Full wwPDB X-ray Structure Validation Report ⓘ

Aug 19, 2023 – 08:40 PM EDT

PDB ID	:	2GJZ
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:

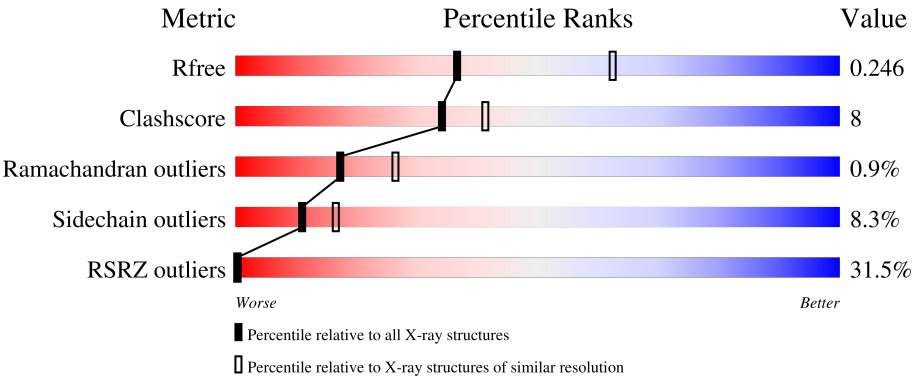
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

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}	130704	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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 <=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	30% 85% 11% .
1	L	217	22% 79% 18% .
2	B	221	31% 75% 23% .
2	H	221	43% 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 (three-letter code: 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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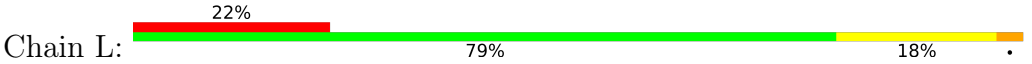
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	9	Total O 9 9	0	0
4	B	9	Total O 9 9	0	0

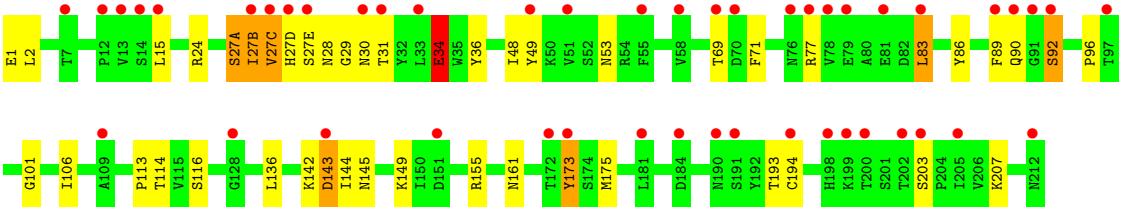
3 Residue-property plots (i)

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

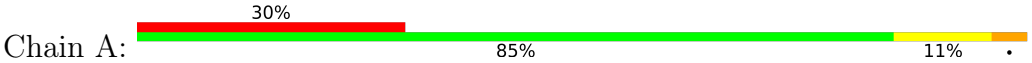
Chain L:

