



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 04:28 AM UTC

PDB ID : 3H3B / pdb_00003h3b
Title : Crystal structure of the single-chain Fv (scFv) fragment of an anti-ErbB2 antibody chA21 in complex with residues 1-192 of ErbB2 extracellular domain
Authors : Zhou, H.; Liu, Y.; Niu, L.; Zhu, J.; Teng, M.
Deposited on : 2009-04-16
Resolution : 2.45 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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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

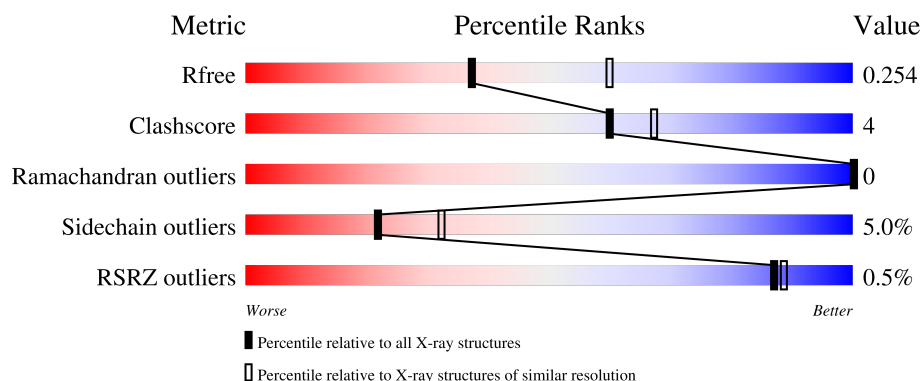
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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}	180053	1190 (2.46-2.46)
Clashscore	190562	1229 (2.46-2.46)
Ramachandran outliers	187476	1218 (2.46-2.46)
Sidechain outliers	187428	1218 (2.46-2.46)
RSRZ outliers	180081	1190 (2.46-2.46)

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	194	 82% 15% ..
1	B	194	 84% 13% ..
2	C	259	 82% 8% • 10%
2	D	259	 80% 9% • 9%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6907 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 Receptor tyrosine-protein kinase erbB-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	193	Total	C	N	O	S	15	2	0
			1522	945	277	289	11			
1	B	189	Total	C	N	O	S	27	2	0
			1499	933	273	282	11			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP P04626
A	0	SER	-	expression tag	UNP P04626
B	-1	GLY	-	expression tag	UNP P04626
B	0	SER	-	expression tag	UNP P04626

- Molecule 2 is a protein called anti-ErbB2 antibody chA21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	234	Total	C	N	O	S	30	0	0
			1816	1152	295	362	7			
2	D	236	Total	C	N	O	S	24	0	0
			1831	1161	298	365	7			

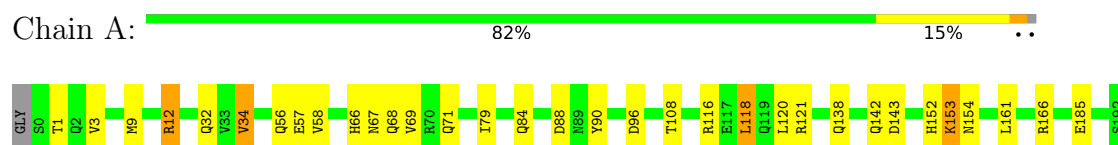
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	68	Total	O	0	0
			68	68		
3	B	48	Total	O	0	0
			48	48		
3	C	54	Total	O	0	0
			54	54		
3	D	69	Total	O	0	0
			69	69		

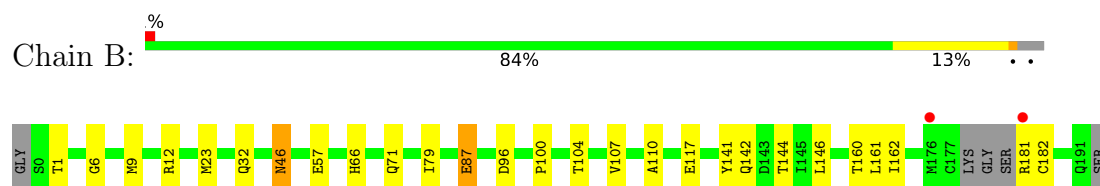
3 Residue-property plots [i](#)

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.

