Full wwPDB X-ray Structure Validation Report (i)

Aug 20, 2020 – 12:13 PM BST

|		
PDB ID	:	6UMG
Title	:	Crystal structure of erenumab Fab bound to the extracellular domain of CGRP receptor
Authors	:	Mohr, C.
Deposited on	:	2019-10-09
Resolution	:	2.70 Å(reported)

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 2.70 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.
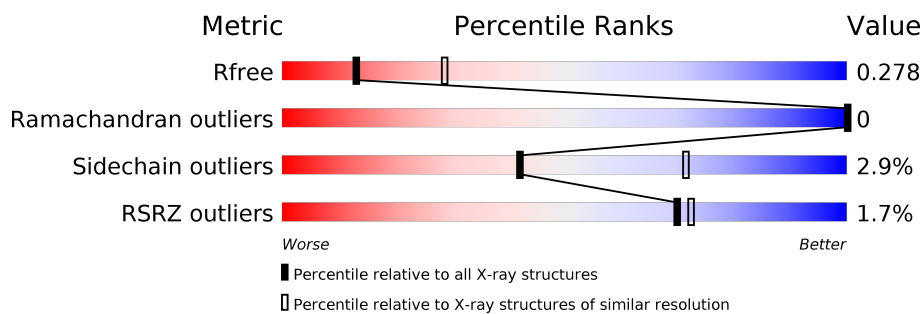
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2808 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 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 <=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	H	237	2% 94% · ·
1	h	237	3% 89% · 8%
2	L	216	97% · ·
2	l	216	% 98% · ·
3	C	139	2% 76% · 20%
3	c	139	4% 78% · 20%
4	R	120	66% · 33%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	r	120	66% · 33%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 9813 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 erenumab Fab heavy chain, IgG1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	228	Total 1728	C 1095	N 292	O 333	S 8	0	0	0
1	h	219	Total 1669	C 1061	N 282	O 319	S 7	0	0	0

- Molecule 2 is a protein called erenumab Fab light chain, IgG1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	214	Total 1592	C 996	N 268	O 324	S 4	0	0	0
2	l	214	Total 1592	C 996	N 268	O 324	S 4	0	0	0

- Molecule 3 is a protein called Calcitonin gene-related peptide type 1 receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	111	Total 906	C 560	N 154	O 183	S 9	0	0	0
3	c	111	Total 901	C 557	N 152	O 183	S 9	0	0	0

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-5	MET	-	expression tag	UNP Q16602
C	-4	SER	-	expression tag	UNP Q16602
C	-3	TYR	-	expression tag	UNP Q16602
C	-2	TYR	-	expression tag	UNP Q16602
C	-1	HIS	-	expression tag	UNP Q16602
C	0	HIS	-	expression tag	UNP Q16602
C	1	HIS	-	expression tag	UNP Q16602
C	2	HIS	-	expression tag	UNP Q16602

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	3	HIS	-	expression tag	UNP Q16602
C	4	HIS	-	expression tag	UNP Q16602
C	5	LEU	-	expression tag	UNP Q16602
C	6	GLU	-	expression tag	UNP Q16602
C	7	SER	-	expression tag	UNP Q16602
C	8	THR	-	expression tag	UNP Q16602
C	9	SER	-	expression tag	UNP Q16602
C	10	LEU	-	expression tag	UNP Q16602
C	11	TYR	-	expression tag	UNP Q16602
C	12	LYS	-	expression tag	UNP Q16602
C	13	LYS	-	expression tag	UNP Q16602
C	14	ALA	-	expression tag	UNP Q16602
C	15	GLY	-	expression tag	UNP Q16602
C	16	SER	-	expression tag	UNP Q16602
C	17	LEU	-	expression tag	UNP Q16602
C	18	VAL	-	expression tag	UNP Q16602
C	19	PRO	-	expression tag	UNP Q16602
C	20	ARG	-	expression tag	UNP Q16602
C	21	GLY	-	expression tag	UNP Q16602
C	22	SER	-	expression tag	UNP Q16602
c	-5	MET	-	expression tag	UNP Q16602
c	-4	SER	-	expression tag	UNP Q16602
c	-3	TYR	-	expression tag	UNP Q16602
c	-2	TYR	-	expression tag	UNP Q16602
c	-1	HIS	-	expression tag	UNP Q16602
c	0	HIS	-	expression tag	UNP Q16602
c	1	HIS	-	expression tag	UNP Q16602
c	2	HIS	-	expression tag	UNP Q16602
c	3	HIS	-	expression tag	UNP Q16602
c	4	HIS	-	expression tag	UNP Q16602
c	5	LEU	-	expression tag	UNP Q16602
c	6	GLU	-	expression tag	UNP Q16602
c	7	SER	-	expression tag	UNP Q16602
c	8	THR	-	expression tag	UNP Q16602
c	9	SER	-	expression tag	UNP Q16602
c	10	LEU	-	expression tag	UNP Q16602
c	11	TYR	-	expression tag	UNP Q16602
c	12	LYS	-	expression tag	UNP Q16602
c	13	LYS	-	expression tag	UNP Q16602
c	14	ALA	-	expression tag	UNP Q16602
c	15	GLY	-	expression tag	UNP Q16602
c	16	SER	-	expression tag	UNP Q16602

