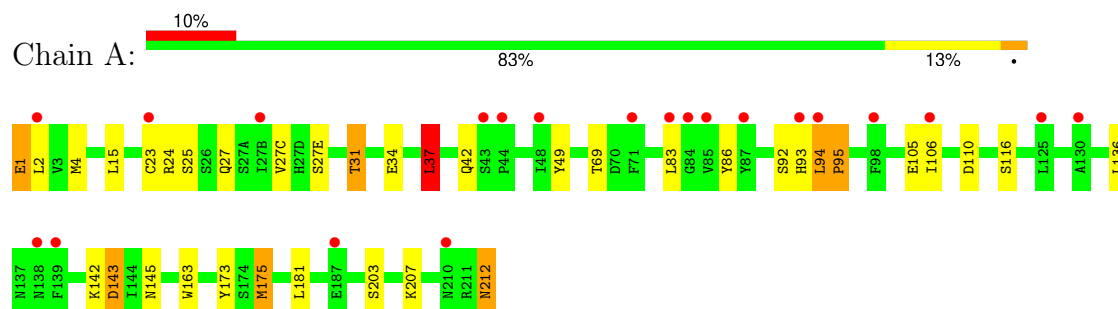
3 Residue-property plots [i](#)

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.

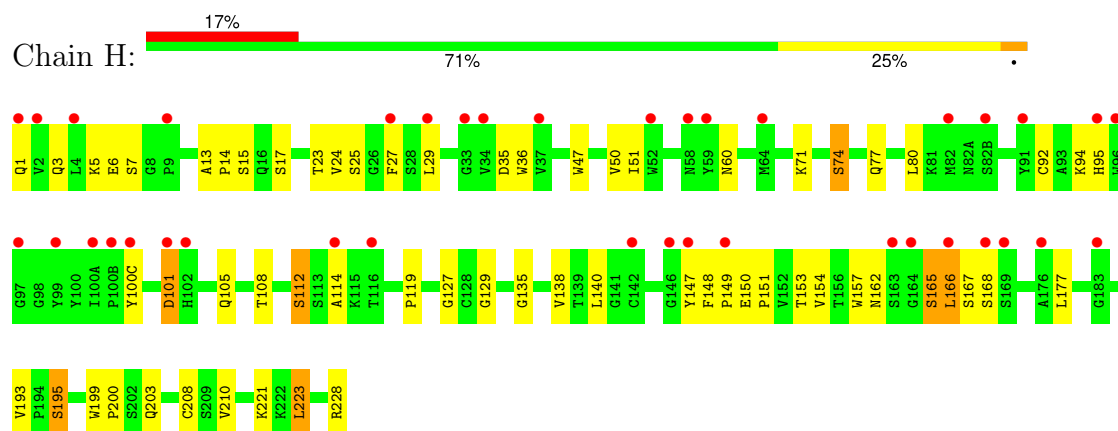
- Molecule 1: Catalytic elimination antibody 13G5 light chain



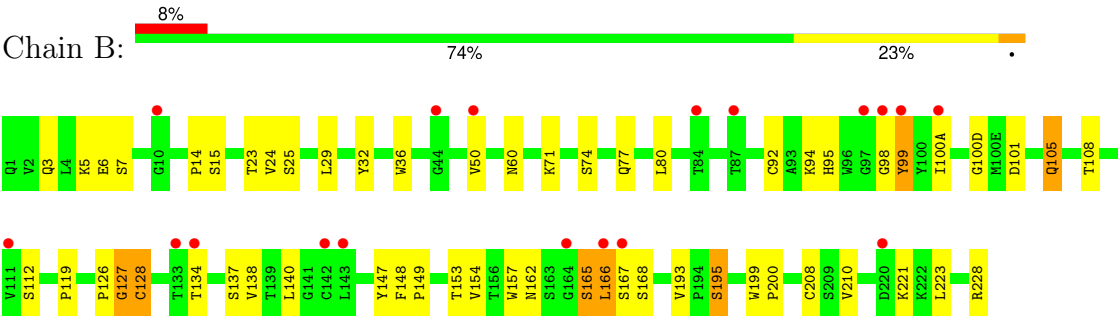
- Molecule 1: Catalytic elimination antibody 13G5 light chain



