



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:02 PM UTC

PDB ID : 1GGB / pdb_00001ggb
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

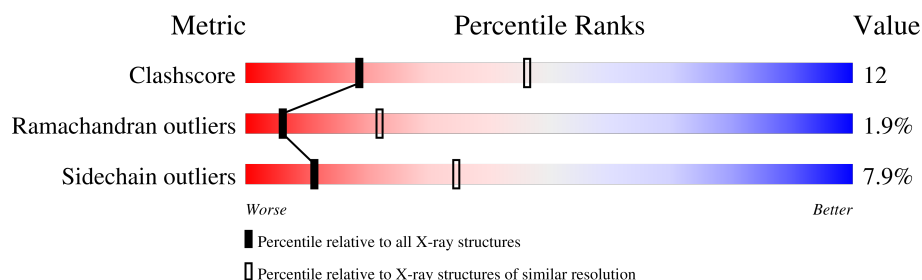
1 Overall quality at a glance

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	
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).

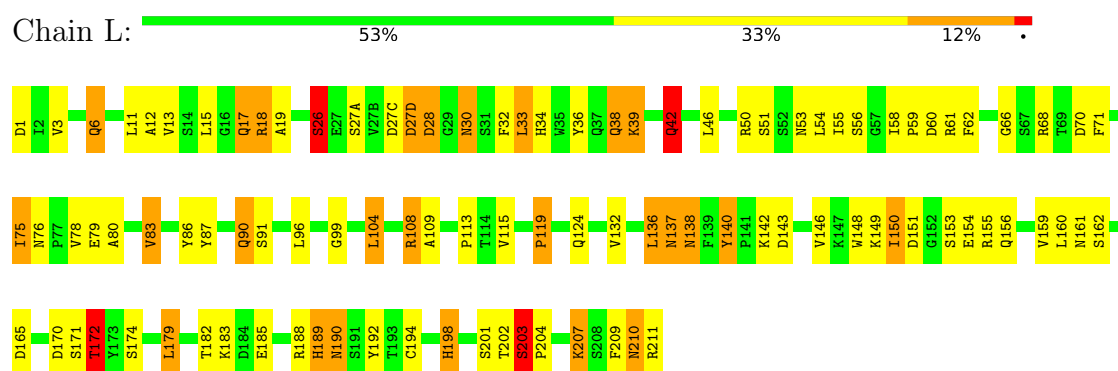
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	215	Total	C	N	O	S	0	0	0
			1628	1031	266	325	6			

3 Residue-property plots

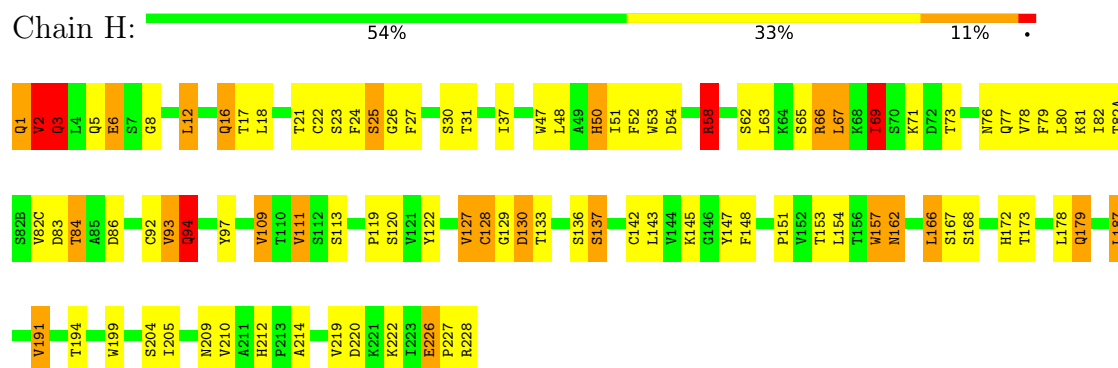
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	123.10Å 119.50Å 109.50Å 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}	0.200 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3291	wwPDB-VP
Average B, all atoms (Å ²)	28.0	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	1.29	12/1699 (0.7%)	2.02	62/2309 (2.7%)
2	H	1.58	18/1670 (1.1%)	2.25	72/2282 (3.2%)
All	All	1.44	30/3369 (0.9%)	2.14	134/4591 (2.9%)

