



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 3, 2025 – 12:14 PM EST

PDB ID : 9BJH
Title : Crystal structure of neutralizing human monoclonal antibody 75C8 in complex with AMA1 DI-DII
Authors : Patel, P.N.; Tang, W.K.; Tolia, N.H.
Deposited on : 2024-04-25
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	:	4.02b-467
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.4

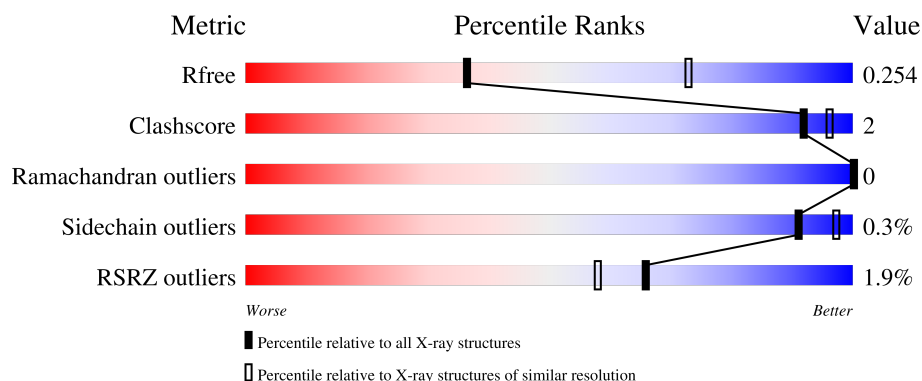
1 Overall quality at a glance

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))
R_{free}	164625	3657 (2.80-2.80)
Clashscore	180529	4123 (2.80-2.80)
Ramachandran outliers	177936	4071 (2.80-2.80)
Sidechain outliers	177891	4073 (2.80-2.80)
RSRZ outliers	164620	3659 (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 $\leq 5\%$. 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	A	347	
1	B	347	
2	H	239	
2	I	239	
3	L	218	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	M	218	<div><div>%</div><div><div></div></div><div>94%</div><div>5% •</div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 22075 atoms, of which 10839 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 Apical membrane antigen 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	285	Total	C	H	N	O	S	0	0	0
			4447	1445	2168	383	436	15			
1	B	283	Total	C	H	N	O	S	0	0	0
			4416	1436	2153	380	432	15			

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	101	GLU	-	expression tag	UNP Q7KQK5
A	102	THR	-	expression tag	UNP Q7KQK5
A	103	GLY	-	expression tag	UNP Q7KQK5
A	164	ALA	THR	engineered mutation	UNP Q7KQK5
A	288	ALA	THR	engineered mutation	UNP Q7KQK5
A	373	ALA	SER	engineered mutation	UNP Q7KQK5
A	423	ALA	SER	engineered mutation	UNP Q7KQK5
A	424	ALA	SER	engineered mutation	UNP Q7KQK5
A	439	GLY	-	expression tag	UNP Q7KQK5
A	440	THR	-	expression tag	UNP Q7KQK5
A	441	LYS	-	expression tag	UNP Q7KQK5
A	442	HIS	-	expression tag	UNP Q7KQK5
A	443	HIS	-	expression tag	UNP Q7KQK5
A	444	HIS	-	expression tag	UNP Q7KQK5
A	445	HIS	-	expression tag	UNP Q7KQK5
A	446	HIS	-	expression tag	UNP Q7KQK5
A	447	HIS	-	expression tag	UNP Q7KQK5
B	101	GLU	-	expression tag	UNP Q7KQK5
B	102	THR	-	expression tag	UNP Q7KQK5
B	103	GLY	-	expression tag	UNP Q7KQK5
B	164	ALA	THR	engineered mutation	UNP Q7KQK5
B	288	ALA	THR	engineered mutation	UNP Q7KQK5
B	373	ALA	SER	engineered mutation	UNP Q7KQK5
B	423	ALA	SER	engineered mutation	UNP Q7KQK5
B	424	ALA	SER	engineered mutation	UNP Q7KQK5