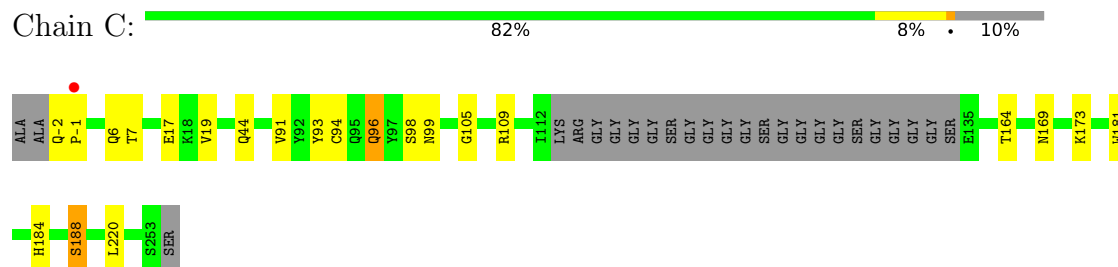
- Molecule 1: Receptor tyrosine-protein kinase erbB-2



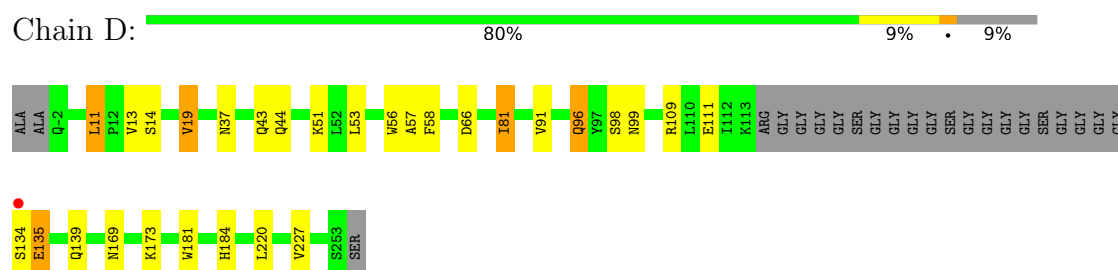
- Molecule 1: Receptor tyrosine-protein kinase erbB-2



- Molecule 2: anti-ErbB2 antibody chA21



- Molecule 2: anti-ErbB2 antibody chA21



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	82.18Å 87.20Å 108.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.91 – 2.45 29.91 – 2.45	Depositor EDS
% Data completeness (in resolution range)	99.2 (29.91-2.45) 99.1 (29.91-2.45)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.53 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.201 , 0.255 0.199 , 0.254	Depositor DCC
R_{free} test set	1458 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	33.5	Xtriage
Anisotropy	0.282	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 33.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6907	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.68% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.48	0/1556	0.81	1/2114 (0.0%)
1	B	0.61	1/1530 (0.1%)	0.86	1/2077 (0.0%)
2	C	0.52	0/1861	0.74	1/2527 (0.0%)
2	D	0.56	2/1876 (0.1%)	0.73	1/2546 (0.0%)
All	All	0.55	3/6823 (0.0%)	0.78	4/9264 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	134	SER	C-N	9.02	1.45	1.33
1	B	6	GLY	C-O	-5.86	1.19	1.24
2	D	227	VAL	C-O	-5.69	1.17	1.24

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	100	PRO	N-CA-C	-7.42	100.29	111.57
2	D	134	SER	CA-CB-OG	6.49	124.08	111.10
2	C	188	SER	N-CA-C	5.68	117.56	111.36
1	A	90	TYR	N-CA-C	5.09	117.19	108.90

There are no chirality outliers.

There are no planarity outliers.

