



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:58 PM GMT

PDB ID : 4K51  
Title : Crystal Structure of the PCI domain of eIF3a  
Authors : Khoshnevis, S.; Neumann, P.; Ficner, R.  
Deposited on : 2013-04-12  
Resolution : 2.65 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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

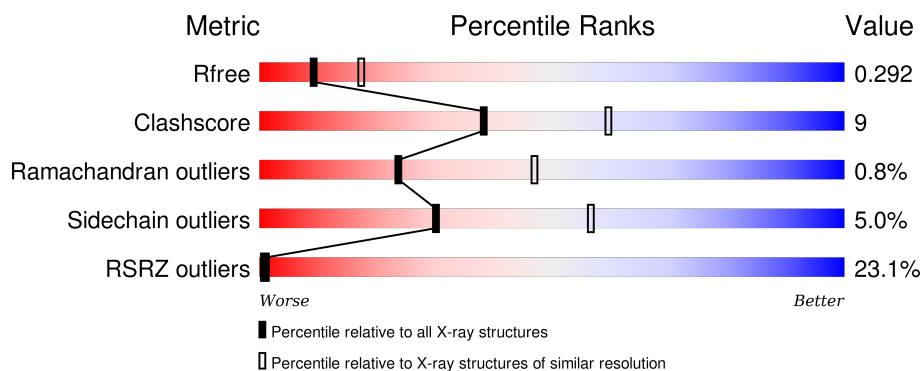
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.65 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))
$R_{free}$	91344	3152 (2.70-2.62)
Clashscore	102246	3524 (2.70-2.62)
Ramachandran outliers	100387	3469 (2.70-2.62)
Sidechain outliers	100360	3469 (2.70-2.62)
RSRZ outliers	91569	3161 (2.70-2.62)

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  $\geq 3$ , 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	224	<div> <div>72%</div> <div>20%</div> <div>5%</div> </div>
1	B	224	<div> <div>38%</div> <div>48%</div> <div>21%</div> <div>29%</div> </div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3032 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 Eukaryotic translation initiation factor 3 subunit A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	213	Total	C	N	O	S	0	0	0
			1739	1127	273	336	3			
1	B	159	Total	C	N	O	S	0	0	0
			1293	844	199	249	1			

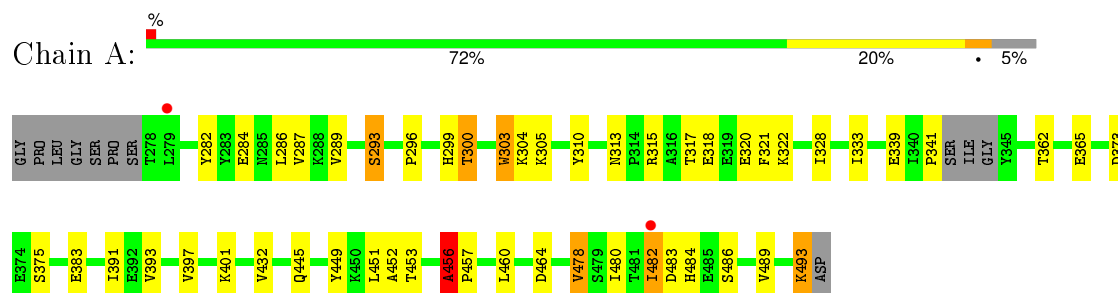
There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	271	GLY	-	EXPRESSION TAG	UNP P38249
A	272	PRO	-	EXPRESSION TAG	UNP P38249
A	273	LEU	-	EXPRESSION TAG	UNP P38249
A	274	GLY	-	EXPRESSION TAG	UNP P38249
A	275	SER	-	EXPRESSION TAG	UNP P38249
B	271	GLY	-	EXPRESSION TAG	UNP P38249
B	272	PRO	-	EXPRESSION TAG	UNP P38249
B	273	LEU	-	EXPRESSION TAG	UNP P38249
B	274	GLY	-	EXPRESSION TAG	UNP P38249
B	275	SER	-	EXPRESSION TAG	UNP P38249

