



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 06:32 am GMT

PDB ID : 1GGC  
Title : MAJOR ANTIGEN-INDUCED DOMAIN REARRANGEMENTS IN AN ANTIBODY  
Authors : Takimoto-Kamimura, M.; Wilson, I.A.  
Deposited on : 1993-07-19  
Resolution : 2.80 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.

---

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

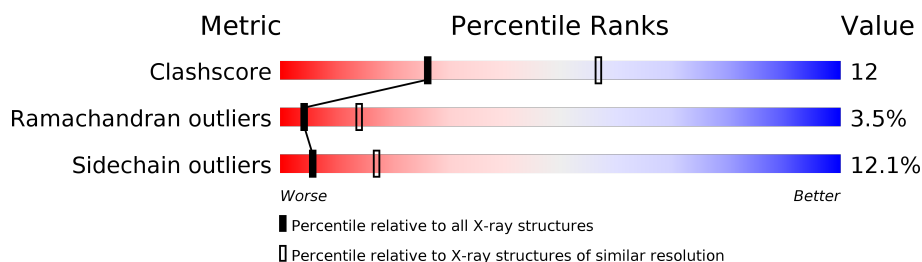
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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))
Clashscore	112137	3033 (2.80-2.80)
Ramachandran outliers	110173	2983 (2.80-2.80)
Sidechain outliers	110143	2985 (2.80-2.80)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	L	215	
2	H	215	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3291 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 IGG2A-KAPPA 50.1 FAB (LIGHT CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	215	Total	C	N	O	S	0	0	0
			1663	1031	283	344	5			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	4	LEU	MET	CONFLICT	EMBL AJ131289
L	7	SER	THR	CONFLICT	EMBL AJ131289
L	9	GLY	ALA	CONFLICT	EMBL AJ131289
L	27A	SER	ASN	CONFLICT	EMBL AJ131289
L	27C	ASP	ARG	CONFLICT	EMBL AJ131289
L	28	ASP	TYR	CONFLICT	EMBL AJ131289
L	33	LEU	MET	CONFLICT	EMBL AJ131289
L	40	PRO	ALA	CONFLICT	EMBL AJ131289
L	51	SER	ALA	CONFLICT	EMBL AJ131289
L	55	ILE	GLU	CONFLICT	EMBL AJ131289
L	60	ASP	ALA	CONFLICT	EMBL AJ131289
L	87	TYR	PHE	CONFLICT	EMBL AJ131289
L	90	GLN	ARG	CONFLICT	EMBL AJ131289
L	94	ASP	VAL	CONFLICT	EMBL AJ131289
L	96	LEU	TRP	CONFLICT	EMBL AJ131289
L	100	ALA	GLY	CONFLICT	EMBL AJ131289

- Molecule 2 is a protein called IGG2A-KAPPA 50.1 FAB (HEAVY CHAIN).

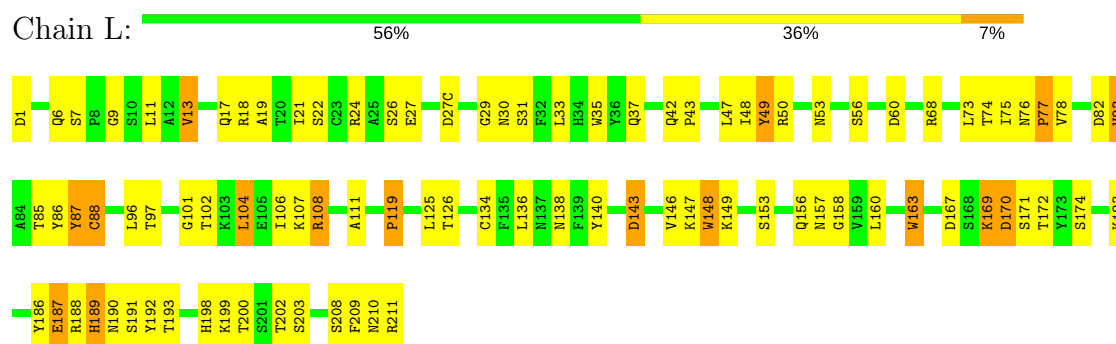
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	215	Total	C	N	O	S	0	0	0
			1628	1031	266	325	6			

### 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.

Note EDS was not executed.

