



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 12:41 am GMT

PDB ID : 5HOG
Title : Crystal structure of the carboxy-terminal domain of yeast Ctf4 bound to Dna2.
Authors : Simon, A.C.; Pellegrini, L.
Deposited on : 2016-01-19
Resolution : 3.09 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

<http://wwpdb.org/validation/2016/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
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

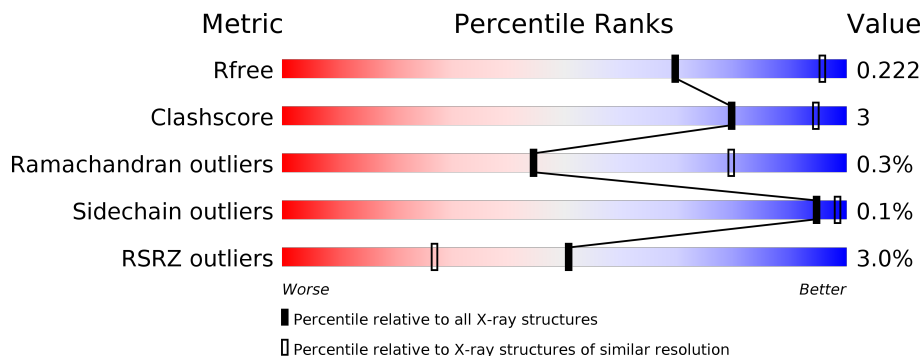
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.09 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}	100719	1001 (3.12-3.08)
Clashscore	112137	1099 (3.12-3.08)
Ramachandran outliers	110173	1057 (3.12-3.08)
Sidechain outliers	110143	1057 (3.12-3.08)
RSRZ outliers	101464	1006 (3.12-3.08)

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. 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	478	<div> <div>79%</div> <div>9%</div> <div>11%</div> </div>
1	B	478	<div> <div>%</div> <div>83%</div> <div>8%</div> <div>10%</div> </div>
1	C	478	<div> <div>4%</div> <div>55%</div> <div>6%</div> <div>38%</div> </div>
2	D	17	<div> <div>35%</div> <div>71%</div> <div>6%</div> <div>24%</div> </div>
2	E	17	<div> <div>41%</div> <div>76%</div> <div>6%</div> <div>18%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9598 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 DNA polymerase alpha-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	425	Total	C	N	O	S	0	1	0
			3425	2199	568	643	15			
1	B	432	Total	C	N	O	S	0	1	0
			3481	2233	578	654	16			
1	C	296	Total	C	N	O	S	0	1	0
			2405	1562	392	440	11			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	450	MET	HIS	conflict	UNP Q01454
A	451	GLY	ASN	conflict	UNP Q01454
A	452	SER	GLU	conflict	UNP Q01454
A	453	SER	HIS	conflict	UNP Q01454
A	454	HIS	SER	conflict	UNP Q01454
A	455	HIS	TYR	conflict	UNP Q01454
A	456	HIS	SER	conflict	UNP Q01454
A	457	HIS	ARG	conflict	UNP Q01454
A	458	HIS	VAL	conflict	UNP Q01454
A	460	SER	LYS	conflict	UNP Q01454
A	461	GLN	THR	conflict	UNP Q01454
A	462	ASP	HIS	conflict	UNP Q01454
A	463	PRO	SER	conflict	UNP Q01454
A	464	GLU	PHE	conflict	UNP Q01454
A	465	ASN	PRO	conflict	UNP Q01454
A	466	LEU	ILE	conflict	UNP Q01454
A	467	TYR	SER	conflict	UNP Q01454
A	468	PHE	LEU	conflict	UNP Q01454
A	469	GLN	ALA	conflict	UNP Q01454
A	470	GLY	ASN	conflict	UNP Q01454
B	450	MET	HIS	conflict	UNP Q01454
B	451	GLY	ASN	conflict	UNP Q01454
B	452	SER	GLU	conflict	UNP Q01454

