



# Full wwPDB X-ray Structure Validation Report i

Feb 26, 2014 – 06:43 PM GMT

PDB ID : 4BSM  
Title : Crystal structure of the Nuclear Export Receptor CRM1 (exportin-1) lacking the C-terminal helical extension at 4.5Å  
Authors : Dian, C.; Bernaudat, F.; Langer, K.; Oliva, M.F.; Fornerod, M.; Schoehn, G.; Muller, C.W.; Petosa, C.  
Deposited on : 2013-06-10  
Resolution : 4.50 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

---

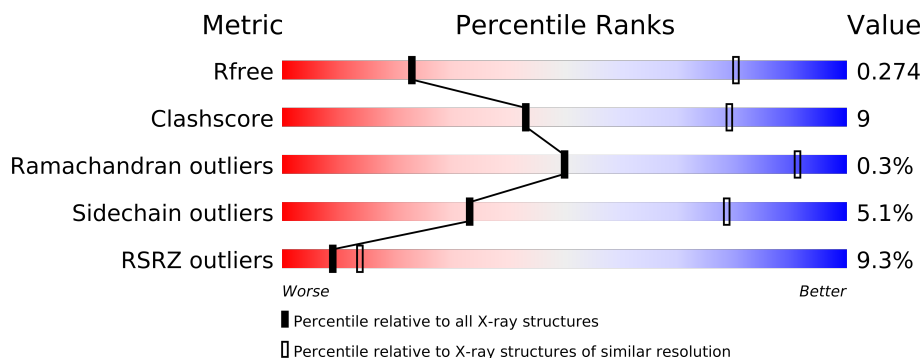
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

# 1 Overall quality at a glance


The reported resolution of this entry is 4.50 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))
$R_{free}$	66092	1029 (5.50-3.50)
Clashscore	79885	1300 (5.50-3.50)
Ramachandran outliers	78287	1222 (5.50-3.50)
Sidechain outliers	78261	1203 (5.50-3.50)
RSRZ outliers	66119	1028 (5.50-3.50)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	1032	

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 6854 atoms, of which 0 are hydrogen and 0 are deuterium.

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 EXPORTIN-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	896	6854	4379	1169	1262	44	0	0	0



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	148.64Å 248.33Å 107.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.59 – 4.50 48.59 – 4.50	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.59-4.50) 99.9 (48.59-4.50)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.47 (at 4.45Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.8_1056)	Depositor
R, $R_{free}$	0.229 , 0.269 0.233 , 0.274	Depositor DCC
$R_{free}$ test set	1212 reflections (10.03%)	DCC
Wilson B-factor (Å <sup>2</sup> )	145.8	Xtriage
Anisotropy	0.606	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 117.7	EDS
Estimated twinning fraction	0.086 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.074 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.36$ , $\langle L^2 \rangle = 0.20$	Xtriage
Outliers	0 of 12100 reflections	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	6854	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	144.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.73% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 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	0.25	0/6978	0.42	0/9473

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6854	0	6542	118	0
All	All	6854	0	6542	118	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 9.

All (118) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:387:SER:HB3	1:A:468:ASP:HA	1.61	0.82
1:A:483:GLN:HG2	1:A:494:LEU:HD13	1.71	0.71
1:A:616:ASN:ND2	1:A:617:ASN:OD1	2.29	0.65
1:A:524:LEU:HD13	1:A:544:ILE:HG12	1.78	0.65
1:A:55:GLU:HG3	1:A:90:ARG:HH22	1.62	0.64

