



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 12:02 AM GMT

PDB ID : 3RMR
Title : Crystal structure of Hyaloperonospora arabidopsidis ATR1 effector domain
Authors : Chou, S.; Krasileva, K.V.; Holton, J.M.; Staskawicz, B.J.; Alber, T.
Deposited on : 2011-04-21
Resolution : 2.30 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

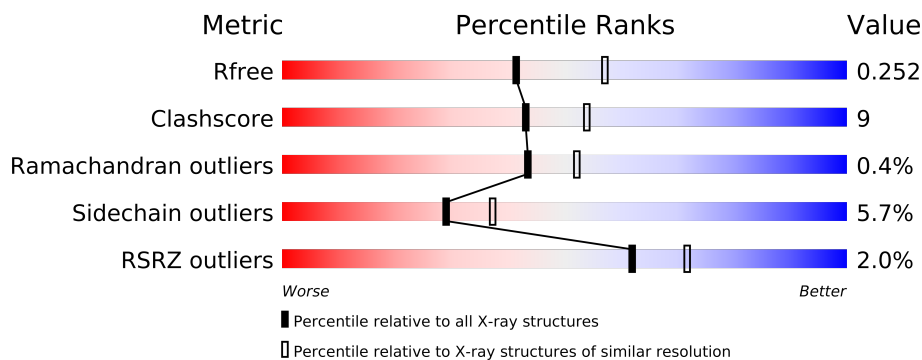
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.30 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	2929 (2.30-2.30)
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)
RSRZ outliers	66119	2930 (2.30-2.30)

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. 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	260	
1	B	260	
1	C	260	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5846 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 Avirulence protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	236	Total	C	N	O	S	Se	0	2	0
			1863	1188	319	351	2	3			
1	B	231	Total	C	N	O	S	Se	0	0	0
			1774	1128	299	342	2	3			
1	C	235	Total	C	N	O	S	Se	0	0	0
			1844	1172	313	354	2	3			

- Molecule 2 is water.

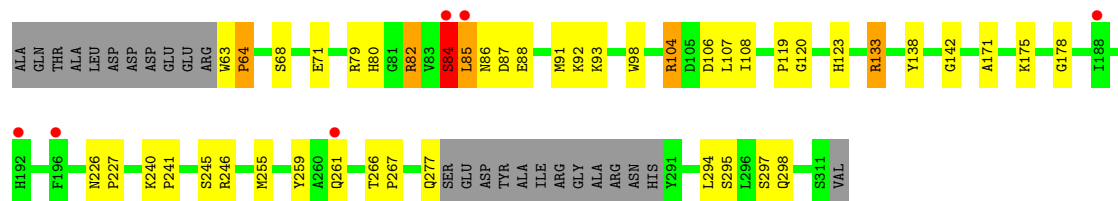
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	113	Total	O	0	0
			113	113		
2	B	114	Total	O	0	0
			114	114		
2	C	138	Total	O	0	0
			138	138		

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.

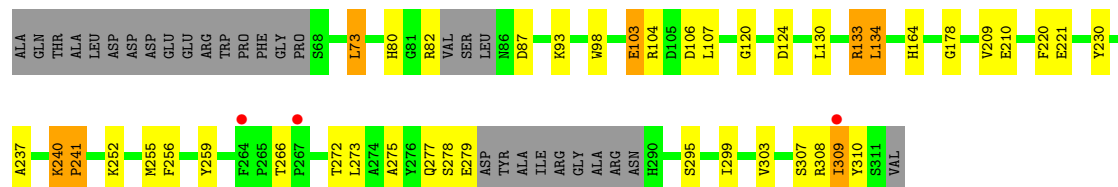
• Molecule 1: Avirulence protein

Chain A: 



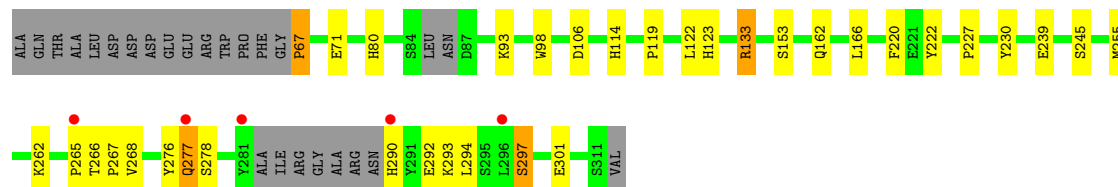
• Molecule 1: Avirulence protein

Chain B: 