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	439	GLY	-	expression tag	UNP Q7KQK5
B	440	THR	-	expression tag	UNP Q7KQK5
B	441	LYS	-	expression tag	UNP Q7KQK5
B	442	HIS	-	expression tag	UNP Q7KQK5
B	443	HIS	-	expression tag	UNP Q7KQK5
B	444	HIS	-	expression tag	UNP Q7KQK5
B	445	HIS	-	expression tag	UNP Q7KQK5
B	446	HIS	-	expression tag	UNP Q7KQK5
B	447	HIS	-	expression tag	UNP Q7KQK5

- Molecule 2 is a protein called 75C8 Fab Heavy Chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	H	222	Total	C	H	N	O	S	0	0	0
			3354	1065	1666	288	330	5			
2	I	217	Total	C	H	N	O	S	0	0	0
			3273	1043	1622	281	322	5			

- Molecule 3 is a protein called 75C8 Fab Light Chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	L	214	Total	C	H	N	O	S	0	0	0
			3269	1043	1608	279	335	4			
3	M	216	Total	C	H	N	O	S	0	0	0
			3295	1051	1622	281	337	4			

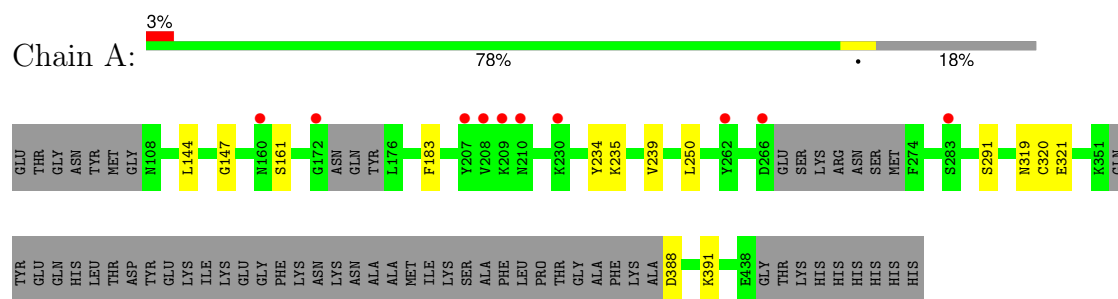
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	O	0	0
			2	2		
4	H	6	Total	O	0	0
			6	6		
4	I	5	Total	O	0	0
			5	5		
4	L	3	Total	O	0	0
			3	3		
4	M	5	Total	O	0	0
			5	5		

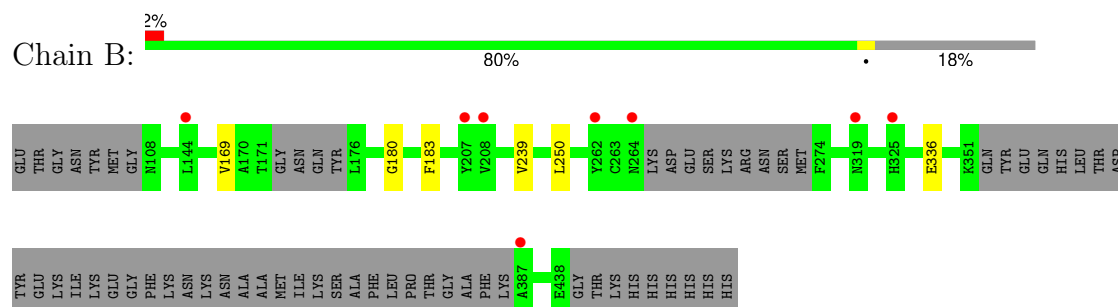
3 Residue-property plots [i](#)

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.