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	A	1522	0	1516	14	0
1	B	1499	0	1500	15	0
2	C	1816	0	1746	13	0
2	D	1831	0	1764	14	0
3	A	68	0	0	0	0
3	B	48	0	0	0	0
3	C	54	0	0	2	0
3	D	69	0	0	0	0
All	All	6907	0	6526	56	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 4.

All (56) 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:D:135:GLU:OE2	2:D:135:GLU:HA	1.62	0.98
1:B:87:GLU:OE1	1:B:87:GLU:HA	1.79	0.83
2:D:169:ASN:HD22	2:D:181:TRP:HE1	1.26	0.81
1:B:87:GLU:OE1	1:B:87:GLU:CA	2.30	0.78
2:C:169:ASN:HD22	2:C:181:TRP:HE1	1.31	0.77
1:B:144:THR:O	1:B:181:ARG:HD3	1.90	0.71
2:C:17:GLU:HG3	3:C:264:HOH:O	1.90	0.71
1:B:9:MET:HE1	1:B:23:MET:HE1	1.74	0.68
2:C:44:GLN:HE22	2:C:173:LYS:HE3	1.61	0.66
1:B:46:ASN:ND2	1:B:46:ASN:H	1.99	0.61
1:B:46:ASN:H	1:B:46:ASN:HD22	1.47	0.60
2:C:6:GLN:HE22	2:C:93:TYR:HA	1.68	0.59
1:A:152:HIS:HD2	1:A:154:ASN:H	1.52	0.58
2:C:96:GLN:HE22	2:C:99:ASN:H	1.50	0.58
1:A:143:ASP:CG	1:A:166:ARG:HH22	2.11	0.57
1:A:143:ASP:OD1	1:A:166:ARG:NH2	2.37	0.57
2:D:44:GLN:HE22	2:D:173:LYS:HE3	1.71	0.55
1:B:146:LEU:HB2	1:B:181:ARG:CZ	2.37	0.54
2:D:91:VAL:HG22	2:D:109:ARG:HG3	1.90	0.53
2:D:19:VAL:HG22	2:D:81:ILE:HG12	1.90	0.53
2:C:96:GLN:NE2	2:C:98:SER:H	2.07	0.53
2:C:6:GLN:NE2	2:C:94:CYS:H	2.07	0.52
2:D:58:PHE:C	2:D:58:PHE:CD1	2.89	0.49
1:A:143:ASP:OD1	1:A:143:ASP:N	2.44	0.49
2:C:44:GLN:NE2	2:C:173:LYS:HE3	2.26	0.48
2:D:96:GLN:NE2	2:D:98:SER:H	2.12	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:107:VAL:HB	1:B:110:ALA:HB3	1.95	0.47
1:A:116:ARG:HH11	1:A:138:GLN:HE21	1.62	0.47
2:C:17:GLU:CG	3:C:264:HOH:O	2.55	0.47
2:D:43:GLN:HB2	2:D:53:LEU:HD11	1.95	0.47
1:B:1:THR:HA	1:B:32:GLN:NE2	2.30	0.46
1:B:160:THR:HG23	1:B:162:ILE:HD12	1.98	0.46
1:A:57:GLU:HB2	1:A:79:ILE:HG23	1.98	0.46
1:B:141:TYR:HB3	1:B:182:CYS:O	2.15	0.46
2:D:56:TRP:O	2:D:57:ALA:HB3	2.16	0.45
2:C:91:VAL:HG22	2:C:109:ARG:HG3	1.99	0.45
1:A:153:LYS:CD	1:A:153:LYS:H	2.29	0.44
1:A:32:GLN:HE21	1:A:56:GLN:HE22	1.65	0.44
2:D:135:GLU:OE2	2:D:135:GLU:CA	2.49	0.43
2:C:-2:GLN:N	2:C:-1:PRO:HD3	2.33	0.43
1:A:34:VAL:HG13	1:A:58:VAL:HA	2.01	0.43
1:A:116:ARG:HH11	1:A:138:GLN:NE2	2.17	0.43
1:A:67:ASN:HB3	1:A:69:VAL:HG12	2.00	0.43
1:B:57:GLU:HG3	1:B:79:ILE:HG23	2.00	0.43
2:C:6:GLN:HE21	2:C:105:GLY:HA3	1.83	0.43
2:D:37:ASN:HB2	2:D:57:ALA:HB2	2.00	0.42
1:B:66:HIS:HA	1:B:96:ASP:O	2.19	0.42
2:D:11:LEU:HD22	2:D:13:VAL:HG13	2.01	0.42
1:A:118:LEU:HD22	1:A:120:LEU:HG	2.01	0.42
2:D:96:GLN:HE22	2:D:99:ASN:H	1.67	0.42
2:C:164:THR:HB	2:C:188:SER:HB3	2.01	0.41
1:A:66:HIS:HA	1:A:96:ASP:O	2.21	0.41
2:D:19:VAL:HG22	2:D:81:ILE:CG1	2.51	0.41
1:A:9:MET:O	1:A:12:ARG:HB3	2.21	0.41
1:B:71:GLN:HG2	1:B:117:GLU:HG3	2.03	0.41
1:B:9:MET:O	1:B:12:ARG:HB2	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	A	193/194 (100%)	184 (95%)	9 (5%)	0	100	100
1	B	187/194 (96%)	179 (96%)	8 (4%)	0	100	100
2	C	230/259 (89%)	223 (97%)	7 (3%)	0	100	100
2	D	232/259 (90%)	223 (96%)	9 (4%)	0	100	100
All	All	842/906 (93%)	809 (96%)	33 (4%)	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	174/172 (101%)	159 (91%)	15 (9%)	10	11
1	B	171/172 (99%)	166 (97%)	5 (3%)	37	52
2	C	202/209 (97%)	197 (98%)	5 (2%)	42	56
2	D	204/209 (98%)	192 (94%)	12 (6%)	18	26
All	All	751/762 (99%)	714 (95%)	37 (5%)	22	33