- Molecule 2: Catalytic elimination antibody 13G5 heavy chain



- Molecule 2: Catalytic elimination antibody 13G5 heavy chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	50.21Å 73.50Å 130.47Å 90.00° 96.33° 90.00°	Depositor
Resolution (Å)	40.00 – 2.65 40.00 – 2.65	Depositor EDS
% Data completeness (in resolution range)	93.0 (40.00-2.65) 92.9 (40.00-2.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.41 (at 2.65Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.213 , 0.250 0.209 , 0.246	Depositor DCC
R_{free} test set	1238 reflections (4.48%)	wwPDB-VP
Wilson B-factor (Å ²)	63.5	Xtriage
Anisotropy	0.020	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 80.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	6706	wwPDB-VP
Average B, all atoms (Å ²)	94.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.13% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.87	2/1723 (0.1%)	0.92	2/2337 (0.1%)
1	L	0.90	3/1723 (0.2%)	0.93	5/2337 (0.2%)
2	B	0.75	0/1697	0.95	2/2324 (0.1%)
2	H	0.74	3/1697 (0.2%)	0.92	2/2324 (0.1%)
All	All	0.82	8/6840 (0.1%)	0.93	11/9322 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	27(E)	SER	C-O	14.16	1.42	1.24
1	L	1	GLU	CD-OE2	11.38	1.47	1.25
2	H	203	GLN	CD-OE1	9.94	1.42	1.23
1	A	27(E)	SER	C-N	9.39	1.46	1.33
2	H	203	GLN	CD-NE2	8.44	1.50	1.33
2	H	153	THR	CB-OG1	6.81	1.54	1.43
1	L	27(E)	SER	C-N	6.50	1.45	1.33
1	A	1	GLU	CD-OE2	5.47	1.35	1.25

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	203	GLN	OE1-CD-NE2	7.93	130.53	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	167	SER	N-CA-C	-7.17	104.40	113.72
2	H	167	SER	N-CA-C	-6.98	104.64	113.72
1	L	37	LEU	CD1-CG-CD2	-6.21	97.15	110.80
1	A	49	TYR	N-CA-C	5.51	121.03	113.97
1	L	49	TYR	CA-C-N	-5.46	115.72	123.03
1	L	49	TYR	C-N-CA	-5.46	115.72	123.03
2	B	137	SER	N-CA-C	5.24	117.04	109.07
1	L	27(A)	SER	CA-CB-OG	-5.22	100.65	111.10
1	A	37	LEU	CD1-CG-CD2	-5.18	99.41	110.80
1	L	27(C)	VAL	N-CA-C	5.06	115.76	108.93