#### • Molecule 1: IGG2A-KAPPA 50.1 FAB (LIGHT CHAIN)



#### • Molecule 2: IGG2A-KAPPA 50.1 FAB (HEAVY CHAIN)



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	83.70Å 110.70Å 56.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.80)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.190 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3291	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	18.0	wwPDB-VP

## 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	L	1.04	2/1699 (0.1%)	1.89	36/2309 (1.6%)
2	H	1.10	0/1670	2.03	52/2282 (2.3%)
All	All	1.07	2/3369 (0.1%)	1.96	88/4591 (1.9%)

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	L	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	7	SER	CA-CB	-5.33	1.45	1.52
1	L	31	SER	CA-CB	-5.04	1.45	1.52

All (88) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	50	ARG	NE-CZ-NH2	-8.99	115.80	120.30
1	L	163	TRP	CD1-CG-CD2	8.92	113.44	106.30
1	L	18	ARG	NE-CZ-NH2	-8.88	115.86	120.30
1	L	49	TYR	CB-CG-CD1	-8.88	115.67	121.00
2	H	36	TRP	CD1-CG-CD2	8.51	113.11	106.30
2	H	32	TYR	CB-CG-CD2	-8.39	115.97	121.00
2	H	199	TRP	CD1-CG-CD2	8.00	112.70	106.30
2	H	220	ASP	CB-CG-OD1	7.97	125.48	118.30
1	L	186	TYR	CB-CG-CD2	-7.77	116.34	121.00
1	L	163	TRP	CE2-CD2-CG	-7.64	101.19	107.30
2	H	59	TYR	CB-CG-CD1	-7.60	116.44	121.00
1	L	50	ARG	NE-CZ-NH1	7.38	123.99	120.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	56	SER	N-CA-CB	-7.14	99.79	110.50
2	H	103	TRP	CD1-CG-CD2	7.05	111.94	106.30
2	H	53	TRP	CE2-CD2-CG	-7.00	101.70	107.30
2	H	36	TRP	CE2-CD2-CG	-6.97	101.72	107.30
1	L	146	VAL	CG1-CB-CG2	-6.96	99.76	110.90
1	L	35	TRP	CD1-CG-CD2	6.85	111.78	106.30
1	L	148	TRP	CG-CD2-CE3	6.84	140.06	133.90
2	H	157	TRP	CD1-CG-CD2	6.76	111.71	106.30
1	L	148	TRP	CE2-CD2-CG	-6.66	101.97	107.30
2	H	47	TRP	CD1-CG-CD2	6.61	111.59	106.30
2	H	53	TRP	CB-CG-CD1	-6.61	118.40	127.00
2	H	92	CYS	CA-CB-SG	-6.53	102.24	114.00
2	H	157	TRP	CE2-CD2-CG	-6.51	102.09	107.30
2	H	36	TRP	CG-CD1-NE1	-6.46	103.64	110.10
1	L	13	VAL	CG1-CB-CG2	-6.39	100.68	110.90
2	H	32	TYR	CG-CD1-CE1	-6.34	116.22	121.30
2	H	129	GLY	N-CA-C	-6.34	97.25	113.10
1	L	35	TRP	CE2-CD2-CG	-6.32	102.24	107.30
1	L	148	TRP	CD1-CG-CD2	6.31	111.34	106.30
2	H	53	TRP	NE1-CE2-CZ2	-6.30	123.47	130.40
2	H	199	TRP	CE2-CD2-CG	-6.29	102.27	107.30
2	H	19	SER	O-C-N	6.29	132.76	122.70
2	H	95	GLU	CA-CB-CG	6.26	127.18	113.40
2	H	47	TRP	CE2-CD2-CG	-6.24	102.31	107.30