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 (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	52	PHE	CA-CB	-9.15	1.38	1.53
2	H	120	SER	CA-CB	-8.28	1.41	1.53
2	H	210	VAL	CA-CB	-7.23	1.45	1.54
1	L	124	GLN	CA-CB	-7.02	1.42	1.53
2	H	78	VAL	CA-CB	-6.94	1.45	1.54
1	L	162	SER	CA-CB	-6.66	1.42	1.53
2	H	222	LYS	CA-CB	-6.45	1.44	1.53
2	H	79	PHE	CA-CB	-6.38	1.41	1.53
2	H	212	HIS	CD2-NE2	-6.30	1.30	1.37
1	L	198	HIS	CD2-NE2	-6.25	1.30	1.37
1	L	83	VAL	CA-CB	6.13	1.61	1.53
1	L	34	HIS	CD2-NE2	-6.09	1.31	1.37
2	H	50	HIS	CD2-NE2	-6.06	1.31	1.37
2	H	142	CYS	CA-CB	-6.06	1.43	1.53
1	L	189	HIS	CG-ND1	-6.02	1.31	1.38
1	L	189	HIS	CD2-NE2	-5.95	1.31	1.37
2	H	220	ASP	CA-CB	-5.93	1.44	1.53
2	H	143	LEU	CA-CB	-5.71	1.44	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	172	HIS	CD2-NE2	-5.66	1.31	1.37
1	L	185	GLU	CA-CB	-5.63	1.44	1.53
2	H	133	THR	CA-CB	5.60	1.62	1.53
2	H	166	LEU	CA-CB	-5.33	1.46	1.53
1	L	198	HIS	CG-ND1	-5.30	1.32	1.38
2	H	6	GLU	CA-CB	-5.30	1.45	1.53
2	H	219	VAL	CA-CB	-5.28	1.47	1.54
1	L	38	GLN	CD-NE2	-5.25	1.22	1.33
2	H	23	SER	CA-CB	-5.23	1.46	1.53
2	H	173	THR	CA-CB	-5.06	1.46	1.53
1	L	34	HIS	CG-ND1	-5.04	1.32	1.38
1	L	162	SER	N-CA	-5.02	1.39	1.46

