Full wwPDB X-ray Structure Validation Report

Jan 31, 2016 – 07:37 PM GMT

PDB ID	:	1GGB
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
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:

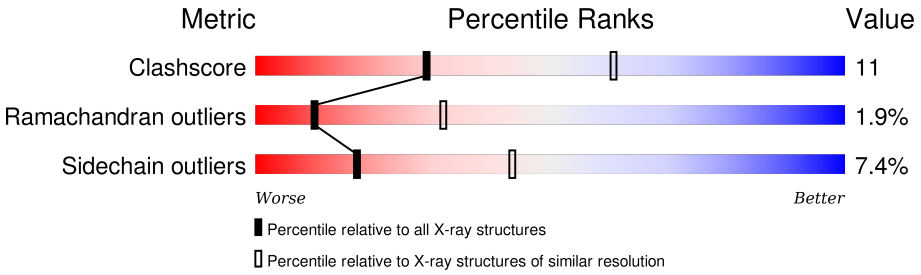
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (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 >=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 <=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	60% 36% •
2	H	215	61% 32% 7% •

2 Entry composition (i)

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			

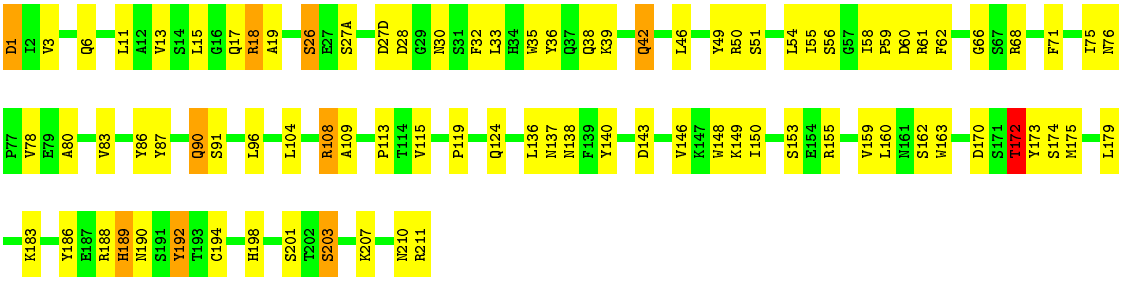
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

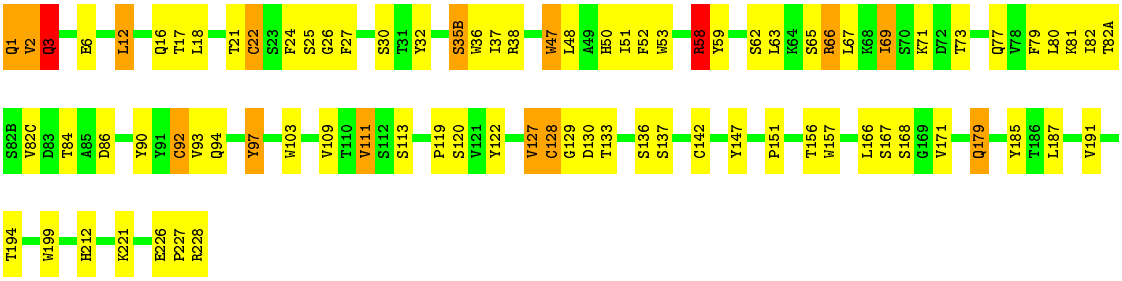
- Molecule 1: IGG2A-KAPPA 50.1 FAB (LIGHT CHAIN)

Chain L:



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

Chain H:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be 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	1.05	2/1699 (0.1%)	1.82	31/2309 (1.3%)
2	H	1.27	6/1670 (0.4%)	2.02	51/2282 (2.2%)
All	All	1.16	8/3369 (0.2%)	1.92	82/4591 (1.8%)

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 (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	120	SER	CA-CB	-8.02	1.41	1.52
2	H	52	PHE	CA-CB	-7.14	1.38	1.53
1	L	162	SER	CA-CB	-7.08	1.42	1.52
2	H	79	PHE	CA-CB	-5.60	1.41	1.53
2	H	35(B)	SER	CA-CB	-5.32	1.45	1.52
1	L	124	GLN	CA-CB	-5.22	1.42	1.53
2	H	157	TRP	CD2-CE2	-5.16	1.35	1.41
2	H	157	TRP	CD1-NE1	-5.05	1.29	1.38