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:809:ASN:OD1	1:A:858:HIS:NE2	2.33	0.62
1:A:600:VAL:HG11	1:A:644:GLN:HB2	1.82	0.61
1:A:56:HIS:N	1:A:57:PRO:HD2	2.16	0.61
1:A:454:TYR:OH	1:A:546:TYR:OH	2.18	0.60
1:A:406:ARG:NH2	1:A:467:LEU:HA	2.15	0.60
1:A:338:GLU:HG2	1:A:408:LEU:HD13	1.84	0.60
1:A:62:ARG:NH1	1:A:75:THR:O	2.33	0.60
1:A:696:VAL:HG12	1:A:758:LEU:HD13	1.83	0.59
1:A:370:LEU:HD11	1:A:457:MET:HG2	1.86	0.58
1:A:485:ASN:OD1	1:A:487:THR:OG1	2.19	0.58
1:A:298:LEU:O	1:A:353:TYR:OH	2.22	0.57
1:A:417:ARG:NH1	1:A:471:ASP:OD2	2.38	0.57
1:A:422:SER:OG	1:A:479:LYS:NZ	2.36	0.57
1:A:388:THR:HG22	1:A:406:ARG:NH1	2.21	0.56
1:A:879:ILE:HG22	1:A:883:LYS:HE3	1.88	0.56
1:A:157:SER:HB2	1:A:208:LEU:HD11	1.87	0.55
1:A:233:LEU:HD23	1:A:270:GLU:HB3	1.89	0.55
1:A:563:LYS:HG3	1:A:610:PHE:HE1	1.72	0.55
1:A:852:LEU:HD11	1:A:874:VAL:HG13	1.89	0.54
1:A:453:LEU:O	1:A:457:MET:HG3	2.08	0.54
1:A:28:LEU:HD13	1:A:71:GLN:HA	1.89	0.54
1:A:458:ARG:HG3	1:A:503:SER:HB2	1.88	0.54
1:A:388:THR:HG23	1:A:467:LEU:O	2.07	0.54
1:A:362:GLU:HB3	1:A:365:ILE:HG22	1.90	0.54
1:A:495:ASN:ND2	1:A:543:ASN:OD1	2.42	0.53
1:A:892:THR:O	1:A:896:ILE:HG13	2.10	0.52
1:A:464:LEU:HA	1:A:467:LEU:HD12	1.91	0.51
1:A:251:ILE:HG21	1:A:289:LEU:HB3	1.93	0.51
1:A:763:VAL:HG11	1:A:807:ILE:HG22	1.93	0.51
1:A:728:ILE:HG23	1:A:745:ILE:HD12	1.93	0.50
1:A:559:TRP:HH2	1:A:610:PHE:HB2	1.77	0.50
1:A:113:THR:HG21	1:A:126:TYR:HE2	1.75	0.50
1:A:116:ASP:OD2	1:A:118:THR:OG1	2.28	0.50
1:A:146:TRP:HB3	1:A:149:PHE:HB2	1.94	0.49
1:A:536:ASN:O	1:A:540:ILE:HG12	2.12	0.49
1:A:199:CYS:SG	1:A:200:ASN:N	2.85	0.49
1:A:360:VAL:HB	1:A:365:ILE:HD13	1.94	0.49
1:A:325:PHE:HD2	1:A:326:LEU:HD22	1.77	0.49
1:A:56:HIS:O	1:A:58:ASP:N	2.46	0.48
1:A:160:SER:OG	1:A:161:GLU:N	2.46	0.48
1:A:495:ASN:HA	1:A:543:ASN:HD21	1.78	0.48
1:A:403:PRO:HG2	1:A:406:ARG:HD2	1.94	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:545:MET:HG3	1:A:583:MET:SD	2.53	0.48
1:A:500:ALA:O	1:A:504:ILE:HG12	2.14	0.47
1:A:379:GLU:OE1	1:A:405:ARG:NH1	2.47	0.47
1:A:559:TRP:CD2	1:A:603:GLN:HG3	2.49	0.47
1:A:57:PRO:O	1:A:60:TRP:NE1	2.48	0.47
1:A:497:LEU:O	1:A:501:ILE:HG12	2.15	0.47
1:A:406:ARG:HH21	1:A:467:LEU:HD23	1.80	0.46
1:A:340:ARG:HD2	1:A:343:LEU:HD23	1.97	0.46
1:A:52:HIS:CE1	1:A:85:ASN:HB3	2.49	0.46
1:A:344:ARG:HG3	1:A:408:LEU:HD21	1.97	0.46
1:A:498:CYS:SG	1:A:543:ASN:HB3	2.55	0.46
1:A:284:VAL:HG21	1:A:340:ARG:HH21	1.80	0.46
1:A:333:HIS:HB3	1:A:336:LEU:HD12	1.97	0.46
1:A:87:ILE:O	1:A:91:TRP:HB2	2.16	0.46
1:A:388:THR:HG22	1:A:406:ARG:HH11	1.81	0.46
1:A:357:VAL:HG12	1:A:365:ILE:HD11	1.98	0.46
1:A:491:TRP:NE1	1:A:536:ASN:OD1	2.49	0.46
1:A:502:GLY:HA3	1:A:546:TYR:CE2	2.51	0.45
1:A:261:ARG:NH1	1:A:314:ASP:OD2	2.49	0.45
1:A:881:ALA:HB3	1:A:893:GLY:HA3	1.98	0.45
1:A:298:LEU:HA	1:A:299:PRO:HD3	1.79	0.45
1:A:206:PHE:CE2	1:A:240:TYR:HB3	2.51	0.45
1:A:739:VAL:HG12	1:A:745:ILE:HG13	1.99	0.45
1:A:879:ILE:HG21	1:A:925:HIS:HB3	1.99	0.45
1:A:491:TRP:CD1	1:A:539:ILE:HG13	2.52	0.45
1:A:353:TYR:O	1:A:357:VAL:HG23	2.17	0.44
1:A:660:LEU:HB2	1:A:661:PRO:HD3	2.00	0.44
1:A:556:ARG:O	1:A:598:HIS:NE2	2.51	0.44
1:A:150:ILE:HD12	1:A:150:ILE:H	1.82	0.44
1:A:119:CYS:SG	1:A:120:VAL:N	2.91	0.44
1:A:388:THR:OG1	1:A:389:SER:N	2.51	0.44
1:A:367:LYS:NZ	1:A:449:ASP:OD1	2.48	0.44
1:A:203:SER:HG	1:A:240:TYR:HE2	1.65	0.44
1:A:247:ILE:HG13	1:A:248:SER:H	1.83	0.44
1:A:40:GLY:O	1:A:44:ARG:HB2	2.17	0.43
1:A:658:MET:SD	1:A:709:GLN:HG2	2.57	0.43
1:A:175:SER:OG	1:A:231:ARG:HG2	2.19	0.43
1:A:317:ASN:O	1:A:321:ASN:ND2	2.51	0.43
1:A:650:GLN:HG3	1:A:651:GLU:N	2.34	0.43
1:A:581:GLN:H	1:A:581:GLN:HG2	1.67	0.43
1:A:251:ILE:HG22	1:A:252:TYR:CD1	2.54	0.43
1:A:693:LYS:O	1:A:697:ARG:HG2	2.19	0.43

