



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 07:48 PM UTC

PDB ID : 1GGC / pdb_00001ggc
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

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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

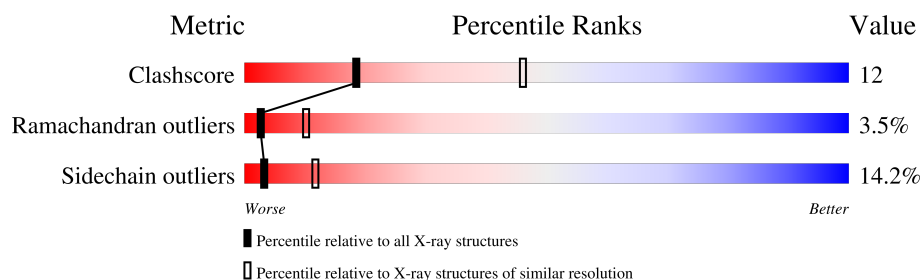
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (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 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	L	215	42% 44% 13%
2	H	215	42% 41% 16%

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

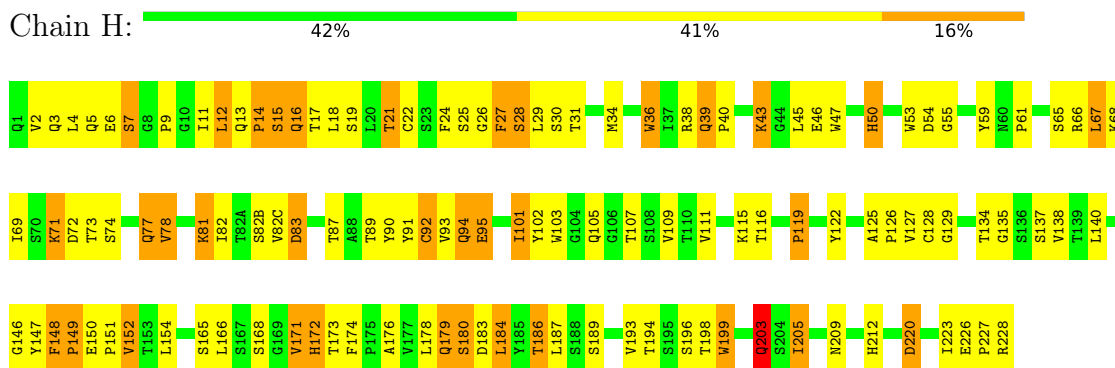
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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, α , β , γ	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 ²)	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	1.33	6/1699 (0.4%)	2.23	84/2309 (3.6%)
2	H	1.37	10/1670 (0.6%)	2.36	83/2282 (3.6%)
All	All	1.35	16/3369 (0.5%)	2.30	167/4591 (3.6%)

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 (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	189	HIS	CD2-NE2	-6.73	1.30	1.37
2	H	212	HIS	CD2-NE2	-6.43	1.30	1.37
1	L	34	HIS	CD2-NE2	-6.05	1.31	1.37
2	H	126	PRO	CA-CB	-5.88	1.45	1.53
1	L	198	HIS	CD2-NE2	-5.83	1.31	1.37
2	H	16	GLN	CA-CB	-5.81	1.44	1.53
1	L	87	TYR	CA-C	-5.50	1.46	1.52
1	L	206	VAL	CA-CB	5.46	1.60	1.54
2	H	12	LEU	CB-CG	-5.40	1.42	1.53
1	L	7	SER	CA-CB	-5.36	1.45	1.53
2	H	50	HIS	CD2-NE2	-5.33	1.31	1.37
2	H	172	HIS	CG-ND1	-5.18	1.32	1.38
2	H	172	HIS	CD2-NE2	-5.17	1.32	1.37
2	H	53	TRP	NE1-CE2	-5.13	1.31	1.37
2	H	39	GLN	CA-CB	-5.11	1.46	1.53
2	H	31	THR	CA-C	-5.02	1.46	1.52