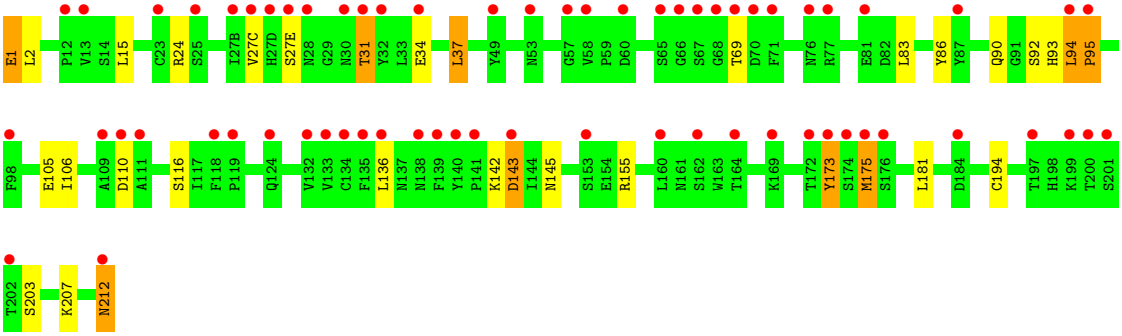




• Molecule 1: Catalytic elimination antibody 13G5 light chain

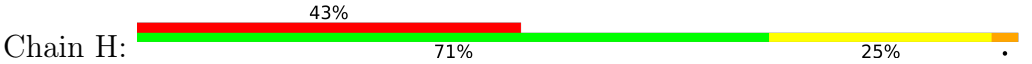
Chain A:

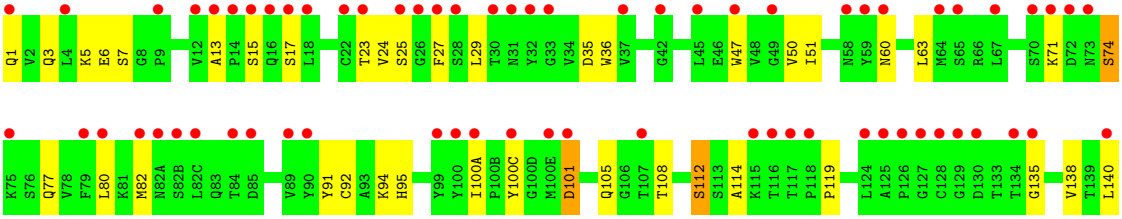


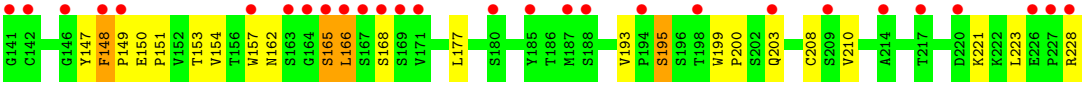


• Molecule 2: Catalytic elimination antibody 13G5 heavy chain

Chain H:

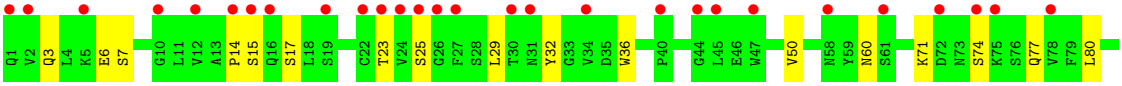


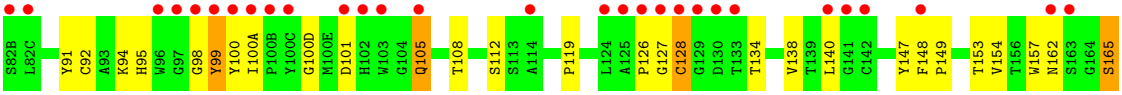


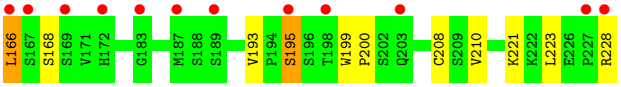


• Molecule 2: Catalytic elimination antibody 13G5 heavy chain

Chain B:







4 Data and refinement statistics (i)

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 35.36 – 2.65	Depositor EDS
% Data completeness (in resolution range)	93.0 (40.00-2.65) 93.0 (35.36-2.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [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 (4.82%)	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)	0.27 , 72.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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

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	0.78	5/1723 (0.3%)	0.73	0/2337
1	L	0.91	8/1723 (0.5%)	0.73	0/2337
2	B	0.67	3/1697 (0.2%)	0.69	0/2324
2	H	0.68	6/1697 (0.4%)	0.69	0/2324
All	All	0.77	22/6840 (0.3%)	0.71	0/9322