All (134) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	136	SER	CA-CB-OG	-12.10	86.91	111.10
2	H	226	GLU	CA-CB-CG	-10.87	92.37	114.10
1	L	189	HIS	CA-CB-CG	-10.36	103.44	113.80
2	H	128	CYS	N-CA-C	10.25	132.64	110.80
2	H	130	ASP	CA-CB-CG	10.03	122.63	112.60
2	H	1	GLN	OE1-CD-NE2	-9.59	113.02	122.60
2	H	3	GLN	N-CA-C	-9.48	93.44	108.90
1	L	28	ASP	CA-CB-CG	8.75	121.35	112.60
2	H	127	VAL	N-CA-C	7.92	121.47	113.47
1	L	17	GLN	OE1-CD-NE2	-7.88	114.72	122.60
2	H	179	GLN	OE1-CD-NE2	-7.67	114.93	122.60
2	H	1	GLN	CG-CD-NE2	7.59	127.78	116.40
2	H	54	ASP	CA-CB-CG	7.52	120.12	112.60
1	L	30	ASN	CA-CB-CG	7.48	120.08	112.60
1	L	137	ASN	N-CA-C	7.43	121.24	109.50
2	H	145	LYS	N-CA-C	7.37	121.14	109.50
1	L	210	ASN	CA-CB-CG	-7.34	105.25	112.60
1	L	204	PRO	N-CA-C	7.29	122.63	111.34
1	L	119	PRO	CA-C-N	7.17	127.22	119.90
1	L	119	PRO	C-N-CA	7.17	127.22	119.90
1	L	165	ASP	CA-CB-CG	7.17	119.77	112.60
1	L	27(D)	ASP	N-CA-C	-7.14	101.76	111.55
1	L	50	ARG	NE-CZ-NH2	-7.08	112.82	119.20
1	L	140	TYR	O-C-N	-7.07	116.86	121.88
2	H	227	PRO	O-C-N	6.87	131.34	123.03
2	H	84	THR	CA-CB-OG1	-6.84	99.34	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	66	ARG	NE-CZ-NH1	6.77	128.27	121.50
2	H	179	GLN	N-CA-C	-6.72	94.46	107.44
1	L	75	ILE	N-CA-C	-6.71	98.92	108.58
2	H	120	SER	CA-CB-OG	-6.68	97.75	111.10
1	L	171	SER	N-CA-C	6.67	120.61	111.54
1	L	172	THR	N-CA-CB	-6.65	100.16	110.46
1	L	138	ASN	OD1-CG-ND2	-6.63	115.97	122.60
2	H	69	ILE	CB-CA-C	-6.59	102.39	111.49
1	L	203	SER	CA-C-N	6.54	126.92	119.92
1	L	203	SER	C-N-CA	6.54	126.92	119.92
1	L	211	ARG	NE-CZ-NH2	-6.52	113.33	119.20
1	L	156	GLN	CB-CG-CD	6.47	123.60	112.60
1	L	159	VAL	CA-C-O	-6.44	113.64	120.53
1	L	155	ARG	NE-CZ-NH2	-6.41	113.43	119.20
2	H	109	VAL	N-CA-C	-6.35	99.23	108.89
2	H	127	VAL	CA-C-N	6.30	133.58	121.54
2	H	127	VAL	C-N-CA	6.30	133.58	121.54
1	L	12	ALA	N-CA-C	-6.25	99.01	109.07
1	L	189	HIS	CA-C-O	-6.25	113.99	120.99
2	H	76	ASN	CB-CG-ND2	6.19	125.69	116.40
1	L	39	LYS	N-CA-C	-6.19	101.11	110.39
1	L	26	SER	CB-CA-C	-6.16	101.21	110.88
1	L	156	GLN	OE1-CD-NE2	-6.15	116.45	122.60
1	L	148	TRP	CG-CD1-NE1	-6.12	102.24	110.20
1	L	113	PRO	O-C-N	-6.12	114.37	122.64
2	H	136	SER	O-C-N	6.09	130.69	122.59
1	L	132	VAL	N-CA-C	-6.08	99.67	108.17
2	H	83	ASP	N-CA-C	-6.03	100.25	109.41
2	H	136	SER	CA-C-O	5.99	129.08	120.51
2	H	66	ARG	NE-CZ-NH2	-5.98	113.82	119.20
2	H	84	THR	N-CA-C	5.95	119.37	111.75
2	H	191	VAL	N-CA-C	-5.95	99.56	108.12
2	H	94	GLN	CG-CD-NE2	5.93	125.29	116.40
2	H	187	LEU	CD1-CG-CD2	-5.86	97.90	110.80
2	H	53	TRP	CG-CD2-CE3	5.86	139.76	133.90
2	H	148	PHE	O-C-N	-5.84	117.28	121.84
2	H	162	ASN	OD1-CG-ND2	-5.83	116.77	122.60
1	L	6	GLN	CA-C-O	-5.81	114.39	121.36
2	H	25	SER	O-C-N	-5.81	116.31	123.33
2	H	214	ALA	CA-C-O	-5.80	113.55	120.10
1	L	150	ILE	N-CA-C	-5.79	99.40	107.80