• Molecule 1: Avirulence protein

Chain C: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	119.43Å 119.43Å 312.57Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	62.35 – 2.30 62.35 – 2.30	Depositor EDS
% Data completeness (in resolution range)	93.5 (62.35-2.30) 97.5 (62.35-2.30)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.03 (at 2.29Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
R, R_{free}	0.223 , 0.260 0.222 , 0.252	Depositor DCC
R_{free} test set	2908 reflections (5.02%)	DCC
Wilson B-factor (Å ²)	45.6	Xtriage
Anisotropy	0.121	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 38.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 57939 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5846	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.42% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities 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	0.41	0/1913	0.54	1/2589 (0.0%)
1	B	0.39	0/1811	0.51	1/2454 (0.0%)
1	C	0.41	0/1884	0.52	1/2548 (0.0%)
All	All	0.40	0/5608	0.52	3/7591 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	67	PRO	N-CA-CB	6.28	110.83	103.30
1	A	64	PRO	N-CA-CB	6.23	110.78	103.30
1	B	241	PRO	N-CA-CB	5.81	110.28	103.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	85	LEU	Peptide

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	1863	0	1795	28	0
1	B	1774	0	1653	36	0
1	C	1844	0	1747	33	0
2	A	113	0	0	4	0
2	B	114	0	0	4	0
2	C	138	0	0	2	1
All	All	5846	0	5195	94	1

