



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 25, 2022 – 10:30 AM EDT

PDB ID : 8D6O  
Title : Nanorana parkeri saxiphilin:F-STX (soaked)  
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Deposited on : 2022-06-06  
Resolution : 2.20 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

<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>.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.31.2  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.2

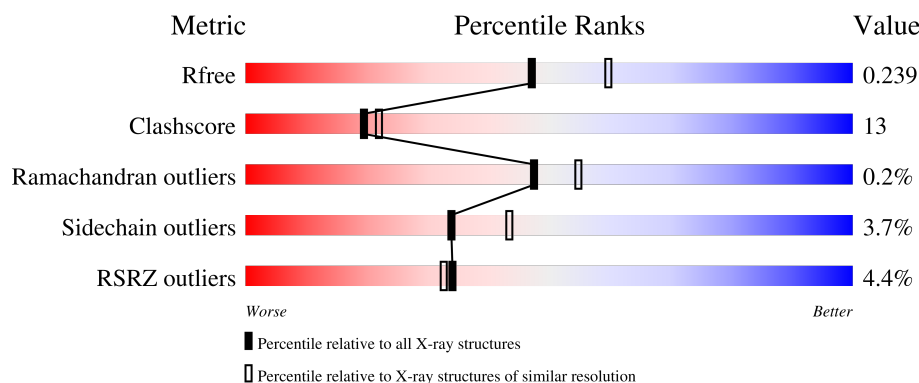
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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))
$R_{free}$	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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  $\geq 3$ , 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	854	<div> <div>4%</div> <div>74%</div> <div>21%</div> <div>• •</div> </div>

## 2 Entry composition [i](#)

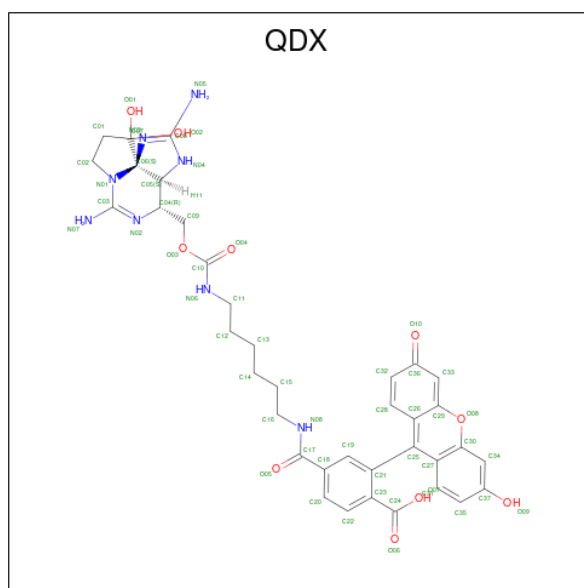
There are 4 unique types of molecules in this entry. The entry contains 6600 atoms, of which 22 are hydrogens and 0 are deuteriums.

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 Saxiphilin.

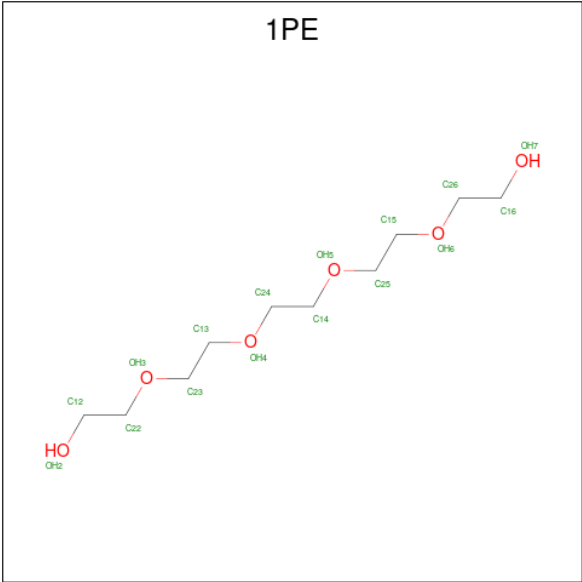
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	819	6346	3973	1096	1218	59	0	0	0