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 (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	1	GLU	CD-OE2	19.39	1.47	1.25
1	L	27(E)	SER	C-O	9.91	1.42	1.23
1	A	1	GLU	CD-OE2	9.18	1.35	1.25
2	H	203	GLN	CD-OE1	8.40	1.42	1.24
1	L	27(A)	SER	CB-OG	7.55	1.52	1.42
2	H	203	GLN	CD-NE2	7.25	1.50	1.32
2	H	91	TYR	CE1-CZ	-6.89	1.29	1.38
1	A	173	TYR	CE1-CZ	-6.34	1.30	1.38
2	H	91	TYR	CG-CD1	-6.27	1.31	1.39
1	L	173	TYR	CE2-CZ	-6.23	1.30	1.38
2	B	91	TYR	CE1-CZ	-6.20	1.30	1.38
1	L	173	TYR	CE1-CZ	-6.00	1.30	1.38
2	H	91	TYR	CE2-CZ	-5.84	1.30	1.38
2	B	91	TYR	CE2-CZ	-5.82	1.30	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	194	CYS	CB-SG	-5.76	1.72	1.81
2	H	153	THR	CB-OG1	5.70	1.54	1.43
1	L	173	TYR	CG-CD1	-5.32	1.32	1.39
1	A	27(E)	SER	C-N	5.27	1.46	1.34
1	L	194	CYS	CB-SG	-5.16	1.73	1.81
1	L	34	GLU	CD-OE1	-5.16	1.20	1.25
1	A	173	TYR	CE2-CZ	-5.09	1.31	1.38
2	B	91	TYR	CG-CD1	-5.06	1.32	1.39

There are no bond angle outliers.

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 (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1684	0	1628	12	0
1	L	1684	0	1628	29	0
2	B	1650	0	1604	28	0
2	H	1650	0	1604	46	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	110	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 8.

All (110) 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
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
1:L:27(D):HIS:C	1:L:28:ASN:N	2.70	0.45
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:L:28:ASN:C	1:L:30:ASN:H	2.22	0.43
2:H:63:LEU:HD22	2:H:82:MET:HE3	2.00	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: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: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
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:14:PRO:HD3	2:B:112:SER:C	2.41	0.41
2:H:148:PHE:CD2	2:H:148:PHE:C	2.94	0.40
1:L:113:PRO:HG3	1:L:144:ILE:HD11	2.04	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 (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	215/217 (99%)	203 (94%)	11 (5%)	1 (0%)	29	43
1	L	215/217 (99%)	205 (95%)	9 (4%)	1 (0%)	29	43
2	B	219/221 (99%)	204 (93%)	12 (6%)	3 (1%)	11	16
2	H	219/221 (99%)	204 (93%)	12 (6%)	3 (1%)	11	16
All	All	868/876 (99%)	816 (94%)	44 (5%)	8 (1%)	17	26

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 (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	194/194 (100%)	176 (91%)	18 (9%)	9	13
1	L	194/194 (100%)	177 (91%)	17 (9%)	10	14
2	B	191/191 (100%)	176 (92%)	15 (8%)	12	19
2	H	191/191 (100%)	177 (93%)	14 (7%)	14	21
All	All	770/770 (100%)	706 (92%)	64 (8%)	11	16

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	2	LEU
1	L	15	LEU
1	L	27(B)	ILE

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Mol	Chain	Res	Type
1	L	27(C)	VAL
1	L	31	THR
1	L	34	GLU
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	155	ARG
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	100(A)	ILE
2	H	105	GLN
2	H	108	THR
2	H	112	SER
2	H	148	PHE
2	H	165	SER
2	H	166	LEU
2	H	195	SER
2	H	221	LYS
1	A	1	GLU
1	A	2	LEU
1	A	15	LEU
1	A	31	THR
1	A	37	LEU
1	A	83	LEU
1	A	90	GLN
1	A	92	SER
1	A	93	HIS
1	A	116	SER
1	A	143	ASP
1	A	145	ASN
1	A	155	ARG
1	A	175	MET

