



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 7, 2020 – 08:04 PM BST

PDB ID : 1I8L
Title : HUMAN B7-1/CTLA-4 CO-STIMULATORY COMPLEX
Authors : Stamper, C.C.; Somers, W.S.; Mosyak, L.
Deposited on : 2001-03-14
Resolution : 3.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

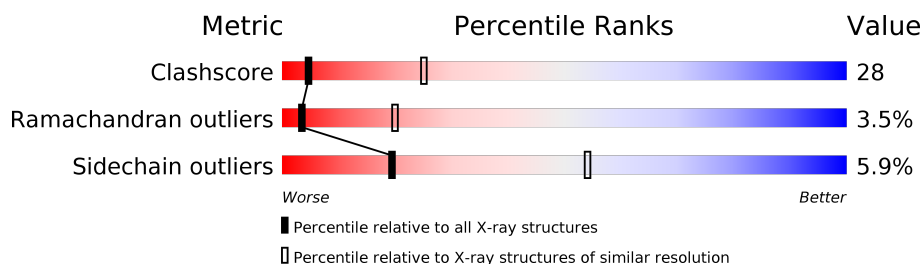
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)

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 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	208	
1	B	208	
2	C	126	
2	D	126	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 5108 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 T LYMPHOCYTE ACTIVATION ANTIGEN CD80.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	199	Total	C	N	O	S	0	0	0
			1574	999	262	303	10			
1	B	199	Total	C	N	O	S	0	0	0
			1564	991	261	302	10			

- Molecule 2 is a protein called CYTOTOXIC T-LYMPHOCYTE PROTEIN 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	118	Total	C	N	O	S	0	0	0
			862	543	140	170	9			
2	D	118	Total	C	N	O	S	0	0	0
			834	527	135	163	9			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is alpha-D-mannopyranose (three-letter code: MAN) (formula: C₆H₁₂O₆).



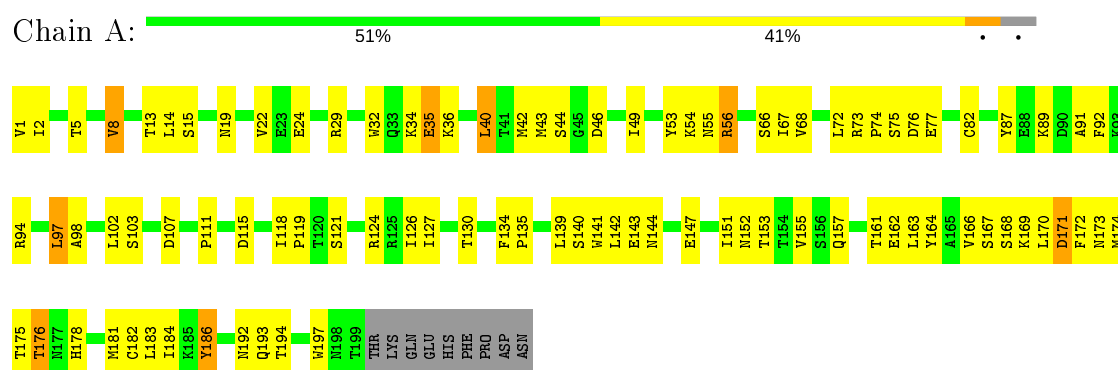
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			11	6	5		
4	B	1	Total	C	O	0	0
			11	6	5		

3 Residue-property plots

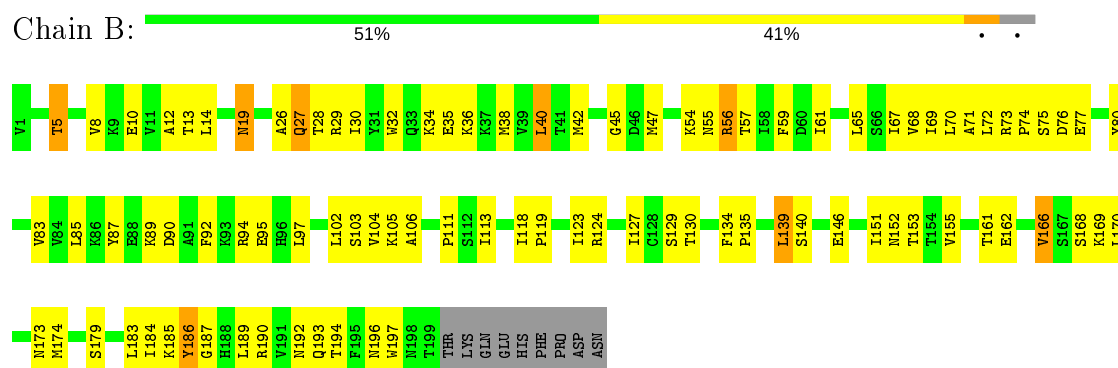
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