All (167) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	127	VAL	N-CA-C	-10.75	99.86	110.72
2	H	220	ASP	CA-CB-CG	10.69	123.29	112.60
2	H	26	GLY	O-C-N	8.82	129.76	122.71
2	H	199	TRP	O-C-N	-8.70	113.48	121.66
1	L	27(C)	ASP	N-CA-C	8.54	121.55	110.53
1	L	170	ASP	CA-CB-CG	8.51	121.11	112.60
2	H	11	ILE	N-CA-C	-8.21	96.23	108.46
2	H	19	SER	O-C-N	8.18	132.76	123.27
1	L	6	GLN	OE1-CD-NE2	-8.10	114.50	122.60
1	L	156	GLN	N-CA-C	7.79	120.86	110.88
1	L	39	LYS	N-CA-C	-7.69	100.40	109.93
1	L	6	GLN	CG-CD-NE2	7.68	127.92	116.40
2	H	16	GLN	N-CA-C	7.65	120.91	110.35
1	L	27(C)	ASP	CA-CB-CG	7.64	120.24	112.60
1	L	126	THR	CA-CB-OG1	-7.54	98.28	109.60
1	L	76	ASN	CA-CB-CG	-7.50	105.11	112.60
1	L	170	ASP	N-CA-C	-7.42	96.23	108.76
2	H	146	GLY	O-C-N	-7.39	115.17	122.41
2	H	94	GLN	OE1-CD-NE2	-7.33	115.27	122.60
1	L	134	CYS	CA-C-N	7.21	132.35	122.19
1	L	134	CYS	C-N-CA	7.21	132.35	122.19
1	L	198	HIS	N-CA-C	7.13	119.91	107.49
2	H	69	ILE	CB-CA-C	-7.11	100.57	111.31
2	H	171	VAL	CB-CA-C	-7.07	99.56	110.95
1	L	119	PRO	N-CA-C	7.04	119.29	110.70
1	L	43	PRO	N-CA-C	7.03	119.28	110.70
2	H	54	ASP	CA-CB-CG	6.97	119.58	112.60
1	L	34	HIS	CB-CG-CD2	-6.97	122.14	131.20
1	L	60	ASP	CA-CB-CG	6.88	119.48	112.60
1	L	113	PRO	N-CA-C	6.84	121.12	110.80
2	H	82(B)	SER	N-CA-C	6.83	120.50	111.28
2	H	59	TYR	CA-C-O	6.82	129.43	121.46
2	H	101	ILE	N-CA-C	6.77	117.53	110.62
2	H	183	ASP	CA-CB-CG	6.76	119.36	112.60
1	L	6	GLN	O-C-N	-6.75	115.10	122.79
2	H	129	GLY	N-CA-C	-6.72	97.25	113.18
2	H	61	PRO	CA-C-O	-6.69	109.39	119.55
1	L	66	GLY	N-CA-C	6.64	118.79	112.08
2	H	53	TRP	CA-C-O	6.64	127.58	120.55
2	H	5	GLN	CB-CG-CD	6.58	123.78	112.60
2	H	50	HIS	CB-CG-ND1	6.57	132.55	122.70
2	H	74	SER	N-CA-C	-6.56	104.31	112.90
1	L	37	GLN	O-C-N	-6.56	114.71	123.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	95	GLU	CA-CB-CG	6.54	127.18	114.10
2	H	105	GLN	N-CA-C	6.49	119.35	111.82
1	L	188	ARG	N-CA-CB	-6.45	101.12	110.47
1	L	75	ILE	N-CA-C	-6.38	97.13	107.28
2	H	193	VAL	O-C-N	-6.36	116.00	123.00
1	L	187	GLU	CA-CB-CG	-6.35	101.40	114.10
2	H	92	CYS	CA-C-O	-6.34	113.38	120.54
2	H	90	TYR	CA-C-O	-6.33	113.38	120.54
1	L	196	ALA	CA-C-O	6.29	127.71	120.60
1	L	16	GLY	CA-C-O	-6.26	112.64	119.59
2	H	9	PRO	O-C-N	-6.25	115.65	123.21
1	L	56	SER	N-CA-CB	-6.23	99.79	109.69
1	L	82	ASP	CA-CB-CG	6.23	118.83	112.60
1	L	208	SER	CA-C-O	-6.21	114.39	121.40
2	H	186	THR	CA-CB-OG1	-6.21	100.29	109.60
1	L	55	ILE	CA-C-O	6.21	127.78	121.58
2	H	152	VAL	CB-CA-C	-6.17	102.01	110.90
1	L	148	TRP	CG-CD2-CE3	6.16	140.06	133.90
2	H	27	PHE	CA-C-O	-6.16	114.44	121.40
1	L	189	HIS	CB-CG-CD2	-6.13	123.22	131.20
1	L	90	GLN	N-CA-C	-6.12	100.93	110.42
2	H	199	TRP	N-CA-C	-6.11	100.91	110.14
2	H	101	ILE	CA-CB-CG1	-6.09	100.04	110.40
1	L	198	HIS	CB-CG-CD2	-6.04	123.34	131.20
1	L	106	ILE	O-C-N	-6.03	116.33	122.54
2	H	50	HIS	CB-CG-CD2	-6.00	123.40	131.20
2	H	93	VAL	O-C-N	-5.99	116.95	123.18
2	H	122	TYR	CA-C-N	5.99	126.49	120.14
2	H	122	TYR	C-N-CA	5.99	126.49	120.14
2	H	174	PHE	CA-CB-CG	-5.98	107.82	113.80
1	L	71	PHE	CA-C-O	-5.93	114.70	121.58
2	H	103	TRP	CA-C-O	-5.87	113.91	120.54
1	L	178	THR	CA-CB-OG1	-5.85	100.82	109.60
1	L	169	LYS	CA-CB-CG	5.85	125.79	114.10
1	L	24	ARG	CA-C-O	-5.80	114.44	120.70
1	L	42	GLN	OE1-CD-NE2	-5.79	116.81	122.60
2	H	150	GLU	O-C-N	-5.77	114.97	121.43
2	H	21	THR	CA-C-O	5.76	127.23	120.20
2	H	178	LEU	N-CA-C	-5.76	101.12	109.59
1	L	89	GLN	O-C-N	-5.75	116.36	123.44
1	L	25	ALA	O-C-N	-5.73	115.94	123.16