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	453	SER	HIS	conflict	UNP Q01454
B	454	HIS	SER	conflict	UNP Q01454
B	455	HIS	TYR	conflict	UNP Q01454
B	456	HIS	SER	conflict	UNP Q01454
B	457	HIS	ARG	conflict	UNP Q01454
B	458	HIS	VAL	conflict	UNP Q01454
B	460	SER	LYS	conflict	UNP Q01454
B	461	GLN	THR	conflict	UNP Q01454
B	462	ASP	HIS	conflict	UNP Q01454
B	463	PRO	SER	conflict	UNP Q01454
B	464	GLU	PHE	conflict	UNP Q01454
B	465	ASN	PRO	conflict	UNP Q01454
B	466	LEU	ILE	conflict	UNP Q01454
B	467	TYR	SER	conflict	UNP Q01454
B	468	PHE	LEU	conflict	UNP Q01454
B	469	GLN	ALA	conflict	UNP Q01454
B	470	GLY	ASN	conflict	UNP Q01454
C	450	MET	HIS	conflict	UNP Q01454
C	451	GLY	ASN	conflict	UNP Q01454
C	452	SER	GLU	conflict	UNP Q01454
C	453	SER	HIS	conflict	UNP Q01454
C	454	HIS	SER	conflict	UNP Q01454
C	455	HIS	TYR	conflict	UNP Q01454
C	456	HIS	SER	conflict	UNP Q01454
C	457	HIS	ARG	conflict	UNP Q01454
C	458	HIS	VAL	conflict	UNP Q01454
C	460	SER	LYS	conflict	UNP Q01454
C	461	GLN	THR	conflict	UNP Q01454
C	462	ASP	HIS	conflict	UNP Q01454
C	463	PRO	SER	conflict	UNP Q01454
C	464	GLU	PHE	conflict	UNP Q01454
C	465	ASN	PRO	conflict	UNP Q01454
C	466	LEU	ILE	conflict	UNP Q01454
C	467	TYR	SER	conflict	UNP Q01454
C	468	PHE	LEU	conflict	UNP Q01454
C	469	GLN	ALA	conflict	UNP Q01454
C	470	GLY	ASN	conflict	UNP Q01454

- Molecule 2 is a protein called Dna2p.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	13	Total	C	N	O	0	0	0
			106	64	17	25			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	14	Total	C	N	O	0	0	0
			110	66	18	26			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	29	Total	O	0	0
			29	29		
3	B	29	Total	O	0	0
			29	29		
3	C	13	Total	O	0	0
			13	13		

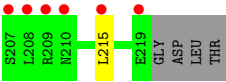
- Molecule 1: DNA polymerase alpha-binding protein



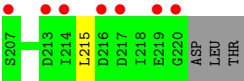
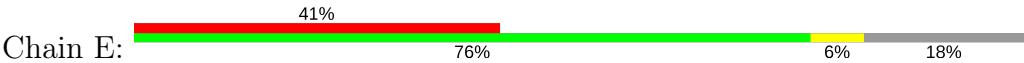
GLU
VAL
LEU
ALA
ALA
LEU
ASN
GLY
ALA
TYR
ASP
LYS
LYS
LEU
LEU
ARG
LEU
PHE
ALA
SER
ALA
CYS
SER
ASP
GLN
ASN
VAL
GLU
LYS
ALA
LEU
SER
LEU
ALA
HIS
GLU
LEU
LYS
GLN
ASP
ARG
ALA
LEU
THR
ALA
ALA
VAL
LYS
ILE
SER
GLU
ARG
ALA
GLU
LEU
PRO
SER
LEU
VAL
LYS

LYS
ILE
ASN
ASN
ILE
ARG
GLU
ALA
ARG
TYR
GLU
GLN
GLN
LEU
LYS

● Molecule 2: Dna2p



● Molecule 2: Dna2p



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α , β , γ	88.68Å 99.55Å 218.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.98 – 3.09 48.98 – 3.09	Depositor EDS
% Data completeness (in resolution range)	99.7 (48.98-3.09) 99.7 (48.98-3.09)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.14 (at 3.07Å)	Xtriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, R_{free}	0.180 , 0.226 0.175 , 0.222	Depositor DCC
R_{free} test set	1817 reflections (5.04%)	DCC
Wilson B-factor (Å ²)	70.7	Xtriage
Anisotropy	0.292	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 47.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9598	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.96% 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	0.25	0/3510	0.42	0/4752
1	B	0.25	0/3567	0.41	0/4828
1	C	0.27	0/2481	0.44	0/3370
2	D	0.20	0/105	0.35	0/141
2	E	0.20	0/109	0.33	0/146
All	All	0.25	0/9772	0.42	0/13237

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	3425	0	3369	27	0
1	B	3481	0	3431	22	0
1	C	2405	0	2326	17	0
2	D	106	0	100	1	0
2	E	110	0	103	1	0
3	A	29	0	0	0	0
3	B	29	0	0	0	0
3	C	13	0	0	0	0
All	All	9598	0	9329	60	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 3.