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	94	LEU	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	1684	0	1628	15	0
1	L	1684	0	1628	33	0
2	B	1650	0	1604	29	0
2	H	1650	0	1604	48	0
3	A	1	0	0	0	0
3	B	3	0	0	0	0
3	H	2	0	0	0	0
3	L	5	0	0	0	0
4	A	9	0	0	0	0
4	B	9	0	0	2	0
4	H	3	0	0	1	0
4	L	6	0	0	0	0
All	All	6706	0	6464	120	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 (120) 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:L:83:LEU:HD11	1:L:106:ILE:CD1	1.77	1.12
1:L:83:LEU:HD11	1:L:106:ILE:HD11	1.24	1.10
1:L:83:LEU:CD1	1:L:106:ILE:HD11	1.87	1.04
2:H:114:ALA:HB3	2:H:148:PHE:CE1	1.95	1.02
2:H:1:GLN:NE2	1:A:110:ASP:OD2	1.98	0.97
2:H:148:PHE:HD2	2:H:149:PRO:CA	1.81	0.93
1:L:83:LEU:HD11	1:L:106:ILE:CG1	1.98	0.92
2:H:148:PHE:CD2	2:H:149:PRO:HA	2.06	0.90
2:H:148:PHE:CD2	2:H:149:PRO:CA	2.55	0.89
2:H:148:PHE:HD2	2:H:149:PRO:N	1.74	0.84
2:H:114:ALA:HB3	2:H:148:PHE:CD1	2.24	0.72
2:H:50:VAL:HG21	2:H:95:HIS:HE1	1.54	0.71
1:L:83:LEU:HD11	1:L:106:ILE:HG13	1.75	0.68
2:B:50:VAL:HG21	2:B:95:HIS:HE1	1.60	0.67
2:H:74:SER:OG	4:H:233:HOH:O	2.13	0.66
1:L:4:MET:HE3	1:L:23:CYS:SG	2.36	0.65
1:A:4:MET:HE3	1:A:23:CYS:SG	2.36	0.65
2:H:148:PHE:CE2	2:H:149:PRO:HB3	2.30	0.65
2:B:100(A):ILE:HG13	4:B:239:HOH:O	1.98	0.64
2:H:138:VAL:HG23	2:H:195:SER:HB2	1.81	0.63
2:B:6:GLU:HG3	2:B:92:CYS:SG	2.40	0.62
2:B:29:LEU:HB3	2:B:71:LYS:HE2	1.82	0.60
1:L:27(D):HIS:CD2	1:L:92:SER:HB3	2.37	0.60
2:H:29:LEU:HB3	2:H:71:LYS:HE2	1.83	0.59
2:H:148:PHE:HE2	2:H:149:PRO:HB3	1.68	0.59
1:L:27(B):ILE:HG21	1:L:71:PHE:CZ	2.39	0.58
1:L:136:LEU:HD12	1:L:136:LEU:N	2.20	0.57
1:L:163:TRP:CZ2	1:L:175:MET:HE2	2.39	0.57
1:A:34:GLU:OE1	2:B:100(D):GLY:HA2	2.04	0.57
2:H:114:ALA:CB	2:H:148:PHE:CD1	2.88	0.57
2:B:94:LYS:HG3	2:B:101:ASP:HB3	1.87	0.56
2:H:94:LYS:HG3	2:H:101:ASP:HB3	1.87	0.56
2:H:228:ARG:O	2:H:228:ARG:HG3	2.05	0.56
2:H:148:PHE:CD2	2:H:149:PRO:N	2.65	0.55
1:L:27(B):ILE:CG2	1:L:71:PHE:HZ	2.20	0.55
2:H:140:LEU:HB3	2:H:223:LEU:HD22	1.89	0.55
2:B:154:VAL:HG22	2:B:210:VAL:HG22	1.88	0.54
1:A:24:ARG:HA	1:A:69:THR:O	2.07	0.54
2:B:148:PHE:CD2	2:B:149:PRO:HA	2.43	0.53
2:B:119:PRO:HB3	2:B:147:TYR:HB3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:TRP:CZ2	1:A:175:MET:HE2	2.44	0.52
2:B:140:LEU:HB3	2:B:223:LEU:HD22	1.91	0.52
2:B:126:PRO:HD3	2:B:140:LEU:HD23	1.90	0.52
2:B:138:VAL:HG23	2:B:195:SER:HB2	1.91	0.52
1:L:143:ASP:OD1	1:L:143:ASP:N	2.43	0.52
1:L:96:PRO:HD2	2:H:47:TRP:CZ3	2.46	0.51
2:B:228:ARG:O	2:B:228:ARG:HG3	2.10	0.51
2:H:166:LEU:CD2	2:H:193:VAL:HG12	2.41	0.51
1:A:136:LEU:HD12	1:A:136:LEU:N	2.26	0.51
2:H:119:PRO:HB3	2:H:147:TYR:HB3	1.92	0.51
2:H:23:THR:HG22	2:H:77:GLN:HG2	1.92	0.50
1:L:27(D):HIS:C	1:L:28:ASN:N	2.70	0.50
2:H:114:ALA:HB3	2:H:148:PHE:HE1	1.62	0.50
1:L:89:PHE:CZ	1:L:96:PRO:HB3	2.47	0.50
1:L:142:LYS:HB2	1:L:173:TYR:CE2	2.47	0.50
2:B:3:GLN:HB2	2:B:25:SER:HB3	1.93	0.50
2:H:6:GLU:HG3	2:H:92:CYS:SG	2.52	0.49
2:H:199:TRP:CG	2:H:200:PRO:HA	2.46	0.49