2	H	90	TYR	CA-CB-CG	-5.71	103.62	113.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	31	SER	CA-CB-OG	-5.71	99.69	111.10
2	H	30	SER	CA-CB-OG	5.67	122.44	111.10
2	H	53	TRP	CB-CG-CD1	-5.66	118.40	126.90
1	L	169	LYS	O-C-N	-5.63	115.36	122.17
2	H	135	GLY	O-C-N	5.62	130.34	122.30
2	H	67	LEU	O-C-N	-5.61	115.90	123.19
2	H	94	GLN	CG-CD-NE2	5.61	124.81	116.40
1	L	149	LYS	CA-CB-CG	-5.60	102.89	114.10
1	L	33	LEU	CA-C-O	-5.59	114.78	120.71
1	L	38	GLN	OE1-CD-NE2	-5.57	117.03	122.60
1	L	208	SER	N-CA-C	5.55	117.62	109.24
2	H	125	ALA	N-CA-C	-5.53	101.95	110.58
1	L	156	GLN	OE1-CD-NE2	-5.53	117.07	122.60
2	H	15	SER	CA-CB-OG	5.52	122.13	111.10
2	H	127	VAL	CA-C-N	5.51	132.06	121.54
2	H	127	VAL	C-N-CA	5.51	132.06	121.54
1	L	150	ILE	CA-C-O	5.50	127.11	120.74
1	L	149	LYS	N-CA-C	5.47	117.77	108.02
1	L	197	THR	N-CA-CB	-5.44	101.03	110.17
1	L	190	ASN	OD1-CG-ND2	-5.44	117.16	122.60
1	L	99	GLY	N-CA-C	-5.43	104.38	113.02
1	L	50	ARG	CA-C-N	5.42	131.90	121.54
1	L	50	ARG	C-N-CA	5.42	131.90	121.54
1	L	102	THR	N-CA-C	-5.42	99.86	109.06
2	H	148	PHE	CB-CA-C	-5.40	102.57	109.92
1	L	38	GLN	CG-CD-NE2	5.40	124.50	116.40
2	H	17	THR	CA-CB-OG1	-5.39	101.52	109.60
1	L	30	ASN	CA-CB-CG	5.39	117.99	112.60
1	L	140	TYR	O-C-N	-5.39	115.81	122.16
1	L	188	ARG	O-C-N	-5.37	115.46	122.39
1	L	82	ASP	CA-C-O	5.36	125.50	119.18
2	H	53	TRP	CG-CD2-CE3	5.35	139.25	133.90
1	L	92	ASN	CB-CG-ND2	5.34	124.42	116.40
2	H	107	THR	CA-CB-OG1	-5.34	101.59	109.60
1	L	34	HIS	CB-CG-ND1	5.33	130.69	122.70
1	L	186	TYR	N-CA-C	-5.33	105.56	111.36
2	H	30	SER	CA-C-N	5.32	128.27	120.71
2	H	30	SER	C-N-CA	5.32	128.27	120.71
2	H	137	SER	CA-C-N	5.32	131.54	121.97
2	H	137	SER	C-N-CA	5.32	131.54	121.97
2	H	71	LYS	O-C-N	-5.32	117.10	123.27
2	H	78	VAL	N-CA-C	-5.31	100.71	108.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	212	HIS	CB-CG-CD2	-5.30	124.31	131.20
2	H	107	THR	CA-CB-CG2	5.29	119.49	110.50
2	H	3	GLN	OE1-CD-NE2	-5.29	117.31	122.60
2	H	92	CYS	CA-CB-SG	-5.29	102.24	114.40
2	H	101	ILE	CA-CB-CG2	5.28	119.48	110.50
1	L	56	SER	CB-CA-C	5.27	118.18	109.70
1	L	91	SER	N-CA-C	-5.27	104.65	111.71
2	H	7	SER	N-CA-C	-5.26	101.30	109.72
2	H	21	THR	N-CA-C	5.26	117.00	108.26
2	H	115	LYS	O-C-N	5.24	129.68	123.33
2	H	165	SER	CA-CB-OG	5.24	121.59	111.10
1	L	156	GLN	CA-C-O	5.23	127.38	121.32
1	L	169	LYS	N-CA-CB	-5.22	102.40	110.13
1	L	117	ILE	O-C-N	-5.22	116.74	122.69
2	H	193	VAL	CA-C-O	-5.22	116.34	121.67
2	H	93	VAL	N-CA-C	5.20	115.46	107.77
2	H	77	GLN	CA-C-O	-5.19	114.69	120.66
1	L	119	PRO	CA-C-N	5.16	125.10	119.78
1	L	119	PRO	C-N-CA	5.16	125.10	119.78
1	L	132	VAL	N-CA-C	-5.16	98.26	107.18
1	L	20	THR	CA-CB-OG1	-5.15	101.87	109.60
1	L	189	HIS	CB-CA-C	-5.15	99.39	110.45
2	H	203	GLN	N-CA-C	-5.13	101.39	109.50
2	H	54	ASP	N-CA-C	-5.12	105.75	112.72
1	L	173	TYR	CA-C-O	-5.10	113.21	120.51
1	L	63	SER	CA-C-O	-5.09	115.36	121.11
1	L	2	ILE	CB-CA-C	5.09	117.22	110.91
1	L	62	PHE	CA-C-N	-5.09	114.82	122.81
1	L	62	PHE	C-N-CA	-5.09	114.82	122.81
2	H	87	THR	CA-C-O	5.08	126.47	120.58
2	H	5	GLN	CG-CD-NE2	-5.06	108.80	116.40
2	H	179	GLN	O-C-N	-5.06	115.86	122.59
2	H	101	ILE	O-C-N	-5.06	116.96	121.87
2	H	36	TRP	CG-CD1-NE1	-5.05	103.64	110.20
2	H	194	THR	O-C-N	-5.05	116.44	122.65
2	H	83	ASP	O-C-N	-5.03	115.89	122.59
1	L	139	PHE	CA-CB-CG	5.02	118.82	113.80
1	L	146	VAL	CG1-CB-CG2	-5.02	99.76	110.80
1	L	53	ASN	OD1-CG-ND2	-5.01	117.59	122.60
1	L	163	TRP	CE2-CD2-CG	-5.01	101.19	107.20