1	L	211	ARG	NE-CZ-NH1	5.79	127.29	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	212	HIS	CB-CG-CD2	-5.78	123.68	131.20
1	L	99	GLY	N-CA-C	-5.73	105.20	112.54
1	L	27(C)	ASP	CA-CB-CG	5.72	118.32	112.60
2	H	227	PRO	CB-CA-C	5.72	118.83	111.46
2	H	5	GLN	OE1-CD-NE2	-5.70	116.90	122.60
2	H	148	PHE	CA-CB-CG	-5.70	108.10	113.80
2	H	122	TYR	CA-C-N	5.69	125.62	119.76
2	H	122	TYR	C-N-CA	5.69	125.62	119.76
2	H	12	LEU	N-CA-CB	-5.68	100.94	110.99
2	H	16	GLN	OE1-CD-NE2	-5.66	116.94	122.60
1	L	207	LYS	N-CA-C	-5.66	99.80	109.24
2	H	53	TRP	CB-CG-CD1	-5.64	118.43	126.90
2	H	67	LEU	O-C-N	-5.63	116.60	123.19
1	L	209	PHE	O-C-N	5.61	129.55	123.10
2	H	93	VAL	N-CA-C	5.59	116.17	108.12
2	H	8	GLY	CA-C-N	5.52	126.75	119.84
2	H	8	GLY	C-N-CA	5.52	126.75	119.84
1	L	194	CYS	CA-CB-SG	-5.52	101.71	114.40
2	H	127	VAL	CA-CB-CG1	-5.51	101.04	110.40
2	H	2	VAL	N-CA-CB	-5.48	102.19	111.23
2	H	199	TRP	CG-CD1-NE1	-5.47	103.09	110.20
1	L	182	THR	N-CA-C	-5.46	103.48	110.53
2	H	3	GLN	OE1-CD-NE2	-5.46	117.14	122.60
2	H	167	SER	O-C-N	-5.44	115.35	122.59
2	H	154	LEU	O-C-N	-5.43	117.14	123.27
1	L	79	GLU	N-CA-C	-5.42	102.17	110.14
1	L	142	LYS	CB-CG-CD	5.42	123.76	111.30
2	H	133	THR	CA-CB-CG2	5.36	119.62	110.50
1	L	190	ASN	OD1-CG-ND2	-5.36	117.24	122.60
1	L	198	HIS	CA-C-O	-5.34	115.07	121.11
2	H	209	ASN	OD1-CG-ND2	-5.34	117.26	122.60
1	L	202	THR	N-CA-CB	-5.34	102.27	110.01
1	L	140	TYR	N-CA-C	-5.33	99.80	108.82
1	L	70	ASP	CA-CB-CG	-5.32	107.28	112.60
1	L	151	ASP	CA-CB-CG	5.32	117.92	112.60
1	L	188	ARG	O-C-N	-5.32	114.79	121.97
1	L	161	ASN	OD1-CG-ND2	-5.32	117.28	122.60
2	H	178	LEU	O-C-N	-5.31	117.17	123.22
2	H	52	PHE	CA-CB-CG	-5.28	108.52	113.80
1	L	26	SER	N-CA-CB	5.26	117.64	110.01
2	H	222	LYS	CB-CG-CD	-5.25	99.21	111.30
2	H	172	HIS	CB-CG-CD2	-5.24	124.39	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	111	VAL	CA-C-O	5.24	126.30	120.59
1	L	53	ASN	CA-C-O	5.23	126.06	120.46
1	L	42	GLN	CA-C-N	5.22	125.76	120.38
1	L	42	GLN	C-N-CA	5.22	125.76	120.38
2	H	145	LYS	CB-CG-CD	-5.22	99.29	111.30
2	H	58	ARG	CB-CG-CD	5.22	123.30	111.30
2	H	12	LEU	N-CA-C	-5.21	100.11	108.55
2	H	153	THR	N-CA-CB	-5.19	102.96	110.84
2	H	212	HIS	N-CA-C	-5.17	97.44	108.93
1	L	198	HIS	CB-CG-CD2	-5.14	124.51	131.20
2	H	93	VAL	O-C-N	-5.14	117.65	123.20
2	H	5	GLN	CB-CG-CD	5.14	121.33	112.60
1	L	1	ASP	N-CA-C	-5.13	96.63	111.00
1	L	189	HIS	CB-CG-CD2	-5.12	124.54	131.20
1	L	201	SER	CA-C-O	5.12	127.09	121.11
2	H	31	THR	N-CA-C	-5.11	102.72	110.28
2	H	172	HIS	CB-CA-C	-5.09	104.76	111.42
2	H	53	TRP	CE2-CD2-CG	-5.08	101.10	107.20
1	L	104	LEU	N-CA-C	-5.05	101.00	109.24
1	L	190	ASN	CB-CG-ND2	5.05	123.98	116.40
2	H	157	TRP	CG-CD1-NE1	-5.04	103.64	110.20
2	H	137	SER	N-CA-C	-5.02	101.22	109.40
1	L	179	LEU	N-CA-C	-5.01	101.00	109.07
1	L	188	ARG	N-CA-C	-5.01	104.09	111.81