2:B:50:VAL:HG21	2:B:95:HIS:CE1	2.43	0.49
2:B:157:TRP:CZ3	2:B:208:CYS:HB3	2.47	0.49
1:L:34:GLU:HB3	1:L:49:TYR:HA	1.95	0.48
1:L:34:GLU:OE1	2:H:100(C):TYR:O	2.32	0.48
1:L:83:LEU:CD1	1:L:106:ILE:CD1	2.60	0.48
2:H:50:VAL:HG21	2:H:95:HIS:CE1	2.41	0.48
1:L:28:ASN:C	1:L:30:ASN:H	2.22	0.48
1:L:27(A):SER:OG	1:L:27(C):VAL:HG23	2.13	0.47
2:H:199:TRP:CD1	2:H:200:PRO:HA	2.50	0.47
2:H:148:PHE:CD2	2:H:149:PRO:CB	2.98	0.47
2:H:140:LEU:HB3	2:H:223:LEU:CD2	2.45	0.46
1:L:27(D):HIS:O	1:L:28:ASN:N	2.49	0.46
1:L:149:LYS:HB2	1:L:193:THR:HB	1.97	0.46
2:H:3:GLN:HB2	2:H:25:SER:HB3	1.96	0.46
1:L:161:ASN:O	2:H:177:LEU:HD11	2.16	0.46
2:B:128:CYS:HA	2:B:228:ARG:H	1.80	0.46
2:B:14:PRO:HD3	2:B:112:SER:C	2.41	0.46
2:H:148:PHE:CD2	2:H:148:PHE:C	2.94	0.46
2:B:36:TRP:CD2	2:B:80:LEU:HD12	2.51	0.45
2:H:35:ASP:OD1	2:H:50:VAL:HB	2.17	0.45
1:A:27(C):VAL:HG22	1:A:31:THR:HB	1.99	0.45
2:B:166:LEU:CD2	2:B:193:VAL:HG12	2.47	0.45
2:B:99:TYR:HB2	4:B:239:HOH:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:148:PHE:HD2	2:H:148:PHE:C	2.25	0.44
1:A:143:ASP:OD1	1:A:143:ASP:N	2.38	0.44
2:H:166:LEU:HD21	2:H:193:VAL:HG12	1.99	0.44
1:L:24:ARG:HA	1:L:69:THR:O	2.18	0.44
2:B:199:TRP:CD1	2:B:200:PRO:HA	2.53	0.44
2:H:135:GLY:O	2:H:195:SER:HB3	2.18	0.44
1:L:27(B):ILE:HG21	1:L:71:PHE:HZ	1.77	0.43
2:H:148:PHE:CD2	2:H:149:PRO:HB3	2.54	0.43
1:A:136:LEU:HD13	1:A:175:MET:HG3	2.01	0.43
2:B:199:TRP:CG	2:B:200:PRO:HA	2.53	0.43
2:H:157:TRP:CZ3	2:H:208:CYS:HB3	2.54	0.43
2:H:162:ASN:O	2:H:165:SER:HB2	2.19	0.43
1:L:27(D):HIS:C	1:L:28:ASN:H	2.27	0.42
1:L:48:ILE:HA	1:L:53:ASN:O	2.19	0.42
2:H:13:ALA:HA	2:H:112:SER:O	2.18	0.42
2:H:154:VAL:HG22	2:H:210:VAL:HG22	2.02	0.42
1:A:37:LEU:HG	1:A:86:TYR:CE2	2.54	0.42
1:A:94:LEU:HB3	1:A:95:PRO:CD	2.49	0.42
1:L:27(D):HIS:O	1:L:29:GLY:N	2.53	0.42
1:A:212:ASN:OD1	1:A:212:ASN:N	2.53	0.42
1:L:86:TYR:O	1:L:101:GLY:HA2	2.20	0.42
2:H:51:ILE:HD13	2:H:71:LYS:HB2	2.01	0.42
1:A:25:SER:C	1:A:27:GLN:H	2.28	0.42
1:A:105:GLU:HG2	1:A:106:ILE:O	2.19	0.41
2:B:23:THR:HG22	2:B:77:GLN:HG2	2.02	0.41
1:L:25:SER:C	1:L:27:GLN:H	2.28	0.41
2:B:140:LEU:HB3	2:B:223:LEU:CD2	2.50	0.41
2:H:24:VAL:HG13	2:H:27:PHE:CE1	2.55	0.41
2:B:105:GLN:HE21	2:B:105:GLN:HB3	1.74	0.41
2:H:150:GLU:HA	2:H:151:PRO:HA	1.84	0.41
2:H:36:TRP:CD2	2:H:80:LEU:HD12	2.55	0.41
2:B:126:PRO:O	2:B:127:GLY:C	2.63	0.41
2:H:127:GLY:C	2:H:129:GLY:H	2.28	0.40
1:L:113:PRO:HG3	1:L:144:ILE:HD11	2.04	0.40
2:H:14:PRO:HD3	2:H:112:SER:C	2.47	0.40
2:B:162:ASN:O	2:B:165:SER:HB2	2.20	0.40
1:L:34:GLU:HG3	1:L:36:TYR:CE1	2.57	0.40
1:A:142:LYS:HD2	1:A:173:TYR:CE2	2.56	0.40
2:B:32:TYR:HD1	2:B:98:GLY:HA2	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	215/217 (99%)	203 (94%)	11 (5%)	1 (0%)	24	39
1	L	215/217 (99%)	205 (95%)	9 (4%)	1 (0%)	24	39
2	B	219/221 (99%)	204 (93%)	12 (6%)	3 (1%)	9	14
2	H	219/221 (99%)	204 (93%)	12 (6%)	3 (1%)	9	14
All	All	868/876 (99%)	816 (94%)	44 (5%)	8 (1%)	14	24

