



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:55 PM UTC

PDB ID : 1A7O / pdb_00001a7o
Title : FV FRAGMENT OF MOUSE MONOCLONAL ANTIBODY D1.3 (BALB/C, IGG1, K) R96L DELETION MUTANT ON VARIANT FOR CHAIN L GLU81->ASP AND CHAIN H LEU312->VAL
Authors : Marks, C.; Henrick, K.; Winter, G.
Deposited on : 1998-03-16
Resolution : 2.00 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)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

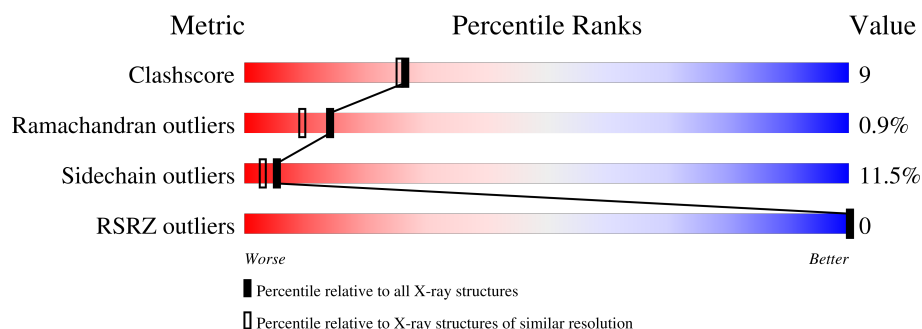
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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 $\leq 5\%$. 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	L	106	
2	H	116	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 1826 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 IGG1-KAPPA D1.3 FV (LIGHT CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	106	Total	C	N	O	S	0	0	0
			802	511	131	158	2			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	3	VAL	GLU	conflict	UNP P01635
L	50	TYR	LYS	conflict	UNP P01635
L	51	THR	ALA	conflict	UNP P01635
L	52	THR	GLN	conflict	UNP P01635
L	81	ASP	GLU	variant	UNP P01635
L	?	-	PRO	deletion	UNP P01635
L	?	-	TRP	deletion	UNP P01635

- Molecule 2 is a protein called IGG1-KAPPA D1.3 FV (HEAVY CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	116	Total	C	N	O	S	0	0	0
			892	560	156	172	4			

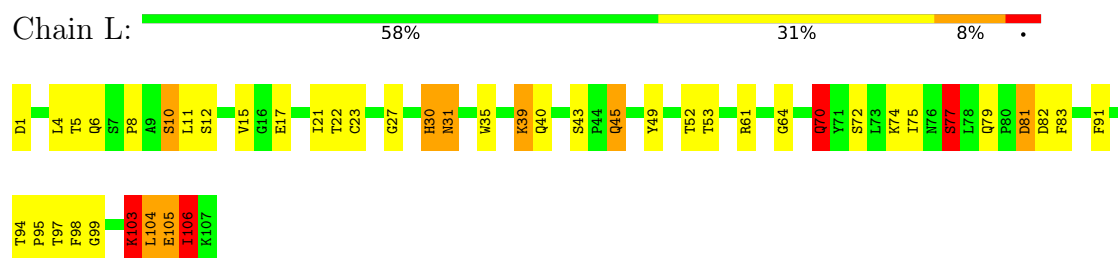
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	L	73	Total	O	0	0
			73	73		
3	H	59	Total	O	0	0
			59	59		

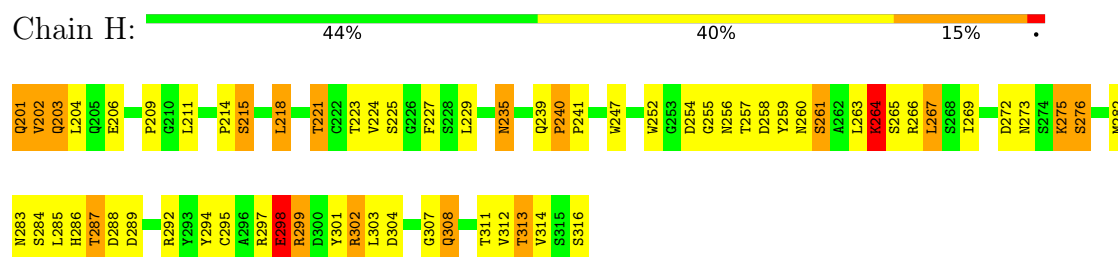
3 Residue-property plots

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 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: IGG1-KAPPA D1.3 FV (LIGHT CHAIN)