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	48	0
All	All	3291	0	3188	78	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 (78) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:L:49:TYR:O	1:L:53:ASN:HB2	2.14	0.47
2:H:154:LEU:HA	2:H:209:ASN:O	2.15	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
1:L:189:HIS:HB2	1:L:192:TYR:OH	2.17	0.43
2:H:81:LYS:HB3	2:H:81:LYS:HE2	1.63	0.43
2:H:27:PHE:HB2	2:H:34:MET:HE3	2.01	0.43
1:L:9:GLY:O	1:L:102:THR:HA	2.18	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
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
1:L:13:VAL:HG21	1:L:78:VAL:HG11	2.01	0.43
2:H:24:PHE:HB2	2:H:27:PHE:CE1	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:180:SER:C	2:H:184:LEU:H	2.28	0.41
2:H:6:GLU:HA	2:H:21:THR:O	2.21	0.41
1:L:19:ALA:O	1:L:74:THR:HA	2.21	0.41
2:H:172:HIS:O	2:H:189:SER:HA	2.20	0.41
1:L:148:TRP:HD1	1:L:156:GLN:HE22	1.68	0.41
2:H:67:LEU:HD23	2:H:82:ILE:HG12	2.02	0.41
1:L:48:ILE:HD13	1:L:48:ILE:HG21	1.84	0.40
1:L:125:LEU:O	1:L:183:LYS:HE2	2.21	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%)	3	11
2	H	213/215 (99%)	189 (89%)	16 (8%)	8 (4%)	2	9
All	All	426/430 (99%)	381 (89%)	30 (7%)	15 (4%)	3	10