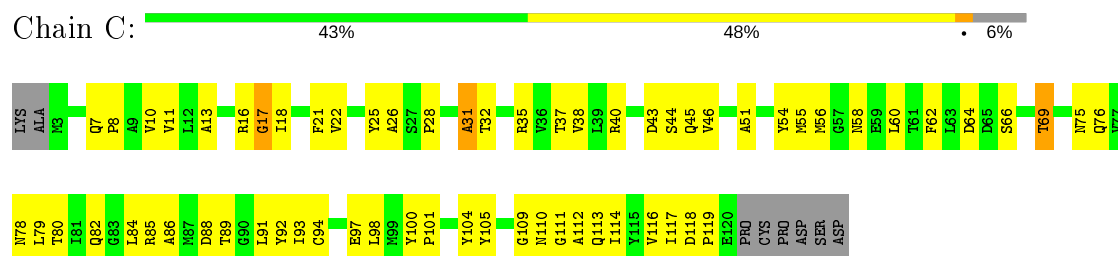
• Molecule 1: T LYMPHOCYTE ACTIVATION ANTIGEN CD80



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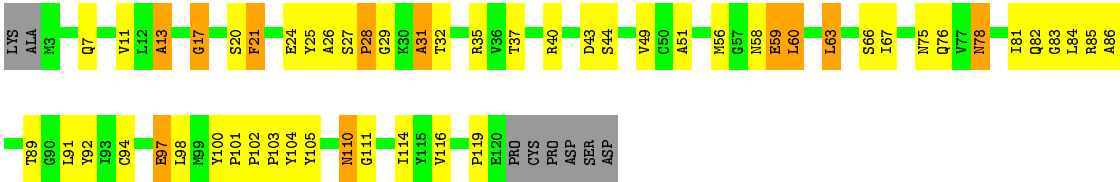


• Molecule 2: CYTOTOXIC T-LYMPHOCYTE PROTEIN 4



• Molecule 2: CYTOTOXIC T-LYMPHOCYTE PROTEIN 4

Chain D: 51% 34% 9% 6%



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	88.60 Å 183.24 Å 230.73 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.77 – 3.00	Depositor
% Data completeness (in resolution range)	82.9 (19.77-3.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.229 , 0.257	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5108	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, MAN

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	0.45	0/1609	0.70	0/2189
1	B	0.44	0/1599	0.72	0/2178
2	C	0.44	0/877	0.73	1/1198 (0.1%)
2	D	0.43	0/848	0.68	0/1161
All	All	0.44	0/4933	0.71	1/6726 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	66	SER	N-CA-C	5.09	124.74	111.00

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	1574	0	1520	96	0
1	B	1564	0	1496	85	0
2	C	862	0	831	50	0
2	D	834	0	795	49	0
3	A	98	0	91	11	0
3	B	98	0	91	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	28	0	26	5	0
3	D	28	0	26	4	0
4	A	11	0	10	1	0
4	B	11	0	10	1	0
All	All	5108	0	4896	281	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 28.

The worst 5 of 281 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:A:192:ASN:HD21	3:A:215:NAG:C1	1.60	1.15
1:A:55:ASN:HD21	3:A:210:NAG:C1	1.64	1.11
1:B:192:ASN:HD21	3:B:215:NAG:C1	1.68	1.05
1:B:152:ASN:HD21	3:B:211:NAG:C1	1.70	1.05
1:B:55:ASN:HD21	3:B:210:NAG:C1	1.74	1.00

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	A	197/208 (95%)	169 (86%)	24 (12%)	4 (2%)	7	34
1	B	197/208 (95%)	168 (85%)	26 (13%)	3 (2%)	10	42
2	C	116/126 (92%)	101 (87%)	9 (8%)	6 (5%)	2	12
2	D	116/126 (92%)	93 (80%)	14 (12%)	9 (8%)	1	4
All	All	626/668 (94%)	531 (85%)	73 (12%)	22 (4%)	3	20

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	8	VAL
1	A	54	LYS
1	A	121	SER
1	B	54	LYS
2	C	16	ARG

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	176/193 (91%)	168 (96%)	8 (4%)	27	64
1	B	174/193 (90%)	161 (92%)	13 (8%)	13	43
2	C	92/104 (88%)	86 (94%)	6 (6%)	17	50
2	D	86/104 (83%)	82 (95%)	4 (5%)	26	63
All	All	528/594 (89%)	497 (94%)	31 (6%)	19	54

5 of 31 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	77	GLU
1	B	139	LEU
2	D	78	ASN
1	B	90	ASP
1	B	166	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	64	ASN
1	B	178	HIS
2	D	78	ASN
1	B	152	ASN
1	B	192	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