• Molecule 2: IGG1-KAPPA D1.3 FV (HEAVY CHAIN)



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	90.42Å 90.42Å 56.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 2.00 6.00 – 2.01	Depositor EDS
% Data completeness (in resolution range)	(Not available) (6.00-2.00) 91.3 (6.00-2.01)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.22 (at 2.00Å)	Xtriage
Refinement program	CCP4	Depositor
R, R_{free}	0.167 , (Not available) 0.172 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	27.1	Xtriage
Anisotropy	0.024	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 89.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	1826	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.13% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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 ⓘ

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	1.21	2/823 (0.2%)	2.32	42/1120 (3.8%)
2	H	1.17	0/912	2.51	62/1238 (5.0%)
All	All	1.19	2/1735 (0.1%)	2.42	104/2358 (4.4%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	52	THR	CA-CB	5.76	1.62	1.54
1	L	53	THR	CA-CB	5.07	1.60	1.53

All (104) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	45	GLN	OE1-CD-NE2	-15.83	106.77	122.60
2	H	201	GLN	CA-CB-CG	-15.60	82.90	114.10
2	H	302	ARG	NE-CZ-NH1	12.80	134.31	121.50
2	H	215	SER	O-C-N	11.65	132.62	121.56
2	H	308	GLN	OE1-CD-NE2	-10.52	112.08	122.60
1	L	70	GLN	OE1-CD-NE2	10.37	132.97	122.60
2	H	302	ARG	NE-CZ-NH2	-9.53	110.62	119.20
1	L	45	GLN	CB-CG-CD	9.36	128.52	112.60
1	L	45	GLN	CG-CD-NE2	9.04	129.96	116.40
2	H	302	ARG	CG-CD-NE	8.54	130.78	112.00
2	H	203	GLN	OE1-CD-NE2	8.25	130.85	122.60
2	H	202	VAL	CB-CA-C	8.11	122.32	111.21
2	H	202	VAL	N-CA-CB	-8.10	99.38	110.56
2	H	286	HIS	CA-CB-CG	-8.06	105.74	113.80
2	H	299	ARG	CA-CB-CG	8.03	130.16	114.10
2	H	201	GLN	CG-CD-NE2	-7.98	104.42	116.40
1	L	97	THR	N-CA-CB	7.97	125.57	111.69
1	L	105	GLU	CA-C-O	7.96	128.96	120.36
1	L	81	ASP	CA-CB-CG	7.94	120.54	112.60
2	H	311	THR	CA-CB-OG1	-7.92	97.71	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	77	SER	CA-C-O	7.89	131.79	120.51
1	L	79	GLN	CB-CA-C	7.70	120.69	108.91
1	L	91	PHE	CA-CB-CG	7.38	121.18	113.80
2	H	264	LYS	CA-C-N	7.31	133.93	121.14
2	H	264	LYS	C-N-CA	7.31	133.93	121.14
1	L	61	ARG	NE-CZ-NH2	7.29	125.76	119.20
2	H	312	VAL	CA-C-O	-7.27	112.76	120.39
1	L	99	GLY	N-CA-C	-7.17	101.31	112.85
2	H	298	GLU	CA-CB-CG	-7.13	99.85	114.10
1	L	79	GLN	OE1-CD-NE2	-7.07	115.53	122.60
1	L	103	LYS	CB-CA-C	-7.00	98.54	110.22
1	L	40	GLN	CG-CD-NE2	6.98	126.88	116.40
2	H	203	GLN	CB-CA-C	6.92	123.43	109.38
2	H	223	THR	CA-CB-OG1	-6.92	99.22	109.60
2	H	285	LEU	O-C-N	6.90	131.35	122.87
2	H	298	GLU	CG-CD-OE1	-6.88	102.58	118.40
2	H	260	ASN	N-CA-C	-6.83	99.55	109.59