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
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 [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	L	191/191 (100%)	161 (84%)	30 (16%)	2	9
2	H	189/189 (100%)	165 (87%)	24 (13%)	4	15
All	All	380/380 (100%)	326 (86%)	54 (14%)	3	12

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	17	GLN
1	L	22	SER
1	L	26	SER
1	L	27	GLU
1	L	27(A)	SER
1	L	27(B)	VAL
1	L	27(C)	ASP
1	L	27(D)	ASP
1	L	30	ASN

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Mol	Chain	Res	Type
1	L	33	LEU
1	L	77	PRO
1	L	85	THR
1	L	96	LEU
1	L	97	THR
1	L	103	LYS
1	L	104	LEU
1	L	106	ILE
1	L	107	LYS
1	L	126	THR
1	L	134	CYS
1	L	136	LEU
1	L	143	ASP
1	L	147	LYS
1	L	159	VAL
1	L	169	LYS
1	L	172	THR
1	L	179	LEU
1	L	202	THR
1	L	203	SER
1	L	206	VAL
2	H	7	SER
2	H	14	PRO
2	H	28	SER
2	H	29	LEU
2	H	46	GLU
2	H	65	SER
2	H	68	LYS
2	H	73	THR
2	H	81	LYS
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	180	SER
2	H	184	LEU
2	H	187	LEU
2	H	196	SER

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Mol	Chain	Res	Type
2	H	203	GLN
2	H	205	ILE
2	H	220	ASP

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

Mol	Chain	Res	Type
1	L	37	GLN
1	L	38	GLN
1	L	42	GLN
1	L	92	ASN
1	L	137	ASN
1	L	145	ASN
1	L	156	GLN
2	H	16	GLN
2	H	39	GLN
2	H	75	ASN
2	H	94	GLN
2	H	105	GLN
2	H	172	HIS
2	H	179	GLN
2	H	203	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 oligosaccharides 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

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.