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
c	17	LEU	-	expression tag	UNP Q16602
c	18	VAL	-	expression tag	UNP Q16602
c	19	PRO	-	expression tag	UNP Q16602
c	20	ARG	-	expression tag	UNP Q16602
c	21	GLY	-	expression tag	UNP Q16602
c	22	SER	-	expression tag	UNP Q16602

- Molecule 4 is a protein called Receptor activity-modifying protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	R	81	665	424	116	117	8	0	0	0
			Total	C	N	O	S			
4	r	81	665	424	116	117	8	0	0	0

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	-2	MET	-	expression tag	UNP O60894
R	-1	SER	-	expression tag	UNP O60894
R	0	TYR	-	expression tag	UNP O60894
R	1	TYR	-	expression tag	UNP O60894
R	2	HIS	-	expression tag	UNP O60894
R	3	HIS	-	expression tag	UNP O60894
R	4	HIS	-	expression tag	UNP O60894
R	5	HIS	-	expression tag	UNP O60894
R	6	HIS	-	expression tag	UNP O60894
R	7	HIS	-	expression tag	UNP O60894
R	8	LEU	-	expression tag	UNP O60894
R	9	GLU	-	expression tag	UNP O60894
R	10	SER	-	expression tag	UNP O60894
R	11	THR	-	expression tag	UNP O60894
R	12	SER	-	expression tag	UNP O60894
R	13	LEU	-	expression tag	UNP O60894
R	14	TYR	-	expression tag	UNP O60894
R	15	LYS	-	expression tag	UNP O60894
R	16	LYS	-	expression tag	UNP O60894
R	17	ALA	-	expression tag	UNP O60894
R	18	GLY	-	expression tag	UNP O60894
R	19	SER	-	expression tag	UNP O60894
R	20	LEU	-	expression tag	UNP O60894
R	21	VAL	-	expression tag	UNP O60894

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
R	22	PRO	-	expression tag	UNP O60894
R	23	ARG	-	expression tag	UNP O60894
R	24	GLY	-	expression tag	UNP O60894
R	25	SER	-	expression tag	UNP O60894
r	-2	MET	-	expression tag	UNP O60894
r	-1	SER	-	expression tag	UNP O60894
r	0	TYR	-	expression tag	UNP O60894
r	1	TYR	-	expression tag	UNP O60894
r	2	HIS	-	expression tag	UNP O60894
r	3	HIS	-	expression tag	UNP O60894
r	4	HIS	-	expression tag	UNP O60894
r	5	HIS	-	expression tag	UNP O60894
r	6	HIS	-	expression tag	UNP O60894
r	7	HIS	-	expression tag	UNP O60894
r	8	LEU	-	expression tag	UNP O60894
r	9	GLU	-	expression tag	UNP O60894
r	10	SER	-	expression tag	UNP O60894
r	11	THR	-	expression tag	UNP O60894
r	12	SER	-	expression tag	UNP O60894
r	13	LEU	-	expression tag	UNP O60894
r	14	TYR	-	expression tag	UNP O60894
r	15	LYS	-	expression tag	UNP O60894
r	16	LYS	-	expression tag	UNP O60894
r	17	ALA	-	expression tag	UNP O60894
r	18	GLY	-	expression tag	UNP O60894
r	19	SER	-	expression tag	UNP O60894
r	20	LEU	-	expression tag	UNP O60894
r	21	VAL	-	expression tag	UNP O60894
r	22	PRO	-	expression tag	UNP O60894
r	23	ARG	-	expression tag	UNP O60894
r	24	GLY	-	expression tag	UNP O60894
r	25	SER	-	expression tag	UNP O60894