All (60) 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:789:GLU:HG3	1:B:818:PRO:HG3	1.72	0.72
1:A:789:GLU:HG3	1:A:818:PRO:HG3	1.73	0.71
1:B:899:VAL:HG13	1:B:911:VAL:HG13	1.77	0.65
1:A:790:ASN:HD21	1:A:815:ILE:HG23	1.67	0.60
1:B:511:TYR:HB2	1:B:530:ASP:HB3	1.85	0.58
1:B:818:PRO:HG2	1:B:821:MET:HB3	1.85	0.57
1:A:899:VAL:HG13	1:A:911:VAL:HG13	1.88	0.55
1:A:511:TYR:HB2	1:A:530:ASP:HB3	1.90	0.54
1:C:617:ALA:HB3	1:C:628:VAL:HB	1.90	0.54
1:C:510:GLN:HG2	1:C:531:LEU:HD23	1.90	0.53
1:A:724:SER:HB2	1:A:742:VAL:HG21	1.91	0.52
1:A:846:GLU:OE2	1:A:852:ASN:ND2	2.43	0.51
1:C:722:LEU:HD21	1:C:774:MET:HE2	1.93	0.51
1:A:634:HIS:CE1	1:B:634:HIS:HA	2.46	0.51
1:B:668:MET:HA	1:B:671:ASP:HB2	1.93	0.50
1:A:739:ASP:OD1	1:A:739:ASP:N	2.45	0.50
1:C:745:LEU:HG	1:C:754:CYS:HA	1.95	0.48
1:A:824:GLU:HA	1:A:869:LEU:HD11	1.95	0.48
1:A:490:ASP:HB3	1:A:506:LYS:HB2	1.94	0.48
1:A:569:ILE:HB	1:B:782:VAL:HG21	1.96	0.48
1:C:597:PHE:HB3	1:C:610:GLU:HB3	1.95	0.48
1:A:685:LYS:NZ	1:A:702:ASN:OD1	2.35	0.47
1:C:558:PRO:HG2	1:C:563:HIS:HB2	1.96	0.47
1:B:790:ASN:HD21	1:B:815:ILE:HG23	1.78	0.47
1:B:739:ASP:OD1	1:B:739:ASP:N	2.47	0.47
1:C:724:SER:HB2	1:C:742:VAL:HG21	1.96	0.47
1:A:508:SER:OG	1:A:509:GLU:N	2.46	0.46
1:C:755:ILE:HG23	1:C:769:PRO:HG2	1.98	0.46
1:C:728:ILE:HD11	1:C:742:VAL:HG23	1.97	0.46
1:A:601:ASN:HB3	1:A:607:PHE:HE2	1.81	0.46
1:B:833:LEU:HB3	1:B:858:LEU:HD21	1.98	0.45
1:A:833:LEU:HB3	1:A:858:LEU:HD21	1.98	0.45
1:C:511:TYR:HB2	1:C:530:ASP:HB3	1.99	0.45
1:B:864:LYS:HE3	2:E:215:LEU:HB3	1.98	0.44
1:A:818:PRO:HG2	1:A:821:MET:HB3	2.00	0.44
1:A:563:HIS:ND1	1:B:880:GLU:OE1	2.34	0.44
1:C:496:MET:HG2	1:C:745:LEU:HD22	1.98	0.44
1:A:552:GLY:O	1:A:570:ILE:N	2.36	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:880:GLU:HB3	1:C:603:PHE:CE1	2.53	0.44
1:A:714:GLU:OE1	1:C:649:ARG:NE	2.45	0.44
1:A:791:LYS:HB2	1:A:791:LYS:HE3	1.81	0.44
1:B:648:LYS:HE2	1:B:650:TYR:CZ	2.53	0.44
1:B:496:MET:HG3	1:B:501:TYR:HB3	2.01	0.43
1:A:866:LEU:HD21	1:A:888:GLU:HB2	2.01	0.43
1:A:698:PHE:CG	1:A:744:PRO:HG3	2.54	0.42
1:A:484:THR:O	1:A:492:ARG:HD2	2.19	0.42
1:B:663:ASN:N	1:B:663:ASN:OD1	2.52	0.42
1:C:698:PHE:CG	1:C:744:PRO:HG3	2.54	0.42
1:B:724:SER:HB2	1:B:742:VAL:HG21	2.02	0.42
1:B:866:LEU:HD21	1:B:888:GLU:HB2	2.02	0.42
1:C:751:THR:HB	1:C:773:GLU:HB3	2.01	0.41
1:B:548:GLN:HG3	1:B:551:THR:H	1.84	0.41
1:A:648:LYS:HB3	1:B:717:LYS:HD3	2.02	0.41
1:C:739:ASP:O	1:C:758:LYS:HA	2.20	0.41
1:C:750:ASP:O	1:C:776:ILE:HG12	2.21	0.41
1:B:866:LEU:HD23	1:B:889:LEU:HD23	2.03	0.41
1:B:704:LEU:HB3	1:B:722:LEU:HB3	2.02	0.41
1:B:702:ASN:HB3	1:B:724:SER:HG	1.86	0.41
1:A:864:LYS:HE3	2:D:215:LEU:HB3	2.03	0.40
1:A:652:LYS:NZ	1:A:655:CYS:SG	2.74	0.40