- Molecule 2 is (2P)-4-({6-([{(3aS,4R,7R,10aS)-2,6-diamino-10,10-dihydroxy-3a,4,9,10-tetrahydro-3H,8H-pyrrolo[1,2-c]purin-4-yl]methoxy}carbonyl)amino]hexyl}carbamoyl)-2-{[4aP,9(9a)P]-6-hydroxy-3-oxo-3H-xanthen-9-yl}benzoic acid (three-letter code: QDX) (formula:  $C_{37}H_{40}N_8O_{10}$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	55	37	8	10	33	0

- Molecule 3 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula:  $C_{10}H_{22}O_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			38	10	22	6		

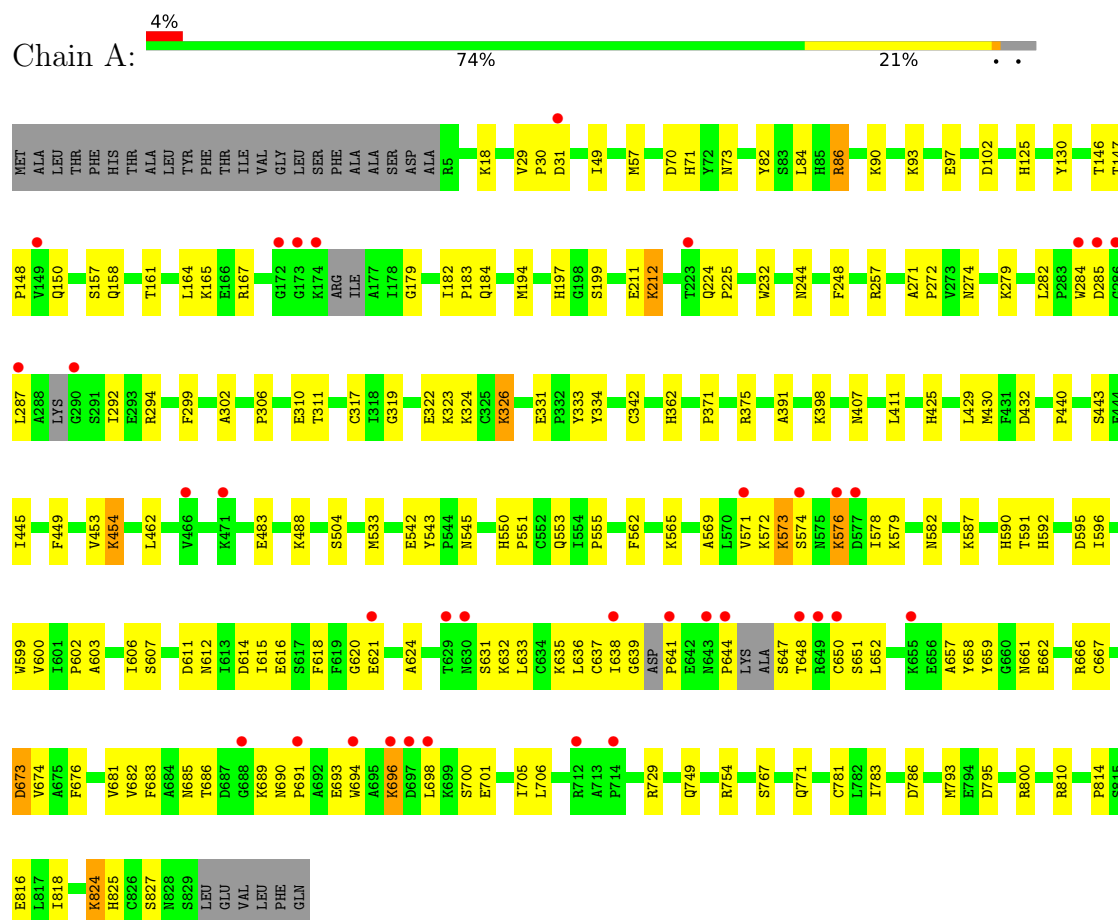
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	161	Total	O	0	0
			161	161		