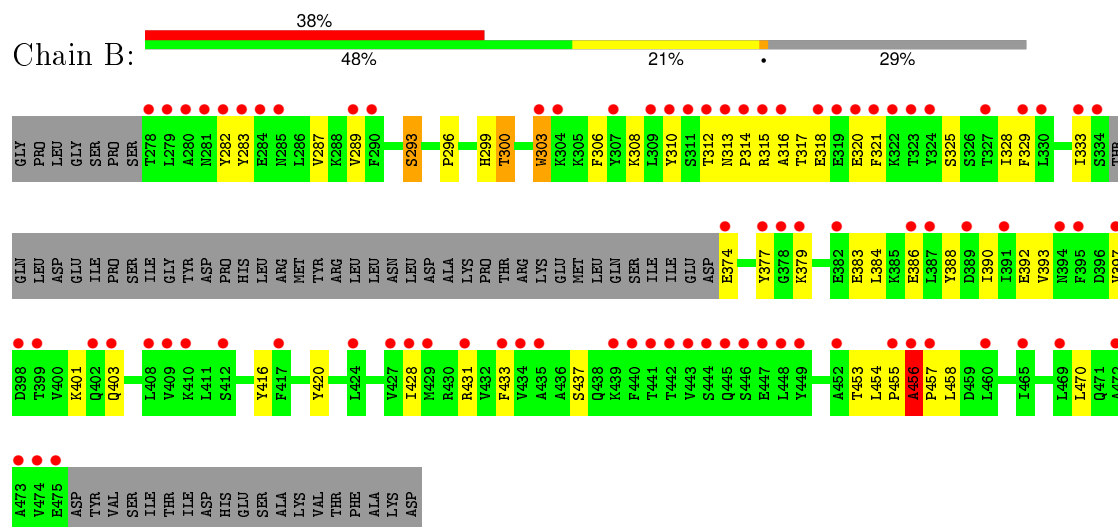
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: Eukaryotic translation initiation factor 3 subunit A



- Molecule 1: Eukaryotic translation initiation factor 3 subunit A



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 21 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	137.14Å 137.14Å 137.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.49 – 2.65 48.49 – 2.65	Depositor EDS
% Data completeness (in resolution range)	99.5 (48.49-2.65) 99.5 (48.49-2.65)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.79 (at 2.65Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, $R_{free}$	0.249 , 0.286 0.252 , 0.292	Depositor DCC
$R_{free}$ test set	630 reflections (5.01%)	DCC
Wilson B-factor (Å <sup>2</sup> )	64.6	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 76.3	EDS
Estimated twinning fraction	0.053 for -l,-k,-h	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 12584 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	3032	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	118.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.11% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.35	0/1775	0.57	1/2408 (0.0%)
1	B	0.32	0/1320	0.63	1/1791 (0.1%)
All	All	0.33	0/3095	0.60	2/4199 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	456	ALA	C-N-CD	7.05	143.21	128.40
1	A	456	ALA	C-N-CD	6.82	142.73	128.40

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	1739	0	1746	28	0
1	B	1293	0	1299	27	0
All	All	3032	0	3045	55	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 9.

