



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 04:10 AM UTC

PDB ID : 8TF7 / pdb_00008tf7
Title : Apo structure of protein crystal of Tri17
Authors : Zhai, R.; Zhang, W.
Deposited on : 2023-07-09
Resolution : 2.45 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	:	4-5-2 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

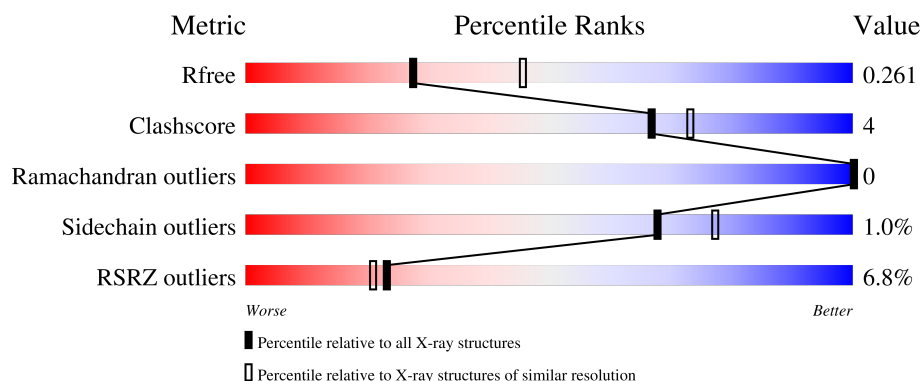
1 Overall quality at a glance

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	565	6% 83% 8% 9%
1	B	565	7% 85% 7% 8%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 15997 atoms, of which 7758 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 AMP-binding protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	516	Total	C	H	N	O	S	0	0	0
			7859	2528	3878	699	741	13			
1	B	517	Total	C	H	N	O	S	0	0	0
			7865	2530	3880	700	742	13			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP A0A5H2UY12
A	557	LEU	-	expression tag	UNP A0A5H2UY12
A	558	GLU	-	expression tag	UNP A0A5H2UY12
A	559	HIS	-	expression tag	UNP A0A5H2UY12
A	560	HIS	-	expression tag	UNP A0A5H2UY12
A	561	HIS	-	expression tag	UNP A0A5H2UY12
A	562	HIS	-	expression tag	UNP A0A5H2UY12
A	563	HIS	-	expression tag	UNP A0A5H2UY12
A	564	HIS	-	expression tag	UNP A0A5H2UY12
A	565	END	-	expression tag	UNP A0A5H2UY12
B	1	MET	-	initiating methionine	UNP A0A5H2UY12
B	557	LEU	-	expression tag	UNP A0A5H2UY12
B	558	GLU	-	expression tag	UNP A0A5H2UY12
B	559	HIS	-	expression tag	UNP A0A5H2UY12
B	560	HIS	-	expression tag	UNP A0A5H2UY12
B	561	HIS	-	expression tag	UNP A0A5H2UY12
B	562	HIS	-	expression tag	UNP A0A5H2UY12
B	563	HIS	-	expression tag	UNP A0A5H2UY12
B	564	HIS	-	expression tag	UNP A0A5H2UY12
B	565	END	-	expression tag	UNP A0A5H2UY12