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	L	203	SER	Peptide
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	47	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	1628	0	1596	33	0
All	All	3291	0	3188	77	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 (77) 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:90:GLN:OE1	1:L:90:GLN:C	2.08	0.95
2:H:119:PRO:HB3	2:H:147:TYR:HB3	1.63	0.80
2:H:2:VAL:HG11	2:H:94:GLN:HE21	1.47	0.78
1:L:6:GLN:NE2	1:L:86:TYR:O	2.26	0.67
1:L:137:ASN:ND2	1:L:174:SER:HB3	2.11	0.65
1:L:119:PRO:HG2	2:H:228:ARG:NH1	2.12	0.65
2:H:2:VAL:HG11	2:H:94:GLN:NE2	2.12	0.64
1:L:54:LEU:HD21	1:L:58:ILE:O	1.96	0.64
2:H:18:LEU:HD23	2:H:82:ILE:HD12	1.81	0.62
1:L:115:VAL:HG22	1:L:136:LEU:HD12	1.81	0.62
1:L:90:GLN:OE1	1:L:91:SER:N	2.32	0.61
1:L:80:ALA:O	1:L:83:VAL:HG12	2.00	0.60
1:L:160:LEU:HD11	2:H:179:GLN:OE1	2.02	0.60
2:H:6:GLU:HG3	2:H:92:CYS:HB2	1.83	0.59
1:L:149:LYS:HA	1:L:153:SER:O	2.02	0.59
2:H:84:THR:HA	2:H:111:VAL:HG23	1.83	0.59
1:L:54:LEU:HG	1:L:58:ILE:HB	1.84	0.57
2:H:58:ARG:HH11	2:H:58:ARG:HG3	1.68	0.57
1:L:90:GLN:C	1:L:90:GLN:CD	2.72	0.57
1:L:90:GLN:OE1	1:L:90:GLN:O	2.24	0.54
2:H:58:ARG:HG3	2:H:58:ARG:NH1	2.23	0.54
1:L:18:ARG:HB3	1:L:76:ASN:OD1	2.08	0.53
1:L:11:LEU:HG	1:L:13:VAL:HG13	1.91	0.53
1:L:39:LYS:HB2	1:L:42:GLN:HG2	1.91	0.52
2:H:166:LEU:HD13	2:H:191:VAL:HG21	1.90	0.52
2:H:1:GLN:HE21	2:H:1:GLN:HA	1.75	0.52
1:L:27(D):ASP:OD1	1:L:30:ASN:HB2	2.10	0.51
1:L:11:LEU:HD23	1:L:104:LEU:HD12	1.93	0.51
1:L:83:VAL:HG23	1:L:104:LEU:O	2.10	0.51
1:L:91:SER:HA	1:L:96:LEU:HD22	1.91	0.51
1:L:115:VAL:HG22	1:L:136:LEU:CD1	2.40	0.51
2:H:37:ILE:HD12	2:H:93:VAL:HG21	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:108:ARG:HD2	1:L:140:TYR:HB2	1.93	0.51
2:H:63:LEU:HB3	2:H:67:LEU:HD11	1.93	0.51
1:L:33:LEU:HD22	1:L:71:PHE:CG	2.46	0.50
1:L:59:PRO:O	1:L:62:PHE:HD2	1.95	0.50
1:L:189:HIS:HB2	1:L:192:TYR:OH	2.13	0.49
1:L:32:PHE:O	1:L:90:GLN:HA	2.13	0.48
1:L:66:GLY:HA3	1:L:71:PHE:HA	1.95	0.48
2:H:18:LEU:O	2:H:81:LYS:HA	2.14	0.48
1:L:137:ASN:HD22	1:L:174:SER:HB3	1.79	0.47
1:L:170:ASP:OD1	1:L:172:THR:HB	2.14	0.47
1:L:61:ARG:HB2	1:L:76:ASN:O	2.14	0.47
1:L:19:ALA:HB3	1:L:75:ILE:HB	1.97	0.46
1:L:108:ARG:HD3	1:L:109:ALA:O	2.15	0.46
1:L:150:ILE:HD11	1:L:179:LEU:HD21	1.98	0.46
2:H:69:ILE:H	2:H:69:ILE:HG13	1.56	0.46
2:H:6:GLU:HA	2:H:21:THR:O	2.16	0.45
2:H:22:CYS:O	2:H:77:GLN:HA	2.17	0.45
2:H:137:SER:HA	2:H:194:THR:HA	1.98	0.45
1:L:207:LYS:HA	1:L:207:LYS:HD3	1.75	0.45
2:H:51:ILE:HD13	2:H:71:LYS:HG3	1.98	0.45
1:L:39:LYS:HB2	1:L:42:GLN:CG	2.47	0.44
1:L:190:ASN:O	1:L:210:ASN:HA	2.18	0.44
2:H:204:SER:C	2:H:205:ILE:HG13	2.43	0.44
1:L:138:ASN:HA	1:L:172:THR:CG2	2.47	0.43
1:L:46:LEU:HG	1:L:55:ILE:HG13	2.00	0.43
1:L:90:GLN:CD	1:L:90:GLN:O	2.61	0.43
1:L:119:PRO:HG2	2:H:228:ARG:CZ	2.48	0.43
2:H:3:GLN:O	2:H:24:PHE:HA	2.18	0.43
2:H:47:TRP:HZ2	2:H:50:HIS:HB2	1.84	0.43
1:L:3:VAL:N	1:L:26:SER:OG	2.52	0.42
1:L:19:ALA:HB2	1:L:78:VAL:CG2	2.50	0.42
2:H:12:LEU:O	2:H:111:VAL:HA	2.19	0.42
2:H:48:LEU:HD12	2:H:80:LEU:HD21	2.01	0.42
1:L:138:ASN:HA	1:L:172:THR:HG23	2.02	0.42
2:H:2:VAL:HG13	2:H:27:PHE:CD1	2.54	0.42
2:H:2:VAL:H	2:H:26:GLY:HA3	1.85	0.41
2:H:17:THR:HG23	2:H:82(A):THR:HA	2.02	0.41
1:L:143:ASP:O	1:L:198:HIS:HD2	2.04	0.41
2:H:16:GLN:O	2:H:82(C):VAL:HG22	2.20	0.41
1:L:27(A):SER:HA	1:L:68:ARG:O	2.20	0.41
1:L:36:TYR:HB2	1:L:87:TYR:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:2:VAL:HA	2:H:25:SER:O	2.20	0.41
2:H:66:ARG:NH2	2:H:86:ASP:OD2	2.54	0.41
1:L:38:GLN:HE21	1:L:87:TYR:HE2	1.69	0.40
2:H:157:TRP:O	2:H:162:ASN:C	2.64	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	L	213/215 (99%)	192 (90%)	18 (8%)	3 (1%)	9	30
2	H	213/215 (99%)	193 (91%)	15 (7%)	5 (2%)	5	18
All	All	426/430 (99%)	385 (90%)	33 (8%)	8 (2%)	6	22