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	168	SER
1	A	95	PRO
2	B	168	SER
2	B	127	GLY
2	H	15	SER
2	H	101	ASP
1	L	77	ARG
2	B	15	SER

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	194/194 (100%)	177 (91%)	17 (9%)	9	15
1	L	194/194 (100%)	178 (92%)	16 (8%)	10	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	191/191 (100%)	176 (92%)	15 (8%)	11	19
2	H	191/191 (100%)	178 (93%)	13 (7%)	14	25
All	All	770/770 (100%)	709 (92%)	61 (8%)	11	19

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	2	LEU
1	L	15	LEU
1	L	31	THR
1	L	33	LEU
1	L	34	GLU
1	L	42	GLN
1	L	83	LEU
1	L	90	GLN
1	L	92	SER
1	L	114	THR
1	L	116	SER
1	L	143	ASP
1	L	145	ASN
1	L	175	MET
1	L	203	SER
1	L	207	LYS
2	H	5	LYS
2	H	7	SER
2	H	17	SER
2	H	60	ASN
2	H	74	SER
2	H	105	GLN
2	H	108	THR
2	H	112	SER
2	H	165	SER
2	H	166	LEU
2	H	195	SER
2	H	221	LYS
2	H	223	LEU
1	A	1	GLU
1	A	2	LEU
1	A	15	LEU
1	A	31	THR
1	A	37	LEU

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Mol	Chain	Res	Type
1	A	42	GLN
1	A	83	LEU
1	A	92	SER
1	A	93	HIS
1	A	116	SER
1	A	143	ASP
1	A	145	ASN
1	A	175	MET
1	A	181	LEU
1	A	203	SER
1	A	207	LYS
1	A	212	ASN
2	B	5	LYS
2	B	7	SER
2	B	24	VAL
2	B	60	ASN
2	B	74	SER
2	B	99	TYR
2	B	105	GLN
2	B	108	THR
2	B	128	CYS
2	B	134	THR
2	B	153	THR
2	B	165	SER
2	B	166	LEU
2	B	195	SER
2	B	221	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	18	GLN
1	L	30	ASN
1	L	42	GLN
1	L	90	GLN
1	L	190	ASN
2	H	105	GLN
1	A	18	GLN
1	A	38	GLN
1	A	42	GLN
1	A	137	ASN
2	B	39	GLN

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Mol	Chain	Res	Type
2	B	105	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 11 are monoatomic - leaving 0 for Mogul analysis.