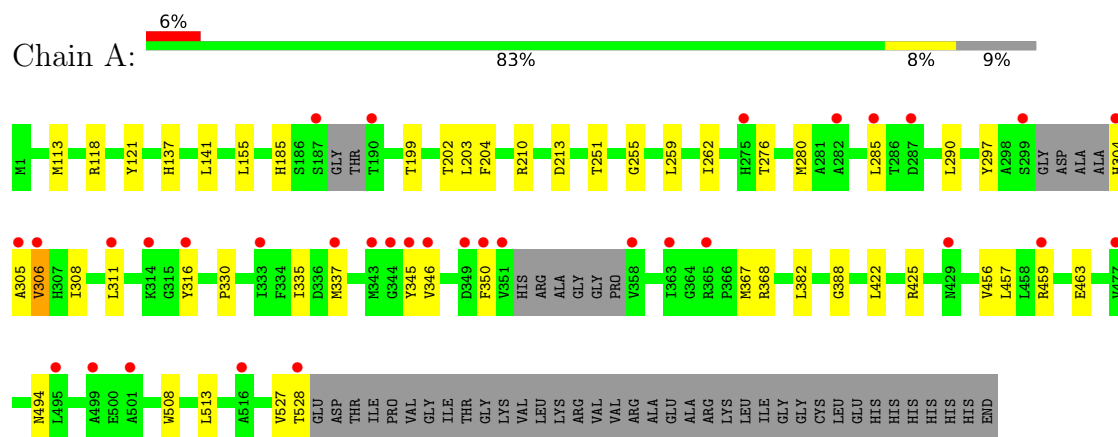
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	127	Total 127	O 127	0	0
2	B	146	Total 146	O 146	0	0

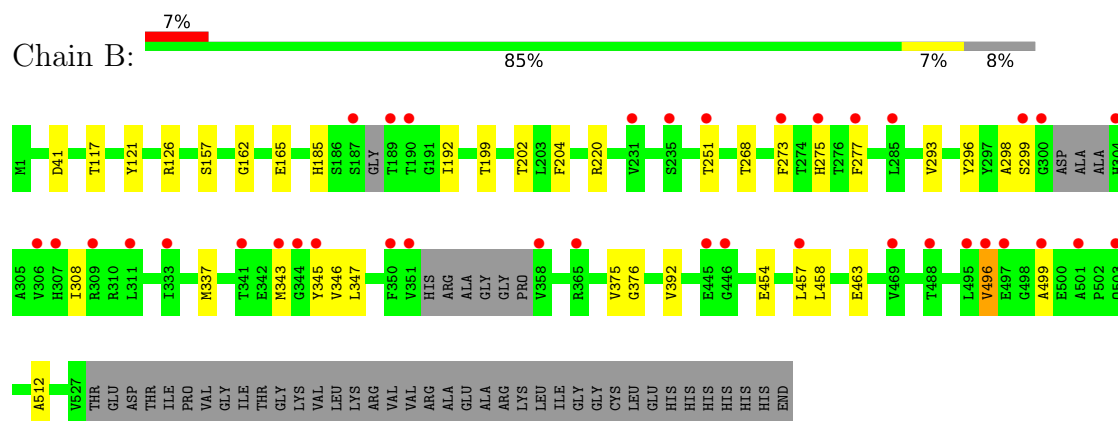
3 Residue-property plots [i](#)

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: AMP-binding protein



• Molecule 1: AMP-binding protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	105.99Å 105.99Å 235.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.34 – 2.45 48.34 – 2.45	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.34-2.45) 100.0 (48.34-2.45)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.16 (at 2.45Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.216 , 0.261 0.215 , 0.261	Depositor DCC
R_{free} test set	2525 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	39.6	Xtriage
Anisotropy	0.443	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 37.0	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	15997	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 7.06% 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	0.22	0/4077	0.38	0/5550
1	B	0.18	0/4081	0.34	0/5555
All	All	0.20	0/8158	0.36	0/11105