2	H	171	VAL	CB-CA-C	-6.23	99.56	111.40
1	L	108	ARG	NE-CZ-NH1	-6.21	117.19	120.30
1	L	49	TYR	CD1-CG-CD2	6.18	124.70	117.90
2	H	135	GLY	CA-C-N	-6.11	103.76	117.20
1	L	188	ARG	NE-CZ-NH2	-6.10	117.25	120.30
1	L	49	TYR	CG-CD1-CE1	-6.04	116.47	121.30
2	H	32	TYR	CD1-CG-CD2	6.03	124.53	117.90
2	H	66	ARG	NE-CZ-NH1	6.00	123.30	120.30
2	H	53	TRP	CG-CD2-CE3	5.94	139.25	133.90
2	H	9	PRO	CA-C-N	5.94	128.07	116.20
2	H	103	TRP	CE2-CD2-CG	-5.89	102.59	107.30
2	H	97	TYR	CB-CG-CD2	-5.81	117.51	121.00
2	H	101	ILE	CA-CB-CG1	-5.77	100.04	111.00
1	L	83	VAL	CG1-CB-CG2	-5.73	101.74	110.90
2	H	146	GLY	CA-C-N	5.72	129.78	117.20
1	L	88	CYS	CA-CB-SG	5.70	124.26	114.00
1	L	163	TRP	CG-CD1-NE1	-5.70	104.40	110.10
2	H	122	TYR	CB-CG-CD1	-5.68	117.59	121.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	169	LYS	CA-CB-CG	5.63	125.79	113.40
1	L	18	ARG	NE-CZ-NH1	5.61	123.11	120.30
2	H	22	CYS	CA-CB-SG	-5.61	103.91	114.00
2	H	69	ILE	CB-CA-C	-5.52	100.57	111.60
1	L	189	HIS	CB-CA-C	-5.51	99.39	110.40
1	L	170	ASP	N-CA-C	-5.47	96.23	111.00
2	H	11	ILE	N-CA-C	-5.47	96.23	111.00
2	H	103	TRP	CA-C-N	5.47	127.14	116.20
2	H	220	ASP	CB-CG-OD2	-5.46	113.38	118.30
1	L	82	ASP	CB-CG-OD1	5.46	123.21	118.30
1	L	187	GLU	CA-CB-CG	-5.46	101.40	113.40
2	H	41	SER	N-CA-CB	-5.46	102.32	110.50
1	L	87	TYR	CB-CG-CD2	-5.43	117.74	121.00
1	L	163	TRP	CB-CG-CD1	-5.41	119.97	127.00
1	L	188	ARG	N-CA-CB	-5.26	101.12	110.60
2	H	47	TRP	CG-CD1-NE1	-5.26	104.84	110.10
1	L	148	TRP	CB-CG-CD1	-5.23	120.20	127.00
2	H	97	TYR	CD1-CG-CD2	5.23	123.65	117.90
2	H	87	THR	CA-C-N	-5.23	105.70	117.20
2	H	178	LEU	CA-CB-CG	5.19	127.24	115.30
2	H	199	TRP	CG-CD1-NE1	-5.17	104.93	110.10
2	H	90	TYR	CA-CB-CG	-5.15	103.62	113.40
2	H	103	TRP	CG-CD1-NE1	-5.15	104.95	110.10
1	L	75	ILE	N-CA-C	-5.14	97.13	111.00
1	L	24	ARG	NE-CZ-NH1	5.11	122.86	120.30
1	L	126	THR	CA-CB-OG1	-5.10	98.28	109.00
2	H	61	PRO	CA-C-N	5.08	128.37	117.20
1	L	27(C)	ASP	CB-CA-C	-5.07	100.26	110.40
2	H	107	THR	CA-CB-CG2	5.07	119.49	112.40
2	H	21	THR	CA-C-N	-5.06	106.07	117.20
2	H	59	TYR	CG-CD1-CE1	-5.05	117.26	121.30
2	H	117	THR	CA-CB-CG2	-5.05	105.34	112.40
2	H	79	PHE	CB-CA-C	-5.03	100.34	110.40
2	H	177	VAL	CG1-CB-CG2	-5.01	102.88	110.90

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	L	140	TYR	Sidechain
1	L	42	GLN	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	L	1663	0	1592	34	0
2	H	1628	0	1596	46	0
All	All	3291	0	3188	76	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 12.