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, 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	217/217 (100%)	1.06	21 (9%) 13 10	87, 95, 101, 104	0
1	L	217/217 (100%)	0.75	6 (2%) 55 48	85, 95, 100, 105	0
2	B	221/221 (100%)	0.93	18 (8%) 18 13	90, 94, 106, 116	0
2	H	221/221 (100%)	1.17	38 (17%) 4 3	90, 94, 104, 116	0
All	All	876/876 (100%)	0.98	83 (9%) 14 11	85, 94, 103, 116	0

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	91	GLY	5.5
2	H	4	LEU	3.7
2	H	164	GLY	3.7
1	A	93	HIS	3.5
1	A	43	SER	3.4
2	B	99	TYR	3.4
1	L	27(B)	ILE	3.3
2	B	167	SER	3.2
2	H	102	HIS	3.2
2	B	100(A)	ILE	3.1
2	B	166	LEU	3.1
1	A	94	LEU	3.0
2	H	97	GLY	2.9
1	A	84	GLY	2.9
1	A	2	LEU	2.9
1	A	125	LEU	2.9
2	H	169	SER	2.7
1	A	87	TYR	2.7
2	H	142	CYS	2.7
2	H	100(A)	ILE	2.7
2	H	100(C)	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
2	B	142	CYS	2.6
2	H	9	PRO	2.6
2	H	59	TYR	2.6
1	A	139	PHE	2.6
2	H	96	TRP	2.6
2	H	64	MET	2.6
2	H	146	GLY	2.6
2	H	176	ALA	2.5
2	H	29	LEU	2.5
2	B	164	GLY	2.5
2	H	52	TRP	2.5
2	H	95	HIS	2.5
2	H	114	ALA	2.5
1	L	97	THR	2.4
2	B	84	THR	2.4
2	B	133	THR	2.4
1	L	83	LEU	2.4
1	A	44	PRO	2.4
2	H	183	GLY	2.4
1	A	210	ASN	2.4
2	B	111	VAL	2.4
1	A	27(B)	ILE	2.4
2	B	134	THR	2.4
2	H	58	ASN	2.4
1	L	92	SER	2.3
2	H	34	VAL	2.3
1	A	98	PHE	2.3
2	H	91	TYR	2.3
2	B	10	GLY	2.3
2	B	98	GLY	2.3
1	A	48	ILE	2.3
2	B	44	GLY	2.3
2	H	166	LEU	2.3
2	H	100(B)	PRO	2.2
2	H	149	PRO	2.2
2	H	33	GLY	2.2
1	A	71	PHE	2.2
1	A	83	LEU	2.2
1	A	85	VAL	2.2
2	H	27	PHE	2.2
1	A	187	GLU	2.2
1	A	138	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
2	H	2	VAL	2.2
2	H	37	VAL	2.1
2	B	220	ASP	2.1
2	H	168	SER	2.1
1	A	106	ILE	2.1
2	B	50	VAL	2.1
1	A	130	ALA	2.1
2	H	82(B)	SER	2.1
2	H	163	SER	2.1
2	H	82	MET	2.1
2	B	97	GLY	2.1
2	H	147	TYR	2.1
2	H	101	ASP	2.0
2	H	1	GLN	2.0
1	A	23	CYS	2.0
2	H	99	TYR	2.0
1	L	55	PHE	2.0
2	H	116	THR	2.0
2	B	87	THR	2.0
2	B	143	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 oligosaccharides 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, 95th 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(Å ²)	Q<0.9
3	ZN	L	214	1/1	0.93	0.23	82,82,82,82	0
3	ZN	B	231	1/1	0.95	0.16	112,112,112,112	0
3	ZN	L	217	1/1	0.96	0.19	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	ZN	B	229	1/1	0.96	0.17	95,95,95,95	0
3	ZN	L	216	1/1	0.96	0.13	81,81,81,81	0
3	ZN	L	213	1/1	0.97	0.16	97,97,97,97	0
3	ZN	B	230	1/1	0.97	0.18	75,75,75,75	0
3	ZN	A	213	1/1	0.97	0.19	57,57,57,57	0
3	ZN	L	215	1/1	0.98	0.19	104,104,104,104	0
3	ZN	H	230	1/1	0.98	0.16	86,86,86,86	0
3	ZN	H	229	1/1	0.99	0.15	73,73,73,73	0

6.5 Other polymers [i](#)

There are no such residues in this entry.