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	3981	3878	3905	32	0
1	B	3985	3880	3908	26	0
2	A	127	0	0	0	0
2	B	146	0	0	1	0
All	All	8239	7758	7813	58	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 (58) 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:B:496:VAL:HG23	1:B:499:ALA:HB2	1.42	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:345:TYR:CE2	1:B:346:VAL:HG22	2.13	0.83
1:B:345:TYR:CD2	1:B:346:VAL:HG22	2.18	0.77
1:B:463:GLU:O	1:B:496:VAL:HG22	1.91	0.70
1:A:494:ASN:OD1	1:A:527:VAL:CG2	2.41	0.68
1:A:210:ARG:CZ	1:A:367:MET:HE2	2.25	0.67
1:B:277:PHE:HB3	1:B:308:ILE:HD11	1.79	0.65
1:A:305:ALA:HB1	1:A:308:ILE:HD11	1.79	0.62
1:A:285:LEU:HD13	1:A:311:LEU:HD23	1.87	0.57
1:A:494:ASN:OD1	1:A:527:VAL:HG21	2.05	0.55
1:A:137:HIS:CE1	1:A:141:LEU:HD11	2.45	0.52
1:A:255:GLY:O	1:A:259:LEU:HG	2.09	0.52
1:A:337:MET:SD	1:A:346:VAL:HG21	2.49	0.52
1:B:273:PHE:HB3	1:B:275:HIS:CD2	2.45	0.51
1:A:297:TYR:HD2	1:A:337:MET:HE2	1.76	0.50
1:A:210:ARG:NH1	1:A:367:MET:HE2	2.28	0.49
1:B:375:VAL:HG12	1:B:376:GLY:O	2.11	0.49
1:B:162:GLY:O	1:B:165:GLU:HG2	2.13	0.49
1:A:457:LEU:HD21	1:A:513:LEU:HD21	1.96	0.47
1:A:316:TYR:CD1	1:A:330:PRO:HA	2.49	0.47
1:B:343:MET:HE3	1:B:392:VAL:HG11	1.97	0.47
1:A:276:THR:O	1:A:280:MET:HG3	2.15	0.46
1:A:259:LEU:CD2	1:A:280:MET:HE3	2.46	0.46
1:A:388:GLY:C	1:A:422:LEU:HD23	2.41	0.46
1:A:345:TYR:CG	1:A:346:VAL:N	2.84	0.45
1:A:382:LEU:O	1:A:425:ARG:NH1	2.48	0.45
1:A:527:VAL:HG23	1:A:528:THR:N	2.31	0.45
1:A:262:ILE:HG21	1:A:290:LEU:HD22	1.99	0.45
1:B:199:THR:OG1	1:B:202:THR:HG23	2.17	0.45
1:A:527:VAL:O	1:A:528:THR:C	2.59	0.45
1:A:305:ALA:O	1:A:306:VAL:HG13	2.18	0.44
1:A:463:GLU:OE1	1:A:508:TRP:HZ2	2.01	0.43
1:B:273:PHE:HB2	1:B:275:HIS:NE2	2.33	0.43
1:A:305:ALA:HB1	1:A:308:ILE:CD1	2.45	0.43
1:A:121:TYR:CZ	1:A:185:HIS:HB3	2.53	0.43
1:B:277:PHE:HB3	1:B:308:ILE:CD1	2.47	0.43
1:A:388:GLY:O	1:A:422:LEU:HD23	2.18	0.43
1:A:456:VAL:HA	1:A:459:ARG:HD2	2.01	0.43
1:B:273:PHE:HB3	1:B:275:HIS:HD2	1.81	0.43
1:A:316:TYR:HD1	1:A:330:PRO:HA	1.82	0.43
1:A:199:THR:OG1	1:A:202:THR:HG23	2.19	0.43
1:B:126:ARG:NH1	2:B:605:HOH:O	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:220:ARG:HD2	1:B:268:THR:HG21	2.01	0.42
1:B:454:GLU:O	1:B:458:LEU:HD12	2.20	0.41
1:A:213:ASP:OD2	1:A:368:ARG:NE	2.51	0.41
1:A:137:HIS:CD2	1:A:155:LEU:HG	2.55	0.41
1:B:121:TYR:CZ	1:B:185:HIS:HB3	2.55	0.41
1:B:298:ALA:O	1:B:337:MET:HG3	2.21	0.41
1:A:335:ILE:HG23	1:A:350:PHE:O	2.21	0.41
1:B:273:PHE:CB	1:B:275:HIS:CD2	3.03	0.41
1:B:293:VAL:HG11	1:B:296:TYR:CZ	2.56	0.41
1:B:343:MET:HE2	1:B:347:LEU:HD12	2.03	0.41
1:B:345:TYR:CG	1:B:346:VAL:N	2.89	0.41
1:A:113:MET:HE3	1:A:118:ARG:HG3	2.03	0.41
1:B:457:LEU:HD23	1:B:512:ALA:HB3	2.03	0.41
1:B:273:PHE:CE1	1:B:299:SER:HB3	2.56	0.40
1:B:117:THR:HG23	1:B:192:ILE:HD13	2.02	0.40
1:B:41:ASP:OD2	1:B:251:THR:HG22	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	508/565 (90%)	491 (97%)	17 (3%)	0	100	100
1	B	509/565 (90%)	493 (97%)	16 (3%)	0	100	100
All	All	1017/1130 (90%)	984 (97%)	33 (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	412/447 (92%)	407 (99%)	5 (1%)	63	74
1	B	412/447 (92%)	409 (99%)	3 (1%)	76	84
All	All	824/894 (92%)	816 (99%)	8 (1%)	68	77

