



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 24, 2022 – 12:31 pm GMT

PDB ID : 6GAP
Title : Crystal structure of the T3D reovirus sigma1 coiled coil tail and body
Authors : Dietrich, M.H.; Stehle, T.
Deposited on : 2018-04-11
Resolution : 2.15 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtrriage (Phenix) : 1.13
EDS : 2.27
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0267
CCP4 : 7.1.010 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.27

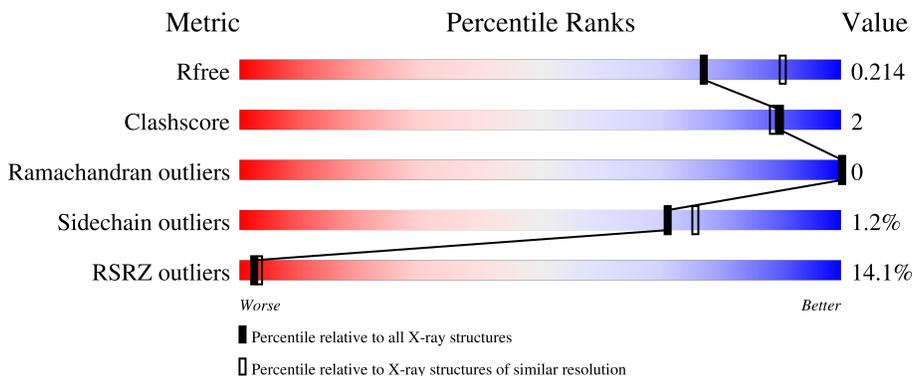
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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	261	 11% 79% 5% 16%
1	B	261	 11% 78% 1% 18%
1	C	261	 12% 77% 5% 18%

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 5186 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 Outer capsid protein sigma-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	218	1606	983	295	326	2	0	1	0
1	B	214	1586	965	295	324	2	0	0	0
1	C	213	1579	962	290	325	2	0	0	0

There are 69 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	MET	-	initiating methionine	UNP P03528
A	3	GLY	-	expression tag	UNP P03528
A	4	SER	-	expression tag	UNP P03528
A	5	SER	-	expression tag	UNP P03528
A	6	HIS	-	expression tag	UNP P03528
A	7	HIS	-	expression tag	UNP P03528
A	8	HIS	-	expression tag	UNP P03528
A	9	HIS	-	expression tag	UNP P03528
A	10	HIS	-	expression tag	UNP P03528
A	11	HIS	-	expression tag	UNP P03528
A	12	SER	-	expression tag	UNP P03528
A	13	SER	-	expression tag	UNP P03528
A	14	GLY	-	expression tag	UNP P03528
A	15	LEU	-	expression tag	UNP P03528
A	16	VAL	-	expression tag	UNP P03528
A	17	PRO	-	expression tag	UNP P03528
A	18	ARG	-	expression tag	UNP P03528
A	19	GLY	-	expression tag	UNP P03528
A	20	SER	-	expression tag	UNP P03528
A	21	HIS	-	expression tag	UNP P03528
A	22	MET	-	expression tag	UNP P03528
A	23	ALA	-	expression tag	UNP P03528
A	24	SER	-	expression tag	UNP P03528