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:96:ARG:HG3	1:A:145:HIS:CE1	2.53	0.42
1:A:257:VAL:HA	1:A:258:PRO:HD3	1.87	0.42
1:A:284:VAL:HG21	1:A:340:ARG:NH2	2.34	0.42
1:A:55:GLU:HB3	1:A:57:PRO:HD2	2.01	0.42
1:A:589:ILE:HG12	1:A:636:ALA:HB2	2.01	0.42
1:A:637:VAL:HA	1:A:640:MET:HE2	2.00	0.42
1:A:168:MET:HE3	1:A:225:THR:HA	2.02	0.42
1:A:165:GLN:HB3	1:A:221:LEU:HD13	2.02	0.42
1:A:305:ARG:HD3	1:A:359:GLU:O	2.19	0.42
1:A:251:ILE:HD11	1:A:290:THR:HG23	2.02	0.42
1:A:527:LEU:HD22	1:A:527:LEU:HA	1.90	0.41
1:A:359:GLU:OE1	1:A:423:ARG:NH2	2.47	0.41
1:A:918:TYR:O	1:A:922:ILE:HG13	2.20	0.41
1:A:899:THR:HG22	1:A:903:ASN:ND2	2.35	0.41
1:A:332:GLU:HB3	1:A:333:HIS:CE1	2.56	0.41
1:A:791:ASN:OD1	1:A:792:VAL:N	2.53	0.41
1:A:915:TYR:O	1:A:919:PHE:HB3	2.21	0.41
1:A:44:ARG:HD3	1:A:44:ARG:N	2.36	0.41
1:A:175:SER:HB3	1:A:232:PHE:CE1	2.56	0.41
1:A:110:ILE:HD11	1:A:134:LEU:HB2	2.02	0.41
1:A:403:PRO:HB2	1:A:406:ARG:HB2	2.02	0.41
1:A:343:LEU:O	1:A:346:THR:OG1	2.31	0.41
1:A:650:GLN:O	1:A:654:ILE:HG13	2.21	0.41
1:A:83:LEU:HD23	1:A:133:ILE:HD13	2.02	0.41
1:A:192:LYS:HA	1:A:192:LYS:HD2	1.89	0.40
1:A:265:LEU:HD22	1:A:265:LEU:HA	1.95	0.40
1:A:188:GLN:O	1:A:192:LYS:HG2	2.21	0.40
1:A:432:VAL:HG21	1:A:542:SER:HB2	2.01	0.40
1:A:867:PRO:HA	1:A:868:PRO:HD3	1.90	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	870/1032 (84%)	834 (96%)	33 (4%)	3 (0%)	50 91