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	203	LEU
1	A	204	PHE
1	A	251	THR
1	A	304	HIS
1	A	306	VAL
1	B	157	SER
1	B	204	PHE
1	B	496	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	HIS
1	A	61	HIS
1	A	307	HIS
1	B	24	HIS
1	B	95	ASN
1	B	156	GLN
1	B	275	HIS

5.3.3 RNA ⓘ

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

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	516/565 (91%)	0.41	33 (6%) 25 23	29, 52, 97, 133	0
1	B	517/565 (91%)	0.36	37 (7%) 21 19	30, 51, 93, 146	0
All	All	1033/1130 (91%)	0.39	70 (6%) 23 21	29, 52, 96, 146	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	345	TYR	9.4
1	A	345	TYR	8.7
1	B	189	THR	7.7
1	A	351	VAL	6.1
1	B	350	PHE	4.8
1	A	304	HIS	4.6
1	B	343	MET	4.5
1	A	306	VAL	4.3
1	B	344	GLY	4.2
1	A	358	VAL	4.1
1	B	285	LEU	4.1
1	A	299	SER	4.1
1	A	459	ARG	4.1
1	B	306	VAL	4.0
1	B	187	SER	4.0
1	B	351	VAL	3.9
1	A	311	LEU	3.8
1	A	190	THR	3.8
1	A	344	GLY	3.7
1	B	235	SER	3.7
1	A	316	TYR	3.7
1	A	343	MET	3.6
1	B	307	HIS	3.5
1	A	275	HIS	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	273	PHE	3.2
1	A	363	ILE	3.2
1	A	429	ASN	3.1
1	A	528	THR	3.1
1	B	304	HIS	3.1
1	B	300	GLY	3.1
1	B	299	SER	3.0
1	B	231	VAL	2.9
1	B	358	VAL	2.9
1	A	501	ALA	2.9
1	A	350	PHE	2.8
1	B	275	HIS	2.8
1	B	333	ILE	2.8
1	B	496	VAL	2.7
1	A	305	ALA	2.7
1	B	497	GLU	2.7
1	A	337	MET	2.6
1	B	445	GLU	2.6
1	B	309	ARG	2.6
1	B	457	LEU	2.6
1	A	287	ASP	2.6
1	A	346	VAL	2.6
1	A	187	SER	2.5
1	B	311	LEU	2.5
1	B	499	ALA	2.5
1	B	190	THR	2.5
1	B	446	GLY	2.4
1	B	365	ARG	2.4
1	A	499	ALA	2.4
1	B	277	PHE	2.3
1	A	285	LEU	2.3
1	B	469	VAL	2.3
1	A	349	ASP	2.2
1	B	341	THR	2.2
1	B	251	THR	2.2
1	A	314	LYS	2.2
1	B	501	ALA	2.1
1	B	503	GLN	2.1
1	A	477	VAL	2.1
1	B	495	LEU	2.1
1	A	495	LEU	2.0
1	B	488	THR	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	365	ARG	2.0
1	A	282	ALA	2.0
1	A	516	ALA	2.0
1	A	333	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 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.