All (82) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	66	ARG	NE-CZ-NH1	15.93	128.27	120.30
1	L	50	ARG	NE-CZ-NH2	-14.95	112.82	120.30
1	L	211	ARG	NE-CZ-NH1	13.99	127.29	120.30
1	L	211	ARG	NE-CZ-NH2	-13.94	113.33	120.30
1	L	155	ARG	NE-CZ-NH2	-13.73	113.43	120.30
2	H	66	ARG	NE-CZ-NH2	-12.96	113.82	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	199	TRP	CD1-CG-CD2	9.77	114.11	106.30
2	H	226	GLU	CA-CB-CG	-9.56	92.37	113.40
1	L	163	TRP	CD1-CG-CD2	9.31	113.75	106.30
2	H	157	TRP	CD1-CG-CD2	9.26	113.70	106.30
1	L	188	ARG	NE-CZ-NH1	9.06	124.83	120.30
2	H	136	SER	CA-CB-OG	-9.00	86.91	111.20
2	H	185	TYR	CB-CG-CD2	-8.70	115.78	121.00
2	H	53	TRP	CD1-CG-CD2	8.56	113.15	106.30
1	L	148	TRP	CD1-CG-CD2	8.40	113.02	106.30
2	H	103	TRP	CD1-CG-CD2	8.38	113.01	106.30
1	L	35	TRP	CD1-CG-CD2	8.23	112.89	106.30
2	H	128	CYS	N-CA-C	8.02	132.64	111.00
1	L	148	TRP	CG-CD1-NE1	-7.86	102.24	110.10
2	H	58	ARG	NE-CZ-NH1	7.78	124.19	120.30
2	H	53	TRP	CE2-CD2-CG	-7.75	101.10	107.30
2	H	136	SER	CA-C-N	-7.74	100.17	117.20
2	H	157	TRP	CE2-CD2-CG	-7.51	101.29	107.30
2	H	199	TRP	CE2-CD2-CG	-7.50	101.30	107.30
1	L	35	TRP	CE2-CD2-CG	-7.45	101.34	107.30
1	L	49	TYR	CB-CG-CD2	-7.37	116.58	121.00
1	L	163	TRP	CE2-CD2-CG	-7.36	101.41	107.30
1	L	113	PRO	CA-C-N	7.31	133.29	117.20
2	H	122	TYR	CB-CG-CD1	-7.13	116.72	121.00
2	H	199	TRP	CG-CD1-NE1	-7.01	103.09	110.10
1	L	186	TYR	CB-CG-CD1	-6.92	116.85	121.00
2	H	38	ARG	NE-CZ-NH1	6.90	123.75	120.30
2	H	36	TRP	CD1-CG-CD2	6.85	111.78	106.30
1	L	194	CYS	CA-CB-SG	-6.83	101.71	114.00
1	L	50	ARG	NE-CZ-NH1	6.75	123.67	120.30
2	H	103	TRP	CE2-CD2-CG	-6.71	101.94	107.30
2	H	53	TRP	CB-CG-CD1	-6.59	118.43	127.00
2	H	127	VAL	CA-CB-CG1	-6.58	101.04	110.90
1	L	148	TRP	CE2-CD2-CG	-6.53	102.08	107.30
2	H	53	TRP	CG-CD2-CE3	6.51	139.76	133.90
2	H	3	GLN	N-CA-C	-6.50	93.44	111.00
2	H	32	TYR	CB-CG-CD2	-6.50	117.10	121.00
2	H	47	TRP	CE2-CD2-CG	-6.50	102.10	107.30
2	H	157	TRP	CG-CD1-NE1	-6.46	103.64	110.10
2	H	47	TRP	CD1-CG-CD2	6.45	111.46	106.30
1	L	163	TRP	CG-CD1-NE1	-6.23	103.87	110.10
2	H	12	LEU	CA-CB-CG	6.23	129.63	115.30
1	L	155	ARG	NE-CZ-NH1	6.19	123.39	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	53	TRP	CG-CD1-NE1	-6.15	103.95	110.10
2	H	36	TRP	CE2-CD2-CG	-6.14	102.39	107.30
2	H	179	GLN	N-CA-C	-6.13	94.46	111.00
2	H	59	TYR	CB-CG-CD1	-6.07	117.36	121.00
1	L	189	HIS	CA-CB-CG	-5.97	103.44	113.60
2	H	111	VAL	CG1-CB-CG2	-5.94	101.40	110.90
1	L	173	TYR	CB-CG-CD1	-5.93	117.44	121.00
2	H	167	SER	CA-C-N	5.93	130.25	117.20
2	H	22	CYS	CA-CB-SG	-5.90	103.37	114.00
2	H	92	CYS	CA-CB-SG	-5.88	103.41	114.00
1	L	201	SER	CA-C-N	-5.84	104.35	117.20
1	L	192	TYR	CB-CG-CD1	-5.58	117.65	121.00
2	H	156	THR	CA-CB-CG2	-5.57	104.60	112.40
2	H	32	TYR	CD1-CG-CD2	5.52	123.97	117.90
2	H	90	TYR	CB-CG-CD1	-5.51	117.69	121.00
2	H	103	TRP	CB-CG-CD1	-5.51	119.84	127.00
1	L	49	TYR	CG-CD1-CE1	-5.41	116.97	121.30
2	H	227	PRO	O-C-N	5.40	131.34	122.70
1	L	148	TRP	CB-CG-CD1	-5.38	120.01	127.00
2	H	122	TYR	CG-CD2-CE2	-5.38	117.00	121.30
1	L	172	THR	N-CA-CB	-5.34	100.16	110.30
1	L	1	ASP	N-CA-C	-5.32	96.63	111.00
2	H	97	TYR	CB-CG-CD1	-5.32	117.81	121.00
1	L	148	TRP	CG-CD2-CE3	5.21	138.59	133.90
1	L	113	PRO	O-C-N	-5.20	114.37	122.70
2	H	221	LYS	CD-CE-NZ	-5.19	99.75	111.70
1	L	175	MET	CG-SD-CE	5.19	108.51	100.20
2	H	133	THR	CA-CB-CG2	5.16	119.62	112.40
1	L	159	VAL	CA-C-N	5.14	128.52	117.20
2	H	171	VAL	CG1-CB-CG2	-5.14	102.68	110.90
2	H	103	TRP	CG-CD1-NE1	-5.09	105.01	110.10
2	H	157	TRP	CB-CG-CD1	-5.05	120.44	127.00
2	H	36	TRP	CG-CD1-NE1	-5.04	105.06	110.10
2	H	212	HIS	N-CA-C	-5.02	97.44	111.00