20 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	NAG	B	216	-	14,14,15	2.12	6 (42%)	17,19,21	3.03	5 (29%)
3	NAG	B	211	-	14,14,15	1.50	3 (21%)	17,19,21	1.45	2 (11%)
3	NAG	A	211	-	14,14,15	1.56	3 (21%)	17,19,21	1.57	4 (23%)
3	NAG	B	215	-	14,14,15	1.52	3 (21%)	17,19,21	1.28	2 (11%)
3	NAG	A	215	-	14,14,15	1.61	3 (21%)	17,19,21	1.51	3 (17%)
3	NAG	A	212	-	14,14,15	2.14	3 (21%)	17,19,21	2.30	7 (41%)
3	NAG	C	128	-	14,14,15	1.95	6 (42%)	17,19,21	1.25	1 (5%)
4	MAN	A	213	-	11,11,12	1.70	5 (45%)	15,15,17	1.10	2 (13%)
3	NAG	D	127	-	14,14,15	1.84	5 (35%)	17,19,21	1.32	2 (11%)
3	NAG	B	210	-	14,14,15	1.89	5 (35%)	17,19,21	1.31	2 (11%)
3	NAG	A	210	-	14,14,15	1.98	6 (42%)	17,19,21	1.28	2 (11%)
3	NAG	B	214	-	14,14,15	2.09	6 (42%)	17,19,21	1.29	1 (5%)
3	NAG	A	214	-	14,14,15	1.97	5 (35%)	17,19,21	2.38	5 (29%)
3	NAG	A	209	-	14,14,15	2.06	6 (42%)	17,19,21	2.41	6 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	C	127	-	14,14,15	1.92	5 (35%)	17,19,21	1.33	3 (17%)
3	NAG	D	128	-	14,14,15	1.92	6 (42%)	17,19,21	1.25	1 (5%)
4	MAN	B	213	-	11,11,12	1.82	4 (36%)	15,15,17	1.08	2 (13%)
3	NAG	B	209	-	14,14,15	1.93	6 (42%)	17,19,21	1.64	5 (29%)
3	NAG	B	212	-	14,14,15	2.37	5 (35%)	17,19,21	2.17	4 (23%)
3	NAG	A	216	-	14,14,15	1.86	3 (21%)	17,19,21	1.46	4 (23%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	B	216	-	-	1/6/23/26	0/1/1/1
3	NAG	B	211	-	-	0/6/23/26	0/1/1/1
3	NAG	A	211	-	-	0/6/23/26	0/1/1/1
3	NAG	B	215	-	-	0/6/23/26	0/1/1/1
3	NAG	A	215	-	-	0/6/23/26	0/1/1/1
3	NAG	A	212	-	-	0/6/23/26	0/1/1/1
3	NAG	C	128	-	-	0/6/23/26	0/1/1/1
4	MAN	A	213	-	-	1/2/19/22	0/1/1/1
3	NAG	D	127	-	-	0/6/23/26	0/1/1/1
3	NAG	B	210	-	-	0/6/23/26	0/1/1/1
3	NAG	A	210	-	-	0/6/23/26	0/1/1/1
3	NAG	B	214	-	-	0/6/23/26	0/1/1/1
3	NAG	A	214	-	-	1/6/23/26	0/1/1/1
3	NAG	A	209	-	-	2/6/23/26	0/1/1/1
3	NAG	C	127	-	-	0/6/23/26	0/1/1/1
3	NAG	D	128	-	-	0/6/23/26	0/1/1/1
4	MAN	B	213	-	-	1/2/19/22	0/1/1/1
3	NAG	B	209	-	-	0/6/23/26	0/1/1/1
3	NAG	B	212	-	-	0/6/23/26	0/1/1/1
3	NAG	A	216	-	-	0/6/23/26	0/1/1/1

The worst 5 of 94 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	212	NAG	C4-C5	5.44	1.64	1.53
3	A	212	NAG	C4-C5	5.27	1.64	1.53
3	B	216	NAG	C1-C2	4.66	1.59	1.52
3	B	212	NAG	C3-C2	4.60	1.62	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	216	NAG	C4-C5	4.28	1.62	1.53

The worst 5 of 63 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	216	NAG	C2-N2-C7	9.17	135.95	122.90
3	A	214	NAG	C2-N2-C7	7.42	133.47	122.90
3	A	209	NAG	C2-N2-C7	7.23	133.19	122.90
3	B	212	NAG	C4-C3-C2	-6.39	101.65	111.02
3	A	212	NAG	C4-C3-C2	-6.07	102.12	111.02

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	214	NAG	C3-C2-N2-C7
3	A	209	NAG	C3-C2-N2-C7
4	A	213	MAN	O5-C5-C6-O6
4	B	213	MAN	O5-C5-C6-O6
3	B	216	NAG	C3-C2-N2-C7

There are no ring outliers.

18 monomers are involved in 33 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	216	NAG	1	0
3	B	211	NAG	5	0
3	A	211	NAG	4	0
3	B	215	NAG	3	0
3	A	215	NAG	3	0
3	A	212	NAG	2	0
3	C	128	NAG	2	0
4	A	213	MAN	1	0
3	D	127	NAG	2	0
3	B	210	NAG	2	0
3	A	210	NAG	2	0
3	A	209	NAG	1	0
3	C	127	NAG	3	0
3	D	128	NAG	2	0
4	B	213	MAN	1	0
3	B	209	NAG	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	212	NAG	2	0
3	A	216	NAG	1	0

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.