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	97	TYR
1	L	60	ASP
2	H	2	VAL
1	L	15	LEU
2	H	128	CYS
2	H	130	ASP
1	L	28	ASP
2	H	129	GLY

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%)	177 (93%)	14 (7%)	13	38
2	H	189/189 (100%)	173 (92%)	16 (8%)	10	31
All	All	380/380 (100%)	350 (92%)	30 (8%)	11	35

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	17	GLN
1	L	18	ARG
1	L	26	SER
1	L	33	LEU
1	L	51	SER
1	L	56	SER
1	L	90	GLN
1	L	108	ARG
1	L	136	LEU
1	L	146	VAL
1	L	154	GLU
1	L	172	THR
1	L	183	LYS
1	L	203	SER
2	H	2	VAL
2	H	3	GLN
2	H	30	SER
2	H	58	ARG
2	H	62	SER
2	H	65	SER
2	H	69	ILE
2	H	73	THR
2	H	94	GLN
2	H	109	VAL
2	H	113	SER
2	H	127	VAL
2	H	151	PRO
2	H	168	SER
2	H	187	LEU
2	H	226	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	38	GLN
1	L	42	GLN
1	L	92	ASN
1	L	137	ASN
1	L	189	HIS
2	H	1	GLN
2	H	3	GLN
2	H	39	GLN
2	H	77	GLN
2	H	94	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](#)

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.