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	54	LYS
1	A	57	PRO
1	A	505	SER

### 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	711/940 (76%)	675 (95%)	36 (5%)	33 79

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	GLU
1	A	62	ARG
1	A	96	ARG
1	A	102	ILE
1	A	119	CYS
1	A	173	LEU
1	A	192	LYS
1	A	265	LEU
1	A	279	TYR
1	A	290	THR
1	A	301	ASN
1	A	332	GLU
1	A	353	TYR
1	A	366	PHE
1	A	380	LEU
1	A	386	PHE
1	A	399	HIS
1	A	408	LEU
1	A	434	GLU
1	A	442	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	524	LEU
1	A	527	LEU
1	A	544	ILE
1	A	553	ARG
1	A	574	HIS
1	A	589	ILE
1	A	598	HIS
1	A	602	VAL
1	A	630	VAL
1	A	634	TYR
1	A	639	TYR
1	A	727	ASN
1	A	875	LEU
1	A	904	VAL
1	A	927	PHE
1	A	931	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	145	HIS
1	A	166	ASN
1	A	215	ASN
1	A	321	ASN
1	A	495	ASN
1	A	543	ASN
1	A	616	ASN
1	A	870	GLN
1	A	916	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	896/1032 (86%)	0.52	83 (9%) 9 14	27, 133, 293, 328	0

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	871	PHE	7.6
1	A	867	PRO	7.1
1	A	954	GLU	5.7
1	A	752	LYS	5.5
1	A	888	ASN	5.4
1	A	872	LYS	5.2
1	A	978	VAL	4.9
1	A	875	LEU	4.4
1	A	868	PRO	4.4
1	A	870	GLN	4.4
1	A	1014	HIS	4.2
1	A	887	ARG	4.1
1	A	974	LEU	4.0
1	A	845	ARG	3.9
1	A	1009	PRO	3.8
1	A	833	MET	3.8
1	A	1013	GLU	3.8
1	A	745	ILE	3.8
1	A	832	ASN	3.8
1	A	874	VAL	3.7
1	A	910	ALA	3.7
1	A	844	HIS	3.6
1	A	869	THR	3.6
1	A	955	GLU	3.6
1	A	842	PRO	3.5
1	A	1017	ASP	3.5
1	A	824	ASP	3.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	956	GLY	3.3
1	A	1012	LYS	3.3
1	A	751	VAL	3.2
1	A	56	HIS	3.2
1	A	1016	ARG	3.1
1	A	823	PHE	3.1
1	A	953	VAL	3.0
1	A	957	LYS	3.0
1	A	920	CYS	3.0
1	A	915	TYR	2.9
1	A	916	GLN	2.9
1	A	905	ALA	2.9
1	A	841	TYR	2.9
1	A	750	THR	2.9
1	A	873	LEU	2.8
1	A	840	GLU	2.8
1	A	917	THR	2.8
1	A	731	ALA	2.8
1	A	843	GLU	2.7
1	A	886	MET	2.7
1	A	1015	LEU	2.7
1	A	1010	ALA	2.7
1	A	746	ARG	2.6
1	A	980	ASN	2.6
1	A	91	TRP	2.6
1	A	826	VAL	2.6
1	A	1011	PHE	2.5
1	A	432	VAL	2.5
1	A	755	THR	2.5
1	A	904	VAL	2.5
1	A	914	PHE	2.5
1	A	748	MET	2.5
1	A	909	ALA	2.4
1	A	975	GLN	2.4
1	A	979	ALA	2.4
1	A	977	TYR	2.4
1	A	782	ASP	2.4
1	A	822	ILE	2.4
1	A	951	ASN	2.3
1	A	889	VAL	2.3
1	A	187	THR	2.3
1	A	827	PHE	2.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	728	ILE	2.2
1	A	918	TYR	2.2
1	A	828	GLU	2.2
1	A	575	GLU	2.2
1	A	749	ARG	2.2
1	A	883	LYS	2.1
1	A	657	TYR	2.1
1	A	742	GLN	2.1
1	A	743	PRO	2.1
1	A	911	ALA	2.1
1	A	431	LEU	2.1
1	A	834	ILE	2.1
1	A	829	CYS	2.1
1	A	92	LYS	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

There are no ligands in this entry.

## 6.5 Other polymers ⓘ

There are no such residues in this entry.