All (76) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:119:PRO:HB3	2:H:147:TYR:HB3	1.59	0.84
2:H:18:LEU:HD23	2:H:82:ILE:HD12	1.62	0.81
2:H:13:GLN:H	2:H:16:GLN:HE22	1.30	0.79
1:L:21:ILE:HD12	1:L:73:LEU:HD23	1.70	0.74
1:L:148:TRP:HB2	1:L:156:GLN:NE2	2.02	0.73
1:L:193:THR:HG23	1:L:208:SER:HB3	1.70	0.72
2:H:39:GLN:HB2	2:H:45:LEU:HD23	1.77	0.66
1:L:148:TRP:HB2	1:L:156:GLN:HE21	1.62	0.64
2:H:140:LEU:HD13	2:H:223:ILE:HG21	1.81	0.61
2:H:4:LEU:HD12	2:H:102:TYR:HD1	1.65	0.61
1:L:119:PRO:HB2	2:H:228:ARG:NH1	2.17	0.60
2:H:28:SER:O	2:H:34:MET:HG2	2.02	0.59
2:H:94:GLN:HE21	2:H:102:TYR:HB3	1.68	0.59
2:H:13:GLN:N	2:H:16:GLN:HE22	1.98	0.58
1:L:83:VAL:HA	1:L:104:LEU:HD23	1.86	0.58
1:L:210:ASN:O	1:L:211:ARG:HG3	2.04	0.57
2:H:173:THR:HG23	2:H:189:SER:HB2	1.86	0.56
2:H:47:TRP:HZ2	2:H:50:HIS:HB2	1.71	0.55
1:L:37:GLN:HB2	1:L:47:LEU:HD11	1.89	0.55
2:H:66:ARG:O	2:H:82:ILE:HA	2.07	0.54
2:H:40:PRO:HB2	2:H:43:LYS:CG	2.38	0.53
1:L:119:PRO:HB2	2:H:228:ARG:HH12	1.73	0.52
1:L:6:GLN:HG2	1:L:88:CYS:SG	2.49	0.52
2:H:6:GLU:HG3	2:H:92:CYS:HB2	1.92	0.52
2:H:179:GLN:NE2	2:H:186:THR:OG1	2.43	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:171:VAL:HG12	2:H:172:HIS:N	2.26	0.51
1:L:160:LEU:HD21	2:H:179:GLN:HB3	1.91	0.50
1:L:6:GLN:OE1	1:L:87:TYR:HA	2.11	0.50
2:H:198:THR:O	2:H:203:GLN:HG3	2.11	0.50
1:L:167:ASP:O	1:L:171:SER:HA	2.12	0.49
1:L:189:HIS:O	1:L:211:ARG:NH1	2.45	0.49
2:H:40:PRO:HB2	2:H:43:LYS:HD2	1.95	0.49
1:L:191:SER:HA	1:L:209:PHE:O	2.13	0.49
2:H:199:TRP:HD1	2:H:205:ILE:HG13	1.78	0.48
1:L:149:LYS:HA	1:L:153:SER:O	2.14	0.48
1:L:11:LEU:HD23	1:L:104:LEU:HD12	1.96	0.47
2:H:154:LEU:HA	2:H:209:ASN:O	2.15	0.47
1:L:49:TYR:O	1:L:53:ASN:HB2	2.14	0.47
2:H:18:LEU:HD13	2:H:109:VAL:HG11	1.96	0.47
2:H:71:LYS:HA	2:H:78:VAL:HA	1.97	0.47
2:H:72:ASP:N	2:H:77:GLN:O	2.49	0.46
1:L:108:ARG:HH12	1:L:111:ALA:HB2	1.80	0.46
2:H:176:ALA:HA	2:H:186:THR:O	2.15	0.45
2:H:199:TRP:CD1	2:H:205:ILE:HG13	2.52	0.45
1:L:190:ASN:HA	1:L:211:ARG:HH11	1.82	0.44
2:H:2:VAL:HA	2:H:25:SER:O	2.17	0.44
2:H:179:GLN:HG2	2:H:184:LEU:O	2.18	0.44
2:H:12:LEU:HD23	2:H:82(C):VAL:HG21	2.00	0.44
2:H:13:GLN:N	2:H:16:GLN:NE2	2.65	0.44
2:H:81:LYS:HB3	2:H:81:LYS:HE2	1.63	0.43
1:L:189:HIS:HB2	1:L:192:TYR:OH	2.17	0.43
2:H:12:LEU:HD12	2:H:12:LEU:HA	1.88	0.43
2:H:22:CYS:HB2	2:H:36:TRP:CZ2	2.53	0.43
1:L:9:GLY:O	1:L:102:THR:HA	2.18	0.43
2:H:226:GLU:HA	2:H:227:PRO:HD3	1.76	0.43
1:L:76:ASN:HA	1:L:77:PRO:HA	1.87	0.43
2:H:24:PHE:HB2	2:H:27:PHE:CE1	2.54	0.43
1:L:13:VAL:HG21	1:L:78:VAL:HG11	2.01	0.43
1:L:183:LYS:O	1:L:187:GLU:HG3	2.19	0.42
2:H:148:PHE:CD1	2:H:149:PRO:HA	2.54	0.42
2:H:83:ASP:O	2:H:111:VAL:HG11	2.19	0.42
1:L:157:ASN:OD1	1:L:158:GLY:N	2.52	0.42
1:L:198:HIS:O	1:L:200:THR:N	2.53	0.42
2:H:38:ARG:HA	2:H:89:THR:O	2.20	0.42
1:L:143:ASP:O	1:L:198:HIS:HD2	2.03	0.42
2:H:22:CYS:O	2:H:77:GLN:HA	2.20	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:86:TYR:O	1:L:101:GLY:HA2	2.19	0.41
2:H:94:GLN:HE21	2:H:102:TYR:CB	2.33	0.41
1:L:43:PRO:HB3	2:H:91:TYR:CE1	2.55	0.41
2:H:6:GLU:HA	2:H:21:THR:O	2.21	0.41
2:H:172:HIS:O	2:H:189:SER:HA	2.20	0.41
1:L:19:ALA:O	1:L:74:THR:HA	2.21	0.41
2:H:67:LEU:HD23	2:H:82:ILE:HG12	2.02	0.41
1:L:148:TRP:HD1	1:L:156:GLN:HE22	1.68	0.41
1:L:125:LEU:O	1:L:183:LYS:HE2	2.21	0.40
1:L:48:ILE:HG21	1:L:48:ILE:HD13	1.84	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	L	213/215 (99%)	192 (90%)	14 (7%)	7 (3%)	4	15
2	H	213/215 (99%)	189 (89%)	16 (8%)	8 (4%)	4	12
All	All	426/430 (99%)	381 (89%)	30 (7%)	15 (4%)	4	14