### 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: Saxiphilin



## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	229.19Å 229.19Å 67.35Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	43.31 – 2.20 43.31 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (43.31-2.20) 99.9 (43.31-2.20)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.65 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, $R_{free}$	0.197 , 0.243 0.194 , 0.239	Depositor DCC
$R_{free}$ test set	3301 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	55.1	Xtriage
Anisotropy	0.385	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 48.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.004 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	6600	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.60% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: QDX, 1PE

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	0.36	0/6488	0.54	0/8771

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	6346	0	6140	161	0
2	A	55	0	0	2	0
3	A	16	22	22	3	0
4	A	161	0	0	13	0
All	All	6578	22	6162	161	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 13.

All (161) 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:A:543:TYR:HB2	1:A:783:ILE:HD12	1.49	0.95
1:A:767:SER:OG	4:A:1001:HOH:O	1.83	0.95
1:A:616:GLU:HG3	1:A:633:LEU:HD11	1.49	0.94
1:A:824:LYS:HE3	1:A:825:HIS:H	1.32	0.93
1:A:165:LYS:HA	1:A:165:LYS:HE2	1.51	0.90
1:A:648:THR:O	1:A:651:SER:OG	1.90	0.90
1:A:662:GLU:HG3	1:A:685:ASN:HD21	1.41	0.82
1:A:225:PRO:O	4:A:1002:HOH:O	1.97	0.81
1:A:638:ILE:HD11	1:A:657:ALA:HB3	1.63	0.79
1:A:824:LYS:HE3	1:A:825:HIS:N	1.97	0.78
1:A:661:ASN:HB3	1:A:681:VAL:HG22	1.67	0.77
1:A:644:PRO:CD	1:A:647:SER:HB3	2.17	0.75
1:A:644:PRO:HD3	1:A:647:SER:HB3	1.70	0.73
1:A:211:GLU:OE1	4:A:1004:HOH:O	2.08	0.72
1:A:73:ASN:HA	1:A:398:LYS:HE3	1.73	0.70
1:A:542:GLU:OE2	4:A:1005:HOH:O	2.09	0.70
1:A:284:TRP:CE3	1:A:292:ILE:HD11	2.27	0.70
1:A:571:VAL:HG12	1:A:674:VAL:HG23	1.74	0.69
1:A:621:GLU:OE2	1:A:635:LYS:HB2	1.93	0.69
1:A:614:ASP:HB3	1:A:616:GLU:OE1	1.93	0.68
1:A:638:ILE:HG23	1:A:658:TYR:HE2	1.59	0.68
1:A:616:GLU:HG3	1:A:633:LEU:CD1	2.22	0.68
1:A:130:TYR:CZ	1:A:147:THR:HG22	2.29	0.68
1:A:454:LYS:HE3	1:A:827:SER:HB3	1.76	0.67
1:A:97:GLU:OE1	4:A:1007:HOH:O	2.13	0.67
1:A:638:ILE:HD11	1:A:657:ALA:CB	2.24	0.67
1:A:454:LYS:HE3	1:A:827:SER:CB	2.25	0.66