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Mol	Chain	Res	Type
1	A	181	LEU
1	A	203	SER
1	A	207	LYS
1	A	212	ASN
2	B	7	SER
2	B	17	SER
2	B	60	ASN
2	B	74	SER
2	B	99	TYR
2	B	100	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 (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	30	ASN
1	L	90	GLN
1	L	137	ASN
2	H	105	GLN
1	A	27	GLN
1	A	137	ASN
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 monosaccharides 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, 95^{th} 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%)	1.71	65 (29%)	0	0	87, 95, 101, 104	0
1	L	217/217 (100%)	1.50	47 (21%)	0	0	85, 95, 100, 105	0
2	B	221/221 (100%)	1.75	69 (31%)	0	0	90, 94, 106, 116	0
2	H	221/221 (100%)	2.16	95 (42%)	0	0	90, 94, 104, 116	0
All	All	876/876 (100%)	1.78	276 (31%)	0	0	85, 94, 103, 116	0

All (276) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	98	GLY	15.3
2	H	1	GLN	8.5
2	B	163	SER	8.2
2	H	166	LEU	7.6
1	A	30	ASN	7.2
2	B	2	VAL	7.2
2	H	228	ARG	6.9
2	H	164	GLY	6.9
2	B	99	TYR	6.8
2	H	82(B)	SER	6.4
2	H	15	SER	6.2
2	H	130	ASP	6.0
1	L	190	ASN	5.9
2	H	146	GLY	5.9
1	A	69	THR	5.8
2	B	228	ARG	5.8
2	H	75	LYS	5.7
1	A	68	GLY	5.7
2	H	203	GLN	5.5
2	H	82	MET	5.2
2	H	99	TYR	5.2

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Mol	Chain	Res	Type	RSRZ
1	A	70	ASP	5.1
2	B	25	SER	5.0
2	B	100(A)	ILE	5.0
2	H	32	TYR	4.9
1	L	184	ASP	4.8
1	L	203	SER	4.8
2	H	64	MET	4.7
2	H	168	SER	4.7
1	A	49	TYR	4.7
2	H	28	SER	4.6
2	H	163	SER	4.6
1	L	172	THR	4.6
1	L	198	HIS	4.5
2	H	26	GLY	4.4
1	L	91	GLY	4.3
2	H	198	THR	4.3
2	H	14	PRO	4.2
2	H	72	ASP	4.2
2	B	1	GLN	4.2
2	H	214	ALA	4.1
2	H	227	PRO	4.1
2	H	85	ASP	4.1
2	B	166	LEU	4.1
1	L	200	THR	4.1
1	A	77	ARG	4.1
1	L	92	SER	4.1
2	B	72	ASP	4.1
2	H	80	LEU	4.0
2	B	82(C)	LEU	4.0
2	B	82(B)	SER	4.0
2	B	10	GLY	4.0
2	H	167	SER	3.9
1	A	27(E)	SER	3.9
2	H	115	LYS	3.8
2	B	127	GLY	3.8
1	A	199	LYS	3.8
2	H	134	THR	3.8
2	H	129	GLY	3.7
2	H	84	THR	3.7
1	A	67	SER	3.7
1	A	143	ASP	3.7
1	A	169	LYS	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	111	ALA	3.6
2	B	128	CYS	3.6
2	H	16	GLN	3.6
1	L	199	LYS	3.6
2	B	100	TYR	3.6
1	A	201	SER	3.5
2	H	70	SER	3.5
1	L	205	ILE	3.5
1	L	7	THR	3.5
2	H	13	ALA	3.5
1	A	71	PHE	3.5
2	H	126	PRO	3.5
2	H	27	PHE	3.5
2	H	100	TYR	3.4
1	A	27(D)	HIS	3.4
1	L	202	THR	3.4
1	L	70	ASP	3.4
1	A	76	ASN	3.4
1	A	172	THR	3.4
2	H	23	THR	3.4
2	H	217	THR	3.3
2	H	100(A)	ILE	3.3
2	H	142	CYS	3.3
1	A	58	VAL	3.3
2	B	14	PRO	3.3
2	B	45	LEU	3.3
2	B	75	LYS	3.3
1	A	27(C)	VAL	3.3
2	B	96	TRP	3.3
2	B	195	SER	3.2
2	B	12	VAL	3.2
1	L	173	TYR	3.2
2	H	9	PRO	3.2
2	B	23	THR	3.2
2	B	30	THR	3.2
2	H	79	PHE	3.2
1	L	212	ASN	3.2
2	B	26	GLY	3.2
1	A	119	PRO	3.1
2	B	16	GLN	3.1
1	L	13	VAL	3.1
2	B	102	HIS	3.1