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	174	SER
1	L	199	LYS
2	H	95	GLU
2	H	116	THR
1	L	138	ASN
2	H	128	CYS
2	H	138	VAL
1	L	29	GLY

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	L	60	ASP
1	L	68	ARG
2	H	14	PRO
2	H	43	LYS
2	H	15	SER
2	H	55	GLY
1	L	119	PRO

### 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	L	191/191 (100%)	167 (87%)	24 (13%)	5	16
2	H	189/189 (100%)	167 (88%)	22 (12%)	6	19
All	All	380/380 (100%)	334 (88%)	46 (12%)	6	17

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	1	ASP
1	L	17	GLN
1	L	22	SER
1	L	26	SER
1	L	27	GLU
1	L	30	ASN
1	L	33	LEU
1	L	77	PRO
1	L	85	THR
1	L	96	LEU
1	L	97	THR
1	L	104	LEU
1	L	106	ILE
1	L	107	LYS
1	L	134	CYS
1	L	136	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	L	143	ASP
1	L	147	LYS
1	L	163	TRP
1	L	169	LYS
1	L	170	ASP
1	L	172	THR
1	L	202	THR
1	L	203	SER
2	H	14	PRO
2	H	28	SER
2	H	29	LEU
2	H	43	LYS
2	H	46	GLU
2	H	65	SER
2	H	73	THR
2	H	82(B)	SER
2	H	101	ILE
2	H	119	PRO
2	H	134	THR
2	H	149	PRO
2	H	151	PRO
2	H	152	VAL
2	H	166	LEU
2	H	168	SER
2	H	178	LEU
2	H	180	SER
2	H	187	LEU
2	H	196	SER
2	H	203	GLN
2	H	220	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	38	GLN
1	L	156	GLN
2	H	16	GLN
2	H	39	GLN
2	H	76	ASN
2	H	94	GLN
2	H	179	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 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

EDS was not executed - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.