All (55) 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:318:GLU:OE1	1:B:379:LYS:NZ	2.27	0.65
1:B:299:HIS:NE2	1:B:420:TYR:OH	2.34	0.61
1:B:401:LYS:HG2	1:B:455:PRO:HD3	1.83	0.60
1:B:289:VAL:O	1:B:293:SER:OG	2.19	0.59
1:A:482:ILE:HG23	1:A:483:ASP:H	1.66	0.59
1:B:433:PHE:O	1:B:437:SER:N	2.33	0.59
1:B:283:TYR:HB3	1:B:306:PHE:HB2	1.89	0.55
1:B:303:TRP:HB3	1:B:328:ILE:HG12	1.91	0.52
1:B:314:PRO:C	1:B:316:ALA:H	2.12	0.51
1:A:303:TRP:HB3	1:A:328:ILE:HG12	1.92	0.51
1:A:478:VAL:HG13	1:A:480:ILE:HG23	1.92	0.51
1:B:296:PRO:O	1:B:300:THR:HG22	2.12	0.49
1:B:390:ILE:HD13	1:B:403:GLN:HB3	1.93	0.49
1:B:310:TYR:OH	1:B:320:GLU:HG3	2.12	0.49
1:A:289:VAL:O	1:A:293:SER:OG	2.29	0.48
1:B:386:GLU:O	1:B:390:ILE:HG13	2.13	0.48
1:A:383:GLU:N	1:A:383:GLU:OE1	2.37	0.48
1:B:283:TYR:O	1:B:287:VAL:HG13	2.14	0.47
1:B:384:LEU:HD11	1:B:416:TYR:CE1	2.49	0.47
1:A:362:THR:HG22	1:A:365:GLU:H	1.80	0.47
1:A:456:ALA:CB	1:A:457:PRO:HD3	2.45	0.47
1:B:383:GLU:OE1	1:B:383:GLU:N	2.43	0.46
1:B:401:LYS:HE3	1:B:453:THR:O	2.15	0.46
1:A:373:ASP:OD1	1:A:375:SER:OG	2.22	0.46
1:A:432:VAL:HG11	1:A:452:ALA:HA	1.98	0.46
1:A:305:LYS:HA	1:A:305:LYS:HD3	1.77	0.46
1:B:313:ASN:OD1	1:B:315:ARG:HG2	2.15	0.46
1:A:449:TYR:O	1:A:453:THR:OG1	2.29	0.46
1:A:456:ALA:HB1	1:A:457:PRO:HD3	1.98	0.45
1:A:296:PRO:O	1:A:300:THR:HG22	2.15	0.45
1:B:388:TYR:O	1:B:392:GLU:HB2	2.17	0.45
1:B:454:LEU:HB2	1:B:458:LEU:HB2	1.99	0.45
1:A:445:GLN:HG2	1:A:489:VAL:HG23	1.98	0.45
1:A:318:GLU:O	1:A:321:PHE:HB2	2.17	0.45
1:B:310:TYR:CZ	1:B:316:ALA:HA	2.53	0.44
1:A:296:PRO:O	1:A:299:HIS:HB3	2.18	0.44
1:A:284:GLU:O	1:A:287:VAL:HG22	2.18	0.44
1:A:310:TYR:OH	1:A:320:GLU:HG3	2.17	0.44
1:A:333:ILE:CG2	1:A:391:ILE:HD11	2.48	0.43
1:A:401:LYS:NZ	1:A:451:LEU:O	2.48	0.43
1:B:374:GLU:HA	1:B:377:TYR:HB3	2.01	0.42
1:A:322:LYS:HB3	1:A:322:LYS:HE2	1.93	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:482:ILE:O	1:A:484:HIS:N	2.45	0.42
1:A:460:LEU:HD13	1:A:464:ASP:HB3	2.01	0.42
1:B:329:PHE:CE2	1:B:333:ILE:HD11	2.55	0.42
1:A:300:THR:O	1:A:304:LYS:HG3	2.20	0.41
1:B:456:ALA:CB	1:B:457:PRO:HD3	2.50	0.41
1:B:470:LEU:HA	1:B:470:LEU:HD23	1.92	0.41
1:A:313:ASN:OD1	1:A:315:ARG:HG2	2.21	0.41
1:A:286:LEU:HA	1:A:286:LEU:HD23	1.92	0.41
1:B:321:PHE:O	1:B:325:SER:OG	2.27	0.41
1:A:339:GLU:O	1:A:341:PRO:HD3	2.22	0.40
1:A:493:LYS:HG2	1:A:493:LYS:H	1.48	0.40
1:B:308:LYS:O	1:B:312:THR:HG23	2.21	0.40
1:B:428:ILE:O	1:B:431:ARG:HB2	2.22	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	209/224 (93%)	193 (92%)	14 (7%)	2 (1%)	19	41
1	B	155/224 (69%)	149 (96%)	5 (3%)	1 (1%)	30	54
All	All	364/448 (81%)	342 (94%)	19 (5%)	3 (1%)	24	47