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Chain	Residue	Modelled	Actual	Comment	Reference
B	2	MET	-	initiating methionine	UNP P03528
B	3	GLY	-	expression tag	UNP P03528
B	4	SER	-	expression tag	UNP P03528
B	5	SER	-	expression tag	UNP P03528
B	6	HIS	-	expression tag	UNP P03528
B	7	HIS	-	expression tag	UNP P03528
B	8	HIS	-	expression tag	UNP P03528
B	9	HIS	-	expression tag	UNP P03528
B	10	HIS	-	expression tag	UNP P03528
B	11	HIS	-	expression tag	UNP P03528
B	12	SER	-	expression tag	UNP P03528
B	13	SER	-	expression tag	UNP P03528
B	14	GLY	-	expression tag	UNP P03528
B	15	LEU	-	expression tag	UNP P03528
B	16	VAL	-	expression tag	UNP P03528
B	17	PRO	-	expression tag	UNP P03528
B	18	ARG	-	expression tag	UNP P03528
B	19	GLY	-	expression tag	UNP P03528
B	20	SER	-	expression tag	UNP P03528
B	21	HIS	-	expression tag	UNP P03528
B	22	MET	-	expression tag	UNP P03528
B	23	ALA	-	expression tag	UNP P03528
B	24	SER	-	expression tag	UNP P03528
C	2	MET	-	initiating methionine	UNP P03528
C	3	GLY	-	expression tag	UNP P03528
C	4	SER	-	expression tag	UNP P03528
C	5	SER	-	expression tag	UNP P03528
C	6	HIS	-	expression tag	UNP P03528
C	7	HIS	-	expression tag	UNP P03528
C	8	HIS	-	expression tag	UNP P03528
C	9	HIS	-	expression tag	UNP P03528
C	10	HIS	-	expression tag	UNP P03528
C	11	HIS	-	expression tag	UNP P03528
C	12	SER	-	expression tag	UNP P03528
C	13	SER	-	expression tag	UNP P03528
C	14	GLY	-	expression tag	UNP P03528
C	15	LEU	-	expression tag	UNP P03528
C	16	VAL	-	expression tag	UNP P03528
C	17	PRO	-	expression tag	UNP P03528
C	18	ARG	-	expression tag	UNP P03528
C	19	GLY	-	expression tag	UNP P03528
C	20	SER	-	expression tag	UNP P03528

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Chain	Residue	Modelled	Actual	Comment	Reference
C	21	HIS	-	expression tag	UNP P03528
C	22	MET	-	expression tag	UNP P03528
C	23	ALA	-	expression tag	UNP P03528
C	24	SER	-	expression tag	UNP P03528

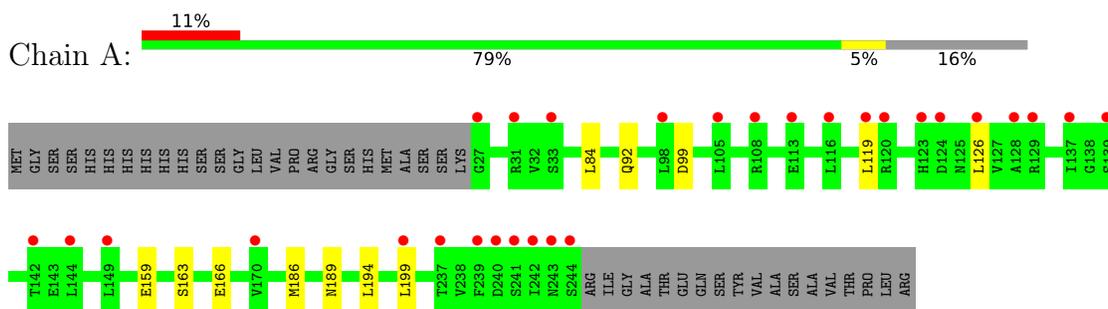
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	148	Total O 148 148	0	0
2	B	119	Total O 119 119	0	0
2	C	148	Total O 148 148	0	0

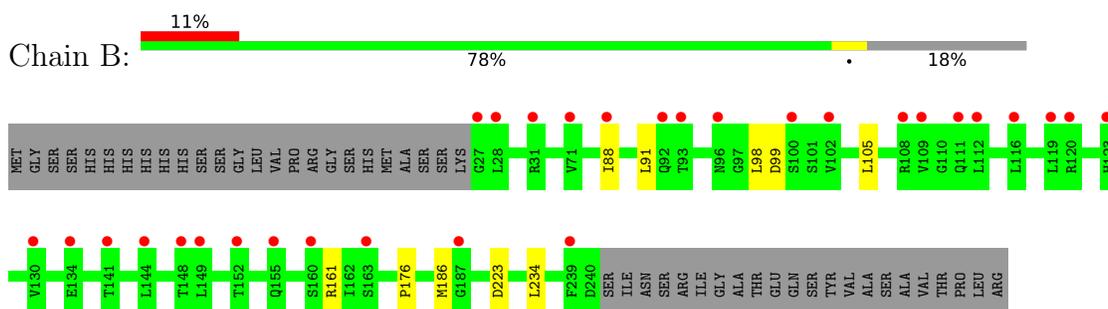
3 Residue-property plots [i](#)

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.