1	L	39	LYS	CA-CB-CG	-6.82	100.45	114.10
2	H	223	THR	O-C-N	6.74	130.90	123.22
2	H	261	SER	O-C-N	6.50	129.01	122.12
2	H	221	THR	CA-CB-OG1	6.48	119.32	109.60
2	H	289	ASP	N-CA-C	-6.44	105.17	113.16
2	H	288	ASP	CB-CA-C	6.40	122.20	110.36
1	L	70	GLN	N-CA-CB	-6.35	100.81	110.77
1	L	4	LEU	O-C-N	6.34	130.85	123.30
2	H	223	THR	CA-C-O	-6.34	113.37	120.54
2	H	314	VAL	O-C-N	6.33	132.06	122.76
1	L	70	GLN	CA-CB-CG	6.31	126.72	114.10
2	H	209	PRO	CA-C-O	-6.20	111.09	118.90
1	L	75	ILE	O-C-N	6.17	129.59	122.99
2	H	258	ASP	CB-CA-C	6.14	121.85	109.38
1	L	21	ILE	CB-CA-C	6.14	119.77	110.62
2	H	239	GLN	O-C-N	6.10	126.51	121.44
2	H	204	LEU	O-C-N	6.09	130.43	123.31
1	L	10	SER	N-CA-CB	6.07	122.81	111.52
1	L	17	GLU	CA-CB-CG	6.01	126.11	114.10
1	L	15	VAL	CA-C-O	-5.84	114.93	121.36
2	H	295	CYS	N-CA-C	-5.83	99.89	109.40
1	L	6	GLN	CA-C-O	-5.77	114.40	120.80
2	H	257	THR	CA-CB-OG1	-5.75	100.97	109.60
2	H	273	ASN	O-C-N	5.75	128.22	122.12
1	L	31	ASN	OD1-CG-ND2	-5.73	116.87	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	267	LEU	N-CA-C	5.73	119.06	109.95
1	L	106	ILE	CB-CG1-CD1	-5.72	101.79	113.80
2	H	307	GLY	N-CA-C	-5.70	103.42	112.66
1	L	94	THR	CA-CB-OG1	-5.66	101.11	109.60
2	H	308	GLN	CG-CD-OE1	5.66	132.11	120.80
2	H	294	TYR	CA-CB-CG	5.64	124.05	113.90
2	H	255	GLY	CA-C-O	-5.64	112.96	119.10
2	H	240	PRO	N-CA-CB	5.59	106.32	103.19
2	H	297	ARG	CA-CB-CG	-5.55	103.00	114.10
2	H	287	THR	CA-CB-OG1	-5.51	101.33	109.60
2	H	316	SER	CA-C-O	-5.51	111.43	120.80
1	L	27	GLY	CA-C-O	-5.51	115.36	121.37
1	L	97	THR	CA-CB-CG2	5.50	119.86	110.50
1	L	23	CYS	CA-C-N	-5.46	114.74	122.94
1	L	23	CYS	C-N-CA	-5.46	114.74	122.94
1	L	30	HIS	N-CA-C	5.45	118.95	111.54
2	H	284	SER	CA-C-O	5.43	128.28	120.51
2	H	203	GLN	CG-CD-NE2	-5.37	108.34	116.40
1	L	98	PHE	CA-CB-CG	5.36	119.16	113.80
1	L	8	PRO	N-CD-CG	-5.33	97.41	103.80
1	L	35	TRP	O-C-N	5.32	129.76	123.27
1	L	82	ASP	CA-CB-CG	5.32	117.92	112.60
2	H	224	VAL	CA-C-N	5.32	131.52	122.37
2	H	224	VAL	C-N-CA	5.32	131.52	122.37
1	L	43	SER	CB-CA-C	5.31	117.82	109.37
2	H	201	GLN	CB-CA-C	-5.30	100.03	110.10
2	H	273	ASN	CA-CB-CG	-5.28	107.32	112.60
2	H	313	THR	CA-CB-OG1	-5.28	101.68	109.60
1	L	104	LEU	O-C-N	5.22	129.26	123.05
1	L	64	GLY	O-C-N	5.20	129.47	122.70
2	H	304	ASP	CA-C-O	-5.17	113.69	119.79
2	H	240	PRO	O-C-N	5.17	123.69	121.31
1	L	103	LYS	O-C-N	5.16	129.07	123.13
2	H	206	GLU	CA-C-O	-5.15	115.20	121.28
2	H	235	ASN	CB-CG-ND2	5.15	124.12	116.40
2	H	292	ARG	N-CA-C	-5.08	100.95	109.24
2	H	201	GLN	CA-C-N	-5.08	114.38	122.50
2	H	201	GLN	C-N-CA	-5.08	114.38	122.50
2	H	215	SER	CA-C-O	-5.05	113.95	119.00
2	H	209	PRO	O-C-N	5.01	129.24	122.37
2	H	263	LEU	N-CA-CB	-5.01	103.28	110.65
1	L	5	THR	CA-CB-OG1	-5.00	102.10	109.60

There are no chirality outliers.

There are no planarity outliers.