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	456	ALA
1	B	456	ALA
1	A	482	ILE



### 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	196/204 (96%)	186 (95%)	10 (5%)	29	55
1	B	145/204 (71%)	138 (95%)	7 (5%)	31	59
All	All	341/408 (84%)	324 (95%)	17 (5%)	30	56

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	282	TYR
1	A	293	SER
1	A	300	THR
1	A	303	TRP
1	A	317	THR
1	A	393	VAL
1	A	397	VAL
1	A	478	VAL
1	A	486	SER
1	A	493	LYS
1	B	282	TYR
1	B	293	SER
1	B	300	THR
1	B	303	TRP
1	B	317	THR
1	B	393	VAL
1	B	397	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	213/224 (95%)	0.35	2 (0%) 85 86	47, 78, 125, 167	0
1	B	159/224 (70%)	2.90	84 (52%) 0 0	104, 165, 241, 272	158 (99%)
All	All	372/448 (83%)	1.44	86 (23%) 1 1	47, 102, 218, 272	158 (42%)

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	444	SER	11.7
1	B	382	GLU	10.9
1	B	311	SER	10.8
1	B	448	LEU	10.1
1	B	440	PHE	10.1
1	B	319	GLU	9.9
1	B	314	PRO	9.3
1	B	397	VAL	8.5
1	B	312	THR	7.7
1	B	443	VAL	7.3
1	B	280	ALA	7.0
1	B	409	VAL	7.0
1	B	472	ALA	6.8
1	B	399	THR	6.7
1	B	408	LEU	6.7
1	B	322	LYS	6.5
1	B	441	THR	6.4
1	B	310	TYR	6.1
1	B	469	LEU	6.0
1	B	475	GLU	5.8
1	B	281	ASN	5.2
1	B	379	LYS	5.2
1	B	445	GLN	5.2
1	B	473	ALA	5.1

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Mol	Chain	Res	Type	RSRZ
1	B	313	ASN	5.0
1	A	482	ILE	4.6
1	B	465	ILE	4.6
1	B	378	GLY	4.6
1	B	474	VAL	4.6
1	B	387	LEU	4.5
1	B	377	TYR	4.4
1	B	329	PHE	4.4
1	B	439	LYS	4.4
1	B	323	THR	4.3
1	B	316	ALA	4.3
1	B	318	GLU	4.2
1	B	321	PHE	4.1
1	B	424	LEU	4.1
1	B	435	ALA	4.0
1	B	386	GLU	4.0
1	B	434	VAL	3.9
1	B	320	GLU	3.9
1	B	330	LEU	3.9
1	B	433	PHE	3.8
1	B	442	THR	3.8
1	B	410	LYS	3.7
1	B	446	SER	3.6
1	B	333	ILE	3.6
1	B	304	LYS	3.6
1	B	334	SER	3.5
1	B	284	GLU	3.5
1	B	279	LEU	3.4
1	B	412	SER	3.3
1	B	449	TYR	3.3
1	B	398	ASP	3.2
1	B	403	GLN	3.2
1	B	457	PRO	3.2
1	B	389	ASP	3.2
1	B	324	TYR	3.2
1	B	456	ALA	3.1
1	B	282	TYR	3.1
1	B	455	PRO	3.0
1	B	307	TYR	2.9
1	B	428	ILE	2.9
1	B	402	GLN	2.8
1	B	290	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	447	GLU	2.7
1	B	431	ARG	2.7
1	B	327	THR	2.7
1	B	427	VAL	2.7
1	B	460	LEU	2.6
1	B	391	ILE	2.6
1	B	278	THR	2.5
1	B	452	ALA	2.5
1	B	395	PHE	2.5
1	B	417	PHE	2.5
1	A	279	LEU	2.5
1	B	374	GLU	2.4
1	B	303	TRP	2.4
1	B	283	TYR	2.4
1	B	309	LEU	2.3
1	B	394	ASN	2.3
1	B	429	MET	2.3
1	B	315	ARG	2.3
1	B	289	VAL	2.3
1	B	285	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.