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	H	19	Total 19	O 19	0	0
5	L	15	Total 15	O 15	0	0
5	C	15	Total 15	O 15	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	R	4	Total 4	O 4	0	0
5	h	12	Total 12	O 12	0	0
5	l	13	Total 13	O 13	0	0
5	c	14	Total 14	O 14	0	0
5	r	3	Total 3	O 3	0	0

# 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.
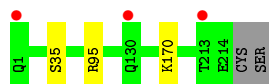
- Molecule 1: erenumab Fab heavy chain, IgG1
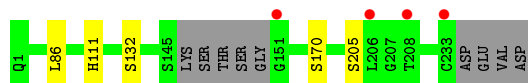
- Molecule 1: erenumab Fab heavy chain, IgG1
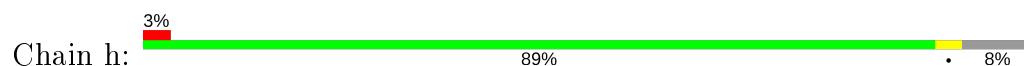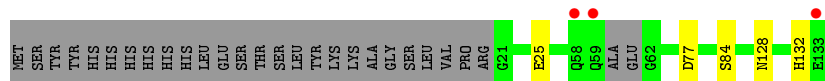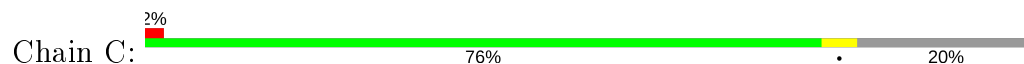

- Molecule 2: erenumab Fab light chain, IgG1

- Molecule 2: erenumab Fab light chain, IgG1

- Molecule 3: Calcitonin gene-related peptide type 1 receptor

- Molecule 3: Calcitonin gene-related peptide type 1 receptor
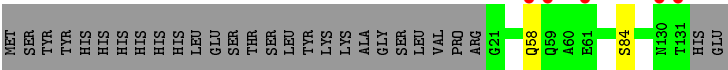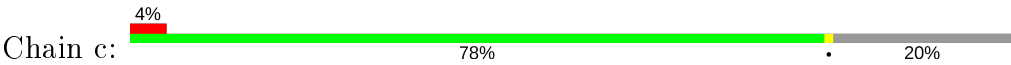
Chain c:

4%

78%   •   20%

MET SER TYR HIS HIS HIS HIS HIS HIS LEU GLU SER THR SER LEU TYR LYS LYS ALA GLY SER LEU VAL PRO ARG G21 Q58 Q59 A60 E61 S84 N130 T131 HIS GLU

● Molecule 4: Receptor activity-modifying protein 1

Chain R:

66%   •   33%

MET SER TYR HIS HIS HIS HIS HIS HIS LEU GLU SER THR SER LEU TYR LYS LYS ALA GLY SER LEU VAL PRO ARG GLY SER A26 R67 R99 I106 SER GLY ARG ALA VAL ARG ASP PRO PRO GLY SER

● Molecule 4: Receptor activity-modifying protein 1

Chain r:

66%   •   33%

MET SER TYR HIS HIS HIS HIS HIS HIS LEU GLU SER THR SER LEU TYR LYS LYS ALA GLY SER LEU VAL PRO ARG GLY SER A26 R67 C82 I106 SER GLY ARG ALA VAL ARG ASP PRO PRO GLY SER
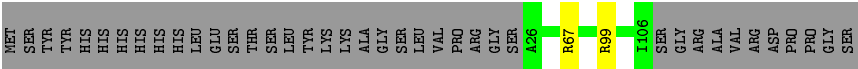
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	70.46Å 112.52Å 77.25Å 90.00° 91.84° 90.00°	Depositor
Resolution (Å)	30.00 – 2.70 26.44 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.7 (30.00-2.70) 99.8 (26.44-2.70)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.26 (at 2.72Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.245 , 0.282 0.242 , 0.278	Depositor DCC
R_{free} test set	1555 reflections (4.70%)	wwPDB-VP
Wilson B-factor (Å^2)	36.0	Xtriage
Anisotropy	0.121	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 2.1	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.127 for h,-k,-l	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	9813	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.70% of the height of the origin peak. No significant pseudotranslation is detected.*