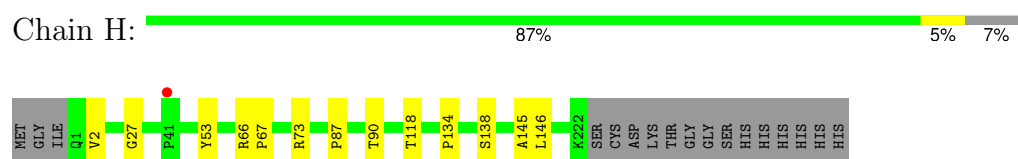
• Molecule 1: Apical membrane antigen 1



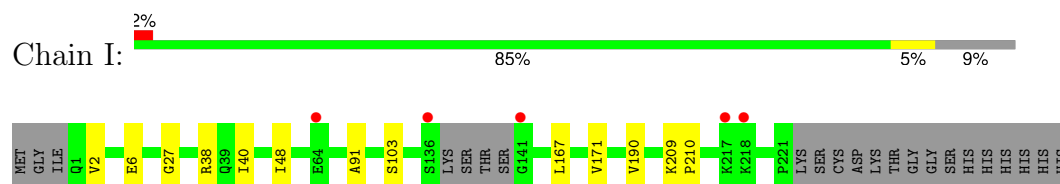
• Molecule 1: Apical membrane antigen 1



• Molecule 2: 75C8 Fab Heavy Chain



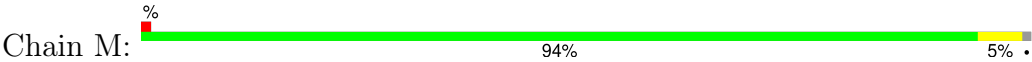
• Molecule 2: 75C8 Fab Heavy Chain



• Molecule 3: 75C8 Fab Light Chain



● Molecule 3: 75C8 Fab Light Chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	54.87Å 71.62Å 132.93Å 94.11° 99.19° 112.39°	Depositor
Resolution (Å)	19.87 – 2.80 19.87 – 2.80	Depositor EDS
% Data completeness (in resolution range)	86.5 (19.87-2.80) 86.4 (19.87-2.80)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.73 (at 2.79Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.211 , 0.253 0.212 , 0.254	Depositor DCC
R_{free} test set	42943 reflections (4.78%)	wwPDB-VP
Wilson B-factor (Å ²)	43.0	Xtriage
Anisotropy	0.480	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 48.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.042 for h,-h-k,-h-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	22075	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.77% 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	A	0.24	0/2337	0.45	0/3166
1	B	0.24	0/2321	0.44	0/3146
2	H	0.25	0/1732	0.51	0/2373
2	I	0.25	0/1694	0.51	0/2322
3	L	0.25	0/1699	0.49	0/2311
3	M	0.26	0/1711	0.49	0/2327
All	All	0.25	0/11494	0.48	0/15645

There are no bond length outliers.

There are no bond angle outliers.

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	A	2279	2168	2166	8	0
1	B	2263	2153	2151	3	0
2	H	1688	1666	1669	7	0
2	I	1651	1622	1625	8	0
3	L	1661	1608	1610	4	0
3	M	1673	1622	1624	5	0
4	A	2	0	0	0	0
4	H	6	0	0	0	0
4	I	5	0	0	0	0
4	L	3	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	M	5	0	0	0	0
All	All	11236	10839	10845	33	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 2.