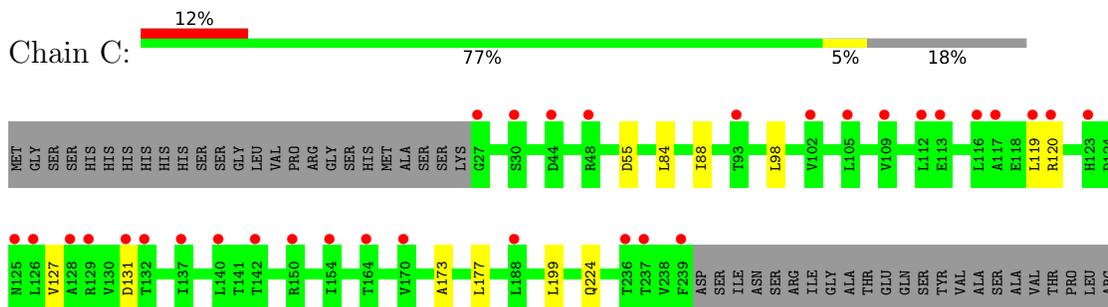
- Molecule 1: Outer capsid protein sigma-1



- Molecule 1: Outer capsid protein sigma-1



- Molecule 1: Outer capsid protein sigma-1



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	350.71Å 41.53Å 63.32Å 90.00° 94.98° 90.00°	Depositor
Resolution (Å)	49.15 – 2.15 49.15 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.15-2.15) 99.9 (49.15-2.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.12 (at 2.16Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.208 , 0.249 0.213 , 0.214	Depositor DCC
R_{free} test set	2513 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	30.4	Xtriage
Anisotropy	0.424	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	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	0.94	EDS
Total number of atoms	5186	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.83% 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	0.49	0/1617	0.60	0/2194
1	B	0.48	0/1593	0.60	0/2161
1	C	0.48	0/1586	0.58	0/2151
All	All	0.48	0/4796	0.59	0/6506

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](#)

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	1606	0	1597	11	0
1	B	1586	0	1581	11	0
1	C	1579	0	1584	10	0
2	A	148	0	0	0	0
2	B	119	0	0	0	0
2	C	148	0	0	1	0
All	All	5186	0	4762	17	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 (17) 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:194:LEU:HD21	1:B:176:PRO:HD3	1.85	0.59
1:B:88:ILE:HD11	1:C:88:ILE:HD11	1.88	0.55
1:B:234:LEU:HD12	1:C:224:GLN:HB3	1.90	0.51
1:C:55:ASP:HB3	2:C:413:HOH:O	2.10	0.51
1:A:84:LEU:HD22	1:C:88:ILE:HD12	1.92	0.49
1:A:199:LEU:HD22	1:B:186:MET:CE	2.42	0.48
1:A:194:LEU:CD2	1:B:176:PRO:HD3	2.42	0.48
1:B:99:ASP:HA	1:C:98:LEU:HD21	1.96	0.47
1:A:99:ASP:HA	1:B:98:LEU:HD21	1.97	0.46
1:A:119:LEU:HD13	1:C:120:ARG:HD2	1.98	0.45
1:B:88:ILE:HD13	1:C:84:LEU:HD22	1.99	0.44
1:A:159:GLU:OE2	1:B:161:ARG:NH2	2.44	0.44
1:A:166:GLU:OE2	1:B:161:ARG:HD2	2.19	0.42
1:A:126:LEU:HD13	1:C:127:VAL:HG22	2.00	0.42
1:A:92:GLN:HG2	1:B:91:LEU:HD13	2.02	0.42
1:A:186:MET:CE	1:C:199:LEU:HD22	2.50	0.41
1:C:173:ALA:HB1	1:C:177:LEU:HB2	2.03	0.41