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

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:277:GLN:NE2	1:C:294:LEU:H	1.35	1.24
1:C:277:GLN:HE22	1:C:294:LEU:H	1.04	0.97
1:C:230:TYR:CG	1:C:255:MSE:HE2	2.05	0.91
1:C:277:GLN:NE2	1:C:294:LEU:N	2.19	0.90
1:C:227:PRO:HA	1:C:255:MSE:HE3	1.60	0.83
1:B:133:ARG:O	1:B:133:ARG:HD3	1.81	0.81
1:C:277:GLN:HE22	1:C:294:LEU:N	1.77	0.80
1:C:220:PHE:CD1	1:C:255:MSE:HE1	2.15	0.80
1:B:279:GLU:O	2:B:383:HOH:O	2.00	0.80
1:C:230:TYR:CD2	1:C:255:MSE:HE2	2.18	0.78
1:B:220:PHE:CD1	1:B:255:MSE:HE1	2.21	0.75
1:A:104:ARG:HD3	1:A:106:ASP:OD1	1.86	0.75
1:B:124:ASP:OD2	2:B:401:HOH:O	2.06	0.73
1:A:82:ARG:HD2	2:A:357:HOH:O	1.86	0.73
1:A:133:ARG:HD3	1:A:133:ARG:O	1.90	0.72
1:B:230:TYR:CD2	1:B:255:MSE:HE2	2.25	0.71
1:A:277:GLN:HE22	1:A:294:LEU:H	1.38	0.70
1:C:277:GLN:HE22	1:C:294:LEU:CB	2.05	0.69
1:B:133:ARG:C	1:B:133:ARG:HD3	2.12	0.68
1:C:277:GLN:HG2	1:C:293:LYS:HB3	1.76	0.68
1:A:133:ARG:HD3	1:A:133:ARG:C	2.15	0.68
1:B:230:TYR:CG	1:B:255:MSE:CE	2.79	0.66
1:C:222:TYR:OH	2:C:362:HOH:O	2.12	0.66
1:C:133:ARG:O	1:C:133:ARG:HD3	1.96	0.65
1:B:230:TYR:HB3	1:B:255:MSE:HE3	1.82	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:299:ILE:O	1:B:303:VAL:HG13	1.99	0.61
1:C:220:PHE:CE1	1:C:255:MSE:HE1	2.35	0.61
1:B:230:TYR:CG	1:B:255:MSE:HE2	2.36	0.60
1:A:85:LEU:CD1	1:A:86:ASN:H	2.14	0.60
1:B:230:TYR:CB	1:B:255:MSE:HE3	2.32	0.59
2:A:313:HOH:O	1:B:82:ARG:HA	2.02	0.59
1:B:164:HIS:CE1	2:B:408:HOH:O	2.56	0.58
1:C:277:GLN:HE22	1:C:294:LEU:HB2	1.68	0.58
1:B:266:THR:HG21	1:B:307:SER:HB3	1.85	0.57
1:B:252:LYS:HE3	1:B:256:PHE:HE2	1.70	0.57
1:C:297:SER:O	1:C:301:GLU:HG3	2.05	0.56
1:A:255:MSE:HE3	1:A:255:MSE:HA	1.88	0.56
1:B:230:TYR:CD2	1:B:255:MSE:CE	2.91	0.54
1:B:309:ILE:HG12	1:B:310:TYR:CD2	2.43	0.53
1:A:171:ALA:O	1:A:175:LYS:HG3	2.08	0.53
1:C:133:ARG:C	1:C:133:ARG:HD3	2.30	0.53
1:C:277:GLN:CG	1:C:293:LYS:HB3	2.39	0.52
1:C:114:HIS:HE1	2:C:427:HOH:O	1.91	0.51
1:A:108:ILE:HD12	1:C:162:GLN:HG3	1.92	0.51
1:A:79[A]:ARG:NH2	2:A:1:HOH:O	2.41	0.50
1:C:230:TYR:HB3	1:C:255:MSE:CE	2.42	0.50
1:A:85:LEU:HD13	1:A:86:ASN:H	1.76	0.50
1:C:80:HIS:CE1	1:C:93:LYS:HD3	2.46	0.50
1:C:227:PRO:HA	1:C:255:MSE:CE	2.37	0.49
1:C:265:PRO:HD2	1:C:268:VAL:HG21	1.94	0.49
1:A:80:HIS:CD2	1:A:93:LYS:HD3	2.48	0.48
1:A:86:ASN:OD1	1:A:88:GLU:HG3	2.12	0.48
1:A:84:SER:O	1:A:85:LEU:HD12	2.13	0.48
1:B:259:TYR:OH	1:B:272:THR:HG21	2.14	0.48
1:B:295:SER:O	1:B:299:ILE:HG13	2.14	0.47
1:B:103:GLU:HG2	1:B:104:ARG:HG2	1.97	0.47
1:A:138:TYR:O	1:A:142:GLY:HA3	2.13	0.47
1:C:227:PRO:HD2	1:C:276:TYR:CD2	2.50	0.47
1:A:68:SER:OG	1:A:71:GLU:HG3	2.16	0.46
1:B:230:TYR:CG	1:B:255:MSE:HE3	2.50	0.46
1:C:67:PRO:HA	1:C:71:GLU:OE1	2.16	0.46
1:C:230:TYR:CB	1:C:255:MSE:CE	2.93	0.46
1:C:230:TYR:CB	1:C:255:MSE:HE2	2.46	0.45
1:B:275:ALA:C	1:B:277:GLN:H	2.20	0.45
1:C:230:TYR:CE2	1:C:255:MSE:HB2	2.51	0.45
1:C:277:GLN:HE22	1:C:294:LEU:CA	2.30	0.44
1:B:221:GLU:OE1	2:B:376:HOH:O	2.21	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:63:TRP:N	2:A:405:HOH:O	2.50	0.44
1:A:87:ASP:O	1:A:91:MSE:HG2	2.17	0.44
1:B:237:ALA:O	1:B:240:LYS:HB2	2.17	0.44
1:B:309:ILE:HD11	1:B:310:TYR:CZ	2.53	0.44
1:B:230:TYR:CE2	1:B:255:MSE:HB2	2.54	0.43
1:A:227:PRO:HG3	1:A:259:TYR:OH	2.17	0.43
1:C:230:TYR:CG	1:C:255:MSE:CE	2.91	0.43
1:B:209:VAL:O	1:B:210:GLU:HB2	2.18	0.43
1:A:104:ARG:HD2	1:A:107[C]:LEU:HG	2.01	0.43
1:A:266:THR:HB	1:A:267:PRO:HD3	2.01	0.43
1:B:73:LEU:HD12	1:B:107:LEU:HD13	2.01	0.42
1:A:226:ASN:C	1:A:226:ASN:OD1	2.57	0.42
1:A:88:GLU:OE1	1:A:92:LYS:NZ	2.51	0.42
1:B:80:HIS:CE1	1:B:93:LYS:HD3	2.54	0.42
1:B:130:LEU:HG	1:B:134:LEU:HD22	2.02	0.42
1:A:295:SER:O	1:A:298:GLN:N	2.53	0.42
1:A:240:LYS:HB3	1:A:241:PRO:HD2	2.02	0.41
1:A:178:GLY:HA2	1:B:120:GLY:HA3	2.02	0.41
1:B:259:TYR:OH	1:B:272:THR:CG2	2.68	0.41
1:C:266:THR:N	1:C:267:PRO:HD2	2.36	0.41
1:C:119:PRO:HD2	1:C:123:HIS:CG	2.56	0.41
1:C:166:LEU:HA	1:C:166:LEU:HD23	1.92	0.41
1:A:119:PRO:HD2	1:A:123:HIS:CG	2.56	0.41
1:A:120:GLY:HA3	1:B:178:GLY:HA2	2.03	0.41
1:B:278:SER:HA	1:B:279:GLU:HA	1.84	0.40
1:B:80:HIS:CE1	1:B:93:LYS:HB3	2.57	0.40
1:B:308:ARG:HG2	1:B:309:ILE:HG22	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:C:369:HOH:O	2:C:374:HOH:O[12_565]	2.09	0.11