All (33) 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)
3:M:152:ASP:OD2	3:M:190:HIS:ND1	2.26	0.68
3:M:2:ILE:HG21	3:M:29:ILE:HD11	1.75	0.67
1:A:147:GLY:O	1:A:291:SER:OG	2.20	0.58
1:A:144:LEU:HD11	1:A:235:LYS:O	2.03	0.58
1:A:388:ASP:OD1	1:A:391:LYS:NZ	2.24	0.57
2:I:38:ARG:HB2	2:I:48:ILE:HD11	1.87	0.55
1:A:319:ASN:ND2	1:A:321:GLU:OE2	2.40	0.55
3:L:21:LEU:HD22	3:L:103:THR:HG21	1.91	0.53
1:B:169:VAL:HG12	1:B:180:GLY:O	2.10	0.52
1:A:319:ASN:OD1	1:A:320:CYS:N	2.43	0.52
2:I:2:VAL:HG22	2:I:27:GLY:HA3	1.90	0.51
1:B:336:GLU:OE1	2:I:103:SER:OG	2.25	0.51
2:H:90:THR:HG23	2:H:118:THR:HA	1.94	0.50
1:A:239:VAL:HG23	1:A:250:LEU:HD11	1.94	0.50
1:A:161:SER:O	2:H:73:ARG:NH2	2.45	0.49
2:H:138:SER:OG	2:H:145:ALA:O	2.28	0.49
3:M:48:LEU:HD23	3:M:59:ILE:HD12	1.97	0.46
2:H:66:ARG:N	2:H:67:PRO:CD	2.80	0.45
2:H:2:VAL:HG22	2:H:27:GLY:HA3	1.99	0.43
1:B:239:VAL:HG23	1:B:250:LEU:HD11	2.00	0.43
2:H:66:ARG:N	2:H:67:PRO:HD2	2.34	0.43
3:L:168:ASP:OD1	3:L:169:SER:N	2.52	0.43
3:M:16:GLY:N	3:M:79:LEU:O	2.45	0.43
2:I:40:ILE:HD13	2:I:91:ALA:HB2	2.01	0.43
2:I:167:LEU:HD21	2:I:190:VAL:HG11	2.00	0.42
3:L:16:GLY:N	3:L:79:LEU:O	2.42	0.42
3:L:19:ALA:HB2	3:L:79:LEU:HD11	2.01	0.42
2:I:209:LYS:N	2:I:210:PRO:HD2	2.35	0.41
2:I:171:VAL:HG22	2:I:190:VAL:HG22	2.02	0.41
3:M:8:PRO:O	3:M:103:THR:HG23	2.20	0.41
1:A:144:LEU:HD13	1:A:234:TYR:CE2	2.55	0.41
2:I:6:GLU:OE1	2:I:6:GLU:N	2.50	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:134:PRO:HG3	2:H:146:LEU:HB3	2.02	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	A	277/347 (80%)	271 (98%)	6 (2%)	0	100	100
1	B	275/347 (79%)	267 (97%)	8 (3%)	0	100	100
2	H	220/239 (92%)	216 (98%)	4 (2%)	0	100	100
2	I	213/239 (89%)	208 (98%)	5 (2%)	0	100	100
3	L	212/218 (97%)	206 (97%)	6 (3%)	0	100	100
3	M	214/218 (98%)	207 (97%)	7 (3%)	0	100	100
All	All	1411/1608 (88%)	1375 (97%)	36 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	A	249/301 (83%)	248 (100%)	1 (0%)	89	96
1	B	247/301 (82%)	246 (100%)	1 (0%)	89	96

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	H	194/208 (93%)	192 (99%)	2 (1%)	73	91
2	I	189/208 (91%)	189 (100%)	0	100	100
3	L	188/191 (98%)	188 (100%)	0	100	100
3	M	189/191 (99%)	189 (100%)	0	100	100
All	All	1256/1400 (90%)	1252 (100%)	4 (0%)	91	97

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	183	PHE
1	B	183	PHE
2	H	53	TYR
2	H	87	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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	A	285/347 (82%)	0.08	10 (3%) 47 39	36, 51, 81, 120	0
1	B	283/347 (81%)	0.16	8 (2%) 55 46	37, 57, 84, 106	0
2	H	222/239 (92%)	-0.11	1 (0%) 87 83	34, 45, 63, 80	0
2	I	217/239 (90%)	0.17	5 (2%) 61 52	36, 55, 87, 105	0
3	L	214/218 (98%)	-0.15	1 (0%) 87 83	36, 50, 67, 92	0
3	M	216/218 (99%)	0.25	3 (1%) 73 66	40, 64, 92, 112	0
All	All	1437/1608 (89%)	0.07	28 (1%) 66 58	34, 52, 86, 120	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	208	VAL	3.4
3	M	0	ILE	3.2
1	B	207	TYR	3.2
1	A	262	TYR	3.1
1	A	230	LYS	3.1
2	I	141	GLY	3.1
1	A	266	ASP	2.9
1	B	208	VAL	2.8
1	B	325	HIS	2.8
3	M	214	GLU	2.7
1	A	207	TYR	2.6
1	A	210	ASN	2.6
2	I	136	SER	2.6
2	H	41	PRO	2.6
3	L	213	GLY	2.4
2	I	217	LYS	2.4
1	B	387	ALA	2.4
1	A	172	GLY	2.3
1	A	283	SER	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	264	ASN	2.3
1	B	262	TYR	2.3
1	B	319	ASN	2.2
3	M	213	GLY	2.2
1	B	144	LEU	2.2
2	I	64	GLU	2.1
1	A	209	LYS	2.0
2	I	218	LYS	2.0
1	A	160	ASN	2.0

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 monosaccharides 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.