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	217/261 (83%)	217 (100%)	0	0	100	100
1	B	212/261 (81%)	211 (100%)	1 (0%)	0	100	100
1	C	211/261 (81%)	209 (99%)	2 (1%)	0	100	100
All	All	640/783 (82%)	637 (100%)	3 (0%)	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	A	172/221 (78%)	170 (99%)	2 (1%)	71	76
1	B	171/221 (77%)	169 (99%)	2 (1%)	71	76
1	C	173/221 (78%)	171 (99%)	2 (1%)	71	76
All	All	516/663 (78%)	510 (99%)	6 (1%)	71	76

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	163	SER
1	A	189	ASN
1	B	105	LEU
1	B	223	ASP
1	C	119	LEU
1	C	131	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	206	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 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

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	218/261 (83%)	1.08	29 (13%) 3 4	21, 40, 83, 112	0
1	B	214/261 (81%)	1.01	30 (14%) 2 3	21, 43, 87, 102	0
1	C	213/261 (81%)	1.06	32 (15%) 2 3	21, 42, 87, 102	0
All	All	645/783 (82%)	1.05	91 (14%) 2 3	21, 42, 86, 112	0

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	27	GLY	10.9
1	B	239	PHE	8.6
1	C	236	THR	8.5
1	A	241	SER	8.1
1	A	242	ILE	7.2
1	A	244	SER	6.9
1	A	239	PHE	5.6
1	C	27	GLY	4.9
1	B	96	ASN	4.7
1	A	240	ASP	4.6
1	C	112	LEU	4.6
1	C	30	SER	4.4
1	A	137	ILE	4.4
1	C	125	ASN	4.4
1	C	120	ARG	4.4
1	B	27	GLY	4.3
1	B	152	THR	4.3
1	A	126	LEU	4.3
1	C	131	ASP	4.2
1	C	239	PHE	4.1
1	C	237	THR	4.1
1	B	160	SER	4.0
1	B	116	LEU	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	124	ASP	3.7
1	C	142	THR	3.7
1	A	120	ARG	3.5
1	C	128	ALA	3.5
1	C	119	LEU	3.5
1	C	113	GLU	3.4
1	C	109	VAL	3.3
1	C	117	ALA	3.2
1	B	108	ARG	3.2
1	A	119	LEU	3.2
1	C	170	VAL	3.2
1	A	98	LEU	3.2
1	C	44	ASP	3.1
1	A	237	THR	3.1
1	B	149	LEU	3.1
1	B	119	LEU	3.1
1	C	140	LEU	3.1
1	C	126	LEU	3.0
1	C	93	THR	3.0
1	B	123	HIS	3.0
1	B	148	THR	2.9
1	C	105	LEU	2.9
1	B	100	SER	2.8
1	A	243	ASN	2.8
1	B	155	GLN	2.7
1	B	120	ARG	2.7
1	B	144	LEU	2.7
1	C	129	ARG	2.6
1	B	28	LEU	2.6
1	A	129	ARG	2.6
1	A	128	ALA	2.6
1	A	144	LEU	2.5
1	A	105	LEU	2.5
1	C	137	ILE	2.4
1	C	116	LEU	2.4
1	C	188	LEU	2.4
1	C	123	HIS	2.4
1	C	102	VAL	2.4
1	A	31	ARG	2.4
1	A	170	VAL	2.4
1	C	48	ARG	2.4
1	A	33	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	134	GLU	2.3
1	B	31	ARG	2.3
1	B	93	THR	2.3
1	A	108	ARG	2.3
1	A	116	LEU	2.2
1	B	112	LEU	2.2
1	B	109	VAL	2.2
1	B	187	GLY	2.2
1	A	123	HIS	2.2
1	A	149	LEU	2.2
1	C	164	THR	2.2
1	B	111	GLN	2.2
1	A	113	GLU	2.2
1	B	130	VAL	2.1
1	A	142	THR	2.1
1	C	154	ILE	2.1
1	C	150	ARG	2.1
1	B	71	VAL	2.1
1	C	132	THR	2.1
1	B	102	VAL	2.1
1	B	92	GLN	2.1
1	A	139	SER	2.0
1	B	141	THR	2.0
1	B	163	SER	2.0
1	A	199	LEU	2.0
1	B	88	ILE	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.