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	802	0	768	10	0
2	H	892	0	856	22	0
3	H	59	0	0	4	0
3	L	73	0	0	1	0
All	All	1826	0	1624	31	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 9.

All (31) 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:49:TYR:OH	3:L:581:HOH:O	1.99	0.80
2:H:203:GLN:HG2	2:H:225:SER:HB2	1.64	0.79
1:L:1:ASP:CB	3:H:600:HOH:O	2.38	0.71
1:L:103:LYS:HB2	1:L:103:LYS:NZ	2.12	0.63
1:L:103:LYS:HG2	1:L:105:GLU:HG3	1.86	0.58
2:H:267:LEU:HD23	2:H:282:MET:HG2	1.86	0.57
2:H:272:ASP:CG	2:H:275:LYS:HG3	2.31	0.56
2:H:211:LEU:CD1	2:H:313:THR:HB	2.36	0.56
2:H:264:LYS:HE2	3:H:526:HOH:O	2.07	0.54
2:H:218:LEU:HD12	2:H:282:MET:HB2	1.90	0.54
2:H:211:LEU:HD12	2:H:313:THR:HB	1.91	0.53
1:L:83:PHE:CE2	1:L:106:ILE:HD12	2.44	0.52
2:H:214:PRO:O	2:H:215:SER:HB2	2.10	0.51
2:H:298:GLU:HG3	2:H:303:LEU:HD23	1.94	0.50
1:L:12:SER:HA	1:L:105:GLU:O	2.13	0.48
2:H:308:GLN:NE2	3:H:471:HOH:O	2.47	0.47
1:L:95:PRO:HG2	2:H:247:TRP:CE2	2.50	0.46
2:H:254:ASP:CG	2:H:256:ASN:HD22	2.24	0.46
2:H:275:LYS:O	2:H:276:SER:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:235:ASN:ND2	2:H:298:GLU:HB2	2.32	0.44
2:H:301:TYR:O	2:H:302:ARG:HB3	2.18	0.44
2:H:240:PRO:HA	2:H:241:PRO:HD3	1.90	0.44
2:H:259:TYR:CE1	2:H:269:ILE:HD12	2.53	0.44
2:H:282:MET:HE2	2:H:282:MET:HB3	1.92	0.44
1:L:10:SER:HB3	1:L:103:LYS:HB3	2.01	0.43
2:H:229:LEU:HB2	3:H:477:HOH:O	2.19	0.43
1:L:30:HIS:O	1:L:31:ASN:HB2	2.19	0.42
2:H:266:ARG:HG2	2:H:283:ASN:O	2.19	0.42
2:H:202:VAL:HG13	2:H:227:PHE:CE1	2.55	0.42
1:L:22:THR:HG23	1:L:70:GLN:HE22	1.84	0.41
2:H:201:GLN:O	2:H:201:GLN:HG2	2.19	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	104/106 (98%)	101 (97%)	2 (2%)	1 (1%)	12	8
2	H	114/116 (98%)	109 (96%)	4 (4%)	1 (1%)	14	9
All	All	218/222 (98%)	210 (96%)	6 (3%)	2 (1%)	14	9

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	77	SER
2	H	264	LYS

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	87/90 (97%)	76 (87%)	11 (13%)	4	2
2	H	96/100 (96%)	86 (90%)	10 (10%)	7	4
All	All	183/190 (96%)	162 (88%)	21 (12%)	5	3

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	11	LEU
1	L	39	LYS
1	L	45	GLN
1	L	70	GLN
1	L	72	SER
1	L	74	LYS
1	L	77	SER
1	L	81	ASP
1	L	103	LYS
1	L	104	LEU
1	L	106	ILE
2	H	218	LEU
2	H	221	THR
2	H	252	TRP
2	H	261	SER
2	H	265	SER
2	H	275	LYS
2	H	276	SER
2	H	287	THR
2	H	298	GLU
2	H	299	ARG

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	HIS

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Mol	Chain	Res	Type
1	L	40	GLN
1	L	45	GLN
1	L	70	GLN
1	L	89	GLN
2	H	203	GLN
2	H	216	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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, 95th 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	L	106/106 (100%)	-0.97	0 100 100	14, 23, 37, 44	7 (6%)
2	H	116/116 (100%)	-0.96	0 100 100	15, 25, 38, 48	3 (2%)
All	All	222/222 (100%)	-0.97	0 100 100	14, 24, 38, 48	10 (4%)

There are no RSRZ outliers to report.

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.