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	THR
1	A	3	VAL
1	A	12	ARG
1	A	34	VAL
1	A	68	GLN
1	A	71	GLN
1	A	84	GLN
1	A	88	ASP
1	A	108	THR
1	A	118	LEU

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Mol	Chain	Res	Type
1	A	121	ARG
1	A	142	GLN
1	A	153	LYS
1	A	161	LEU
1	A	185	GLU
1	B	46	ASN
1	B	87	GLU
1	B	104	THR
1	B	142	GLN
1	B	161	LEU
2	C	7	THR
2	C	19	VAL
2	C	96	GLN
2	C	184	HIS
2	C	220	LEU
2	D	11	LEU
2	D	14	SER
2	D	19	VAL
2	D	51	LYS
2	D	66	ASP
2	D	81	ILE
2	D	96	GLN
2	D	111	GLU
2	D	135	GLU
2	D	139	GLN
2	D	184	HIS
2	D	220	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	ASN
1	A	56	GLN
1	A	68	GLN
1	A	138	GLN
1	A	152	HIS
1	B	20	HIS
1	B	26	HIS
1	B	32	GLN
1	B	46	ASN
2	C	6	GLN
2	C	44	GLN

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Mol	Chain	Res	Type
2	C	96	GLN
2	C	169	ASN
2	C	174	ASN
2	C	184	HIS
2	D	35	GLN
2	D	43	GLN
2	D	44	GLN
2	D	95	GLN
2	D	96	GLN
2	D	169	ASN
2	D	174	ASN

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	A	193/194 (99%)	-0.17	0 100 100	13, 21, 33, 36	9 (4%)
1	B	189/194 (97%)	-0.01	2 (1%) 78 79	10, 23, 38, 44	10 (5%)
2	C	234/259 (90%)	-0.02	1 (0%) 88 89	13, 25, 31, 33	9 (3%)
2	D	236/259 (91%)	-0.06	1 (0%) 88 89	14, 24, 36, 39	9 (3%)
All	All	852/906 (94%)	-0.06	4 (0%) 87 88	10, 24, 35, 44	37 (4%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	134	SER	4.5
1	B	176	MET	2.3
2	C	-1	PRO	2.2
1	B	181	ARG	2.1

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.