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Mol	Chain	Res	Type	RSRZ
2	H	209	SER	3.1
2	B	126	PRO	3.1
1	L	27(C)	VAL	3.1
2	H	42	GLY	3.1
2	H	73	ASN	3.1
1	L	27(B)	ILE	3.1
1	L	77	ARG	3.1
1	A	31	THR	3.1
1	A	202	THR	3.1
2	B	24	VAL	3.1
2	B	97	GLY	3.0
2	B	162	ASN	3.0
1	L	69	THR	3.0
2	H	4	LEU	3.0
2	H	60	ASN	3.0
2	H	17	SER	3.0
2	B	61	SER	3.0
2	H	25	SER	3.0
1	A	141	PRO	3.0
2	H	18	LEU	2.9
2	H	118	PRO	2.9
1	L	79	GLU	2.9
1	A	28	ASN	2.9
1	A	184	ASP	2.9
1	L	81	GLU	2.9
2	B	100(C)	TYR	2.9
2	H	47	TRP	2.9
2	B	15	SER	2.9
1	L	109	ALA	2.9
1	L	83	LEU	2.8
1	A	118	PHE	2.8
1	A	60	ASP	2.8
2	H	71	LYS	2.8
1	A	173	TYR	2.8
1	A	53	ASN	2.8
2	H	82(A)	ASN	2.8
1	A	34	GLU	2.8
1	A	81	GLU	2.8
2	B	19	SER	2.7
1	L	15	LEU	2.7
2	B	167	SER	2.7
2	H	67	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
2	H	31	ASN	2.7
2	B	31	ASN	2.7
2	B	34	VAL	2.7
1	L	27(D)	HIS	2.7
2	H	141	GLY	2.7
1	A	32	TYR	2.7
1	A	134	CYS	2.7
2	H	127	GLY	2.7
2	H	22	CYS	2.7
2	H	45	LEU	2.7
1	L	14	SER	2.7
2	H	65	SER	2.7
2	B	227	PRO	2.7
2	H	128	CYS	2.7
1	A	25	SER	2.7
2	H	180	SER	2.7
2	B	5	LYS	2.7
2	H	101	ASP	2.7
2	H	185	TYR	2.7
2	B	22	CYS	2.6
1	A	12	PRO	2.6
2	H	157	TRP	2.6
2	B	133	THR	2.6
2	B	198	THR	2.6
1	A	133	VAL	2.6
2	H	82(C)	LEU	2.6
2	H	169	SER	2.6
2	B	141	GLY	2.6
1	L	194	CYS	2.6
1	L	31	THR	2.5
1	A	200	THR	2.5
1	L	89	PHE	2.5
1	A	135	PHE	2.5
2	B	169	SER	2.5
1	L	143	ASP	2.5
1	A	57	GLY	2.5
2	B	140	LEU	2.5
2	H	149	PRO	2.5
2	H	220	ASP	2.5
1	A	153	SER	2.5
2	B	74	SER	2.5
1	L	78	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	124	GLN	2.5
2	B	105	GLN	2.5
1	L	151	ASP	2.5
1	A	164	THR	2.4
2	H	116	THR	2.4
1	A	176	SER	2.4
2	B	58	ASN	2.4
1	A	66	GLY	2.4
1	L	33	LEU	2.4
1	L	191	SER	2.4
1	A	132	VAL	2.4
2	H	59	TYR	2.4
1	A	138	ASN	2.4
2	H	30	THR	2.4
1	L	27(E)	SER	2.4
1	A	95	PRO	2.4
2	B	101	ASP	2.4
1	A	140	TYR	2.3
2	B	129	GLY	2.3
2	H	226	GLU	2.3
2	B	27	PHE	2.3