---

[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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	H	0.34	0/1771	0.52	0/2407
1	h	0.35	0/1711	0.56	0/2325
2	L	0.28	0/1630	0.48	0/2226
2	l	0.28	0/1630	0.48	0/2226
3	C	0.32	0/929	0.52	0/1263
3	c	0.32	0/924	0.53	0/1258
4	R	0.32	0/684	0.44	0/927
4	r	0.30	0/684	0.49	0/927
All	All	0.31	0/9963	0.51	0/13559

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 (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	H	224/237 (94%)	216 (96%)	8 (4%)	0	100	100
1	h	213/237 (90%)	206 (97%)	7 (3%)	0	100	100
2	L	212/216 (98%)	205 (97%)	7 (3%)	0	100	100
2	l	212/216 (98%)	201 (95%)	11 (5%)	0	100	100
3	C	107/139 (77%)	102 (95%)	5 (5%)	0	100	100
3	c	109/139 (78%)	106 (97%)	3 (3%)	0	100	100
4	R	79/120 (66%)	79 (100%)	0	0	100	100
4	r	79/120 (66%)	79 (100%)	0	0	100	100
All	All	1235/1424 (87%)	1194 (97%)	41 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	H	193/201 (96%)	188 (97%)	5 (3%)	46	75
1	h	185/201 (92%)	177 (96%)	8 (4%)	29	57
2	L	180/182 (99%)	176 (98%)	4 (2%)	52	79
2	l	180/182 (99%)	177 (98%)	3 (2%)	60	84
3	C	101/126 (80%)	96 (95%)	5 (5%)	24	51
3	c	100/126 (79%)	98 (98%)	2 (2%)	55	81
4	R	68/101 (67%)	66 (97%)	2 (3%)	42	71
4	r	68/101 (67%)	66 (97%)	2 (3%)	42	71
All	All	1075/1220 (88%)	1044 (97%)	31 (3%)	42	71

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	86	LEU
1	H	111	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	132	SER
1	H	170	SER
1	H	205	SER
2	L	1	GLN
2	L	35	SER
2	L	174	ASN
2	L	213	THR
3	C	25	GLU
3	C	77	ASP
3	C	84	SER
3	C	128	ASN
3	C	132	HIS
4	R	67	ARG
4	R	99	ARG
1	h	43	LYS
1	h	86	LEU
1	h	111	HIS
1	h	137	SER
1	h	170	SER
1	h	172	ASN
1	h	205	SER
1	h	229	GLU
2	l	35	SER
2	l	95	ARG
2	l	170	LYS
3	c	58	GLN
3	c	84	SER
4	r	67	ARG
4	r	82	CYS

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

Mol	Chain	Res	Type
1	H	111	HIS
1	H	122	GLN
1	H	188	GLN
2	L	198	GLN
3	C	58	GLN
3	C	128	ASN
1	h	111	HIS
1	h	172	ASN
1	h	188	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	c	58	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 monosaccharides 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(Å²)	Q<0.9
1	H	228/237 (96%)	-0.17	4 (1%)	68	70	24, 33, 62, 76	0
1	h	219/237 (92%)	-0.05	6 (2%)	54	55	25, 35, 65, 72	0
2	L	214/216 (99%)	-0.23	0	100	100	27, 34, 45, 58	0
2	l	214/216 (99%)	-0.22	3 (1%)	75	77	27, 36, 49, 57	0
3	C	111/139 (79%)	-0.16	3 (2%)	54	55	26, 35, 53, 68	0
3	c	111/139 (79%)	-0.08	5 (4%)	33	31	27, 36, 52, 62	0
4	R	81/120 (67%)	-0.16	0	100	100	30, 37, 42, 48	0
4	r	81/120 (67%)	-0.13	0	100	100	31, 40, 47, 51	0
All	All	1259/1424 (88%)	-0.16	21 (1%)	70	72	24, 35, 57, 76	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	208	THR	7.4
1	h	208	THR	5.7
1	H	233	CYS	4.9
1	h	144	SER	4.1
3	c	59	GLN	3.5
1	h	131	ALA	3.0
2	l	213	THR	2.9
3	C	133	GLU	2.8
3	C	58	GLN	2.7
3	C	59	GLN	2.7
3	c	58	GLN	2.5
1	H	206	LEU	2.5
3	c	130	ASN	2.5
3	c	131	THR	2.4
1	H	151	GLY	2.4
2	l	130	GLN	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	l	1	GLN	2.2
1	h	189	SER	2.2
3	c	61	GLU	2.1
1	h	151	GLY	2.1
1	h	206	LEU	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.