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 (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	L	1663	0	1592	46	0
2	H	1628	0	1596	31	0
All	All	3291	0	3188	74	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 11.

All (74) 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	0.90
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:HG3	2:H:58:ARG:HH11	1.68	0.57
1:L:90:GLN:O	1:L:90:GLN:OE1	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:HA	2:H:1:GLN:HE21	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:L:83:VAL:HG23	1:L:104:LEU:O	2.10	0.51
2:H:37:ILE:HD12	2:H:93:VAL:HG21	1.91	0.51
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:59:PRO:O	1:L:62:PHE:HD2	1.95	0.50
1:L:33:LEU:HD22	1:L:71:PHE:CG	2.46	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
2:H:18:LEU:O	2:H:81:LYS:HA	2.14	0.48
1:L:66:GLY:HA3	1:L:71:PHE:HA	1.95	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:108:ARG:HD3	1:L:109:ALA:O	2.15	0.46
1:L:19:ALA:HB3	1:L:75:ILE:HB	1.97	0.46
1:L:150:ILE:HD11	1:L:179:LEU:HD21	1.98	0.46
2:H:69:ILE:HG13	2:H:69:ILE:H	1.56	0.46
2:H:6:GLU:HA	2:H:21:THR:O	2.16	0.45
2:H:137:SER:HA	2:H:194:THR:HA	1.98	0.45
2:H:22:CYS:O	2:H:77:GLN:HA	2.17	0.45
1:L:207:LYS:HD3	1:L:207:LYS:HA	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
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: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
2:H:2:VAL:HG13	2:H:27:PHE:CD1	2.54	0.42
1:L:138:ASN:HA	1:L:172:THR:HG23	2.02	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:90:GLN:CD	1:L:90:GLN:C	2.72	0.41
1:L:27(A):SER:HA	1:L:68:ARG:O	2.20	0.41
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:36:TYR:HB2	1:L:87:TYR:HB2	2.02	0.41
1:L:38:GLN:HE21	1:L:87:TYR:HE2	1.69	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%)	14 42
2	H	213/215 (99%)	193 (91%)	15 (7%)	5 (2%)	8 26
All	All	426/430 (99%)	385 (90%)	33 (8%)	8 (2%)	10 32

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%)	179 (94%)	12 (6%)	22 53
2	H	189/189 (100%)	173 (92%)	16 (8%)	13 36
All	All	380/380 (100%)	352 (93%)	28 (7%)	17 43

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	1	ASP
1	L	17	GLN
1	L	18	ARG
1	L	26	SER
1	L	51	SER
1	L	56	SER
1	L	90	GLN
1	L	108	ARG
1	L	146	VAL
1	L	172	THR
1	L	183	LYS
1	L	203	SER
2	H	1	GLN
2	H	3	GLN
2	H	30	SER
2	H	35(B)	SER
2	H	58	ARG
2	H	62	SER
2	H	65	SER
2	H	69	ILE
2	H	73	THR
2	H	109	VAL
2	H	113	SER
2	H	127	VAL
2	H	142	CYS
2	H	151	PRO
2	H	168	SER

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Mol	Chain	Res	Type
2	H	187	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	38	GLN
1	L	137	ASN
1	L	189	HIS
2	H	1	GLN
2	H	39	GLN
2	H	94	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 carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.