1	A	174	SER	2.3
2	H	148	PHE	2.3
1	L	90	GLN	2.3
2	B	103	TRP	2.3
2	H	49	GLY	2.3
2	H	188	SER	2.3
2	B	203	GLN	2.3
2	B	142	CYS	2.3
2	H	12	VAL	2.3
1	A	65	SER	2.3
2	H	58	ASN	2.3
2	H	140	LEU	2.3
2	H	165	SER	2.3
1	L	55	PHE	2.3
2	H	171	VAL	2.3
2	B	189	SER	2.2
1	A	87	TYR	2.2
1	L	58	VAL	2.2
2	B	44	GLY	2.2
2	B	47	TRP	2.2
2	B	78	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	L	76	ASN	2.2
2	H	107	THR	2.2
2	H	33	GLY	2.2
2	H	100(C)	TYR	2.2
2	B	125	ALA	2.2
2	B	148	PHE	2.2
2	H	194	PRO	2.2
1	A	175	MET	2.2
1	L	128	GLY	2.2
1	L	12	PRO	2.2
1	A	160	LEU	2.2
1	A	197	THR	2.2
1	A	139	PHE	2.2
1	A	23	CYS	2.2
1	A	13	VAL	2.1
2	B	130	ASP	2.1
1	L	97	THR	2.1
2	H	117	THR	2.1
2	B	40	PRO	2.1
2	B	100(B)	PRO	2.1
2	H	90	TYR	2.1
2	H	135	GLY	2.1
2	B	124	LEU	2.1
2	B	114	ALA	2.1
1	A	162	SER	2.1
1	L	30	ASN	2.1
1	A	136	LEU	2.1
1	A	27(B)	ILE	2.1
2	H	100(E)	MET	2.1
2	B	183	GLY	2.1
2	H	124	LEU	2.1
2	B	172	HIS	2.1
1	A	98	PHE	2.1
1	L	181	LEU	2.0
2	H	37	VAL	2.0
2	H	89	VAL	2.0
2	H	187	MET	2.0
2	B	187	MET	2.0
1	L	51	VAL	2.0
1	L	49	TYR	2.0
1	A	110	ASP	2.0
1	A	109	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	212	ASN	2.0
2	H	125	ALA	2.0
1	A	94	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 monosaccharides 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^{th} 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	216	1/1	0.90	0.08	81,81,81,81	0
3	ZN	L	214	1/1	0.94	0.12	82,82,82,82	0
3	ZN	B	229	1/1	0.94	0.13	95,95,95,95	0
3	ZN	B	231	1/1	0.94	0.22	112,112,112,112	0
3	ZN	A	213	1/1	0.96	0.07	57,57,57,57	0
3	ZN	L	213	1/1	0.97	0.09	97,97,97,97	0
3	ZN	L	217	1/1	0.97	0.16	81,81,81,81	0
3	ZN	B	230	1/1	0.97	0.06	75,75,75,75	0
3	ZN	H	229	1/1	0.97	0.04	73,73,73,73	0
3	ZN	L	215	1/1	0.98	0.14	104,104,104,104	0
3	ZN	H	230	1/1	0.99	0.13	86,86,86,86	0

6.5 Other polymers (i)

There are no such residues in this entry.