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	235/260 (90%)	226 (96%)	7 (3%)	2 (1%)	25	26
1	B	225/260 (86%)	215 (96%)	9 (4%)	1 (0%)	43	52
1	C	229/260 (88%)	223 (97%)	6 (3%)	0	100	100
All	All	689/780 (88%)	664 (96%)	22 (3%)	3 (0%)	43	52

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	64	PRO
1	A	84	SER
1	B	241	PRO

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	194/218 (89%)	185 (95%)	9 (5%)	37	48
1	B	178/218 (82%)	168 (94%)	10 (6%)	30	38
1	C	190/218 (87%)	177 (93%)	13 (7%)	22	28
All	All	562/654 (86%)	530 (94%)	32 (6%)	29	37

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	82	ARG
1	A	84	SER
1	A	98	TRP
1	A	104	ARG
1	A	133	ARG
1	A	245	SER
1	A	246	ARG
1	A	261	GLN
1	A	297	SER
1	B	73	LEU
1	B	87	ASP
1	B	98	TRP

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Mol	Chain	Res	Type
1	B	103	GLU
1	B	106	ASP
1	B	133	ARG
1	B	134	LEU
1	B	240	LYS
1	B	273	LEU
1	B	309	ILE
1	C	98	TRP
1	C	106	ASP
1	C	122	LEU
1	C	133	ARG
1	C	153	SER
1	C	239	GLU
1	C	245	SER
1	C	262	LYS
1	C	277	GLN
1	C	278	SER
1	C	290	HIS
1	C	292	GLU
1	C	297	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	277	GLN
1	B	236	HIS
1	C	114	HIS
1	C	277	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, 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	236/260 (90%)	0.23	6 (2%) 54 65	28, 47, 71, 90	0
1	B	231/260 (88%)	0.22	3 (1%) 74 82	27, 48, 72, 92	0
1	C	235/260 (90%)	0.25	5 (2%) 60 70	24, 40, 68, 101	0
All	All	702/780 (90%)	0.23	14 (1%) 62 72	24, 45, 71, 101	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	281	TYR	4.8
1	A	85	LEU	4.8
1	C	290	HIS	4.3
1	C	296	LEU	3.1
1	A	84	SER	2.9
1	A	192	HIS	2.6
1	A	196	PHE	2.4
1	B	309	ILE	2.3
1	C	277	GLN	2.2
1	B	264	PHE	2.2
1	B	267	PRO	2.2
1	C	265	PRO	2.1
1	A	188	ILE	2.1
1	A	261	GLN	2.1

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.