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	420/478 (88%)	401 (96%)	18 (4%)	1 (0%)	51	84
1	B	429/478 (90%)	413 (96%)	15 (4%)	1 (0%)	51	84
1	C	293/478 (61%)	275 (94%)	17 (6%)	1 (0%)	44	79

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	11/17 (65%)	11 (100%)	0	0	100	100
2	E	12/17 (71%)	11 (92%)	1 (8%)	0	100	100
All	All	1165/1468 (79%)	1111 (95%)	51 (4%)	3 (0%)	44	79

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	749	TYR
1	C	749	TYR
1	A	749	TYR

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	378/422 (90%)	378 (100%)	0	100	100
1	B	385/422 (91%)	384 (100%)	1 (0%)	94	97
1	C	267/422 (63%)	267 (100%)	0	100	100
2	D	13/16 (81%)	13 (100%)	0	100	100
2	E	13/16 (81%)	13 (100%)	0	100	100
All	All	1056/1298 (81%)	1055 (100%)	1 (0%)	94	98

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	852	ASN

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

Mol	Chain	Res	Type
1	A	634	HIS

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 carbohydrates 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	425/478 (88%)	-0.16	1 (0%) 94 89	38, 60, 103, 128	0
1	B	432/478 (90%)	-0.13	4 (0%) 84 69	40, 61, 108, 140	0
1	C	296/478 (61%)	-0.00	17 (5%) 24 11	46, 69, 126, 162	0
2	D	13/17 (76%)	2.22	6 (46%) 0 0	120, 130, 144, 145	0
2	E	14/17 (82%)	2.06	7 (50%) 0 0	121, 135, 145, 148	0
All	All	1180/1468 (80%)	-0.05	35 (2%) 51 27	38, 63, 120, 162	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	207	SER	4.8
1	C	733	GLY	4.4
2	D	208	LEU	4.1
2	E	207	SER	3.8
1	B	666	SER	3.6
2	D	210	ASN	3.5
2	D	209	ARG	3.4
1	C	732	SER	3.3
1	B	927	LYS	3.3
1	C	673	ASN	3.1
1	C	736	GLU	2.9
1	B	665	ASN	2.8
2	E	220	GLY	2.8
2	D	215	LEU	2.7
1	C	729	TRP	2.7
1	C	731	MET	2.6
1	A	510	GLN	2.6
1	B	926	LEU	2.5
1	C	735	LYS	2.5
1	C	724	SER	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	E	217	ASP	2.4
2	E	219	GLU	2.3
1	C	726	MET	2.3
1	C	737	THR	2.3
1	C	672	ALA	2.3
2	D	219	GLU	2.3
1	C	740	ILE	2.3
1	C	734	GLY	2.2
2	E	213	ASP	2.2
1	C	739	ASP	2.1
2	E	216	ASP	2.1
1	C	730	LYS	2.1
2	E	214	ILE	2.1
1	C	738	THR	2.1
1	C	725	ASN	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 carbohydrates 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.