1:A:682:VAL:O	1:A:686:THR:HG23	1.95	0.66
1:A:483:GLU:OE2	4:A:1008:HOH:O	2.14	0.65
1:A:161:THR:OG1	1:A:164:LEU:HD12	1.97	0.64
1:A:244:ASN:ND2	4:A:1006:HOH:O	2.13	0.64
1:A:638:ILE:HG23	1:A:658:TYR:CE2	2.33	0.63
1:A:449:PHE:O	1:A:825:HIS:HE1	1.81	0.63
1:A:824:LYS:CE	1:A:825:HIS:H	2.09	0.63
1:A:274:ASN:HB3	3:A:902:1PE:C14	2.29	0.62
1:A:225:PRO:HG3	1:A:362:HIS:ND1	2.15	0.62
1:A:587:LYS:NZ	1:A:621:GLU:OE1	2.33	0.61
1:A:279:LYS:HE3	1:A:371:PRO:O	2.01	0.60
1:A:147:THR:HB	1:A:148:PRO:HD2	1.84	0.60
1:A:224:GLN:HG3	1:A:225:PRO:HD2	1.83	0.60
1:A:587:LYS:HB2	1:A:673:ASP:OD1	2.02	0.59
1:A:603:ALA:HB1	1:A:615:ILE:HD11	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:ASN:HB3	3:A:902:1PE:H141	1.85	0.58
1:A:587:LYS:HE3	1:A:636:LEU:HD11	1.84	0.58
1:A:84:LEU:HD22	1:A:824:LYS:HE2	1.87	0.57
1:A:147:THR:O	1:A:150:GLN:HG2	2.05	0.56
1:A:587:LYS:NZ	1:A:621:GLU:HB3	2.21	0.56
1:A:693:GLU:H	1:A:693:GLU:CD	2.08	0.56
1:A:693:GLU:OE1	1:A:693:GLU:N	2.31	0.56
1:A:49:ILE:CD1	1:A:57:MET:HG2	2.35	0.56
1:A:543:TYR:CB	1:A:783:ILE:HD12	2.31	0.56
1:A:572:LYS:HB2	1:A:572:LYS:HZ3	1.71	0.55
1:A:661:ASN:HB3	1:A:681:VAL:CG2	2.36	0.55
1:A:578:ILE:O	1:A:578:ILE:HG23	2.08	0.54
1:A:407:ASN:OD1	1:A:440:PRO:HB3	2.08	0.54
1:A:29:VAL:O	4:A:1009:HOH:O	2.19	0.53
1:A:84:LEU:HD21	1:A:825:HIS:O	2.09	0.53
1:A:682:VAL:HG13	1:A:683:PHE:CD1	2.44	0.53
1:A:690:ASN:HD22	1:A:691:PRO:HD2	1.73	0.53
1:A:212:LYS:O	1:A:212:LYS:HD3	2.09	0.52
1:A:146:THR:HB	1:A:150:GLN:HG3	1.91	0.52
1:A:411:LEU:HD12	1:A:411:LEU:O	2.09	0.52
1:A:662:GLU:HG3	1:A:685:ASN:ND2	2.18	0.52
1:A:317:CYS:HB3	1:A:331:GLU:OE1	2.10	0.51
1:A:652:LEU:HA	1:A:659:TYR:CE2	2.46	0.51
1:A:661:ASN:O	1:A:681:VAL:HG11	2.10	0.51
1:A:274:ASN:HB3	3:A:902:1PE:H142	1.91	0.51
1:A:693:GLU:O	1:A:696:LYS:HB2	2.10	0.51
1:A:86:ARG:HG3	1:A:232:TRP:NE1	2.26	0.51
1:A:638:ILE:HD12	1:A:639:GLY:O	2.10	0.50
1:A:814:PRO:HD2	1:A:818:ILE:HD12	1.94	0.50
1:A:553:GLN:O	1:A:555:PRO:HD3	2.10	0.50
1:A:824:LYS:HE3	1:A:824:LYS:CA	2.41	0.49
1:A:542:GLU:OE2	1:A:729:ARG:HD3	2.12	0.49
1:A:533:MET:HE2	4:A:1042:HOH:O	2.12	0.49
1:A:639:GLY:C	1:A:647:SER:HA	2.33	0.49
1:A:795:ASP:OD1	2:A:901:QDX:N05	2.45	0.49
1:A:454:LYS:H	1:A:454:LYS:CD	2.25	0.48
1:A:562:PHE:HB2	2:A:901:QDX:O04	2.13	0.48
1:A:606:ILE:HD12	1:A:618:PHE:CE2	2.47	0.48
1:A:685:ASN:HD22	1:A:694:TRP:HH2	1.60	0.48
1:A:167:ARG:NH1	1:A:183:PRO:O	2.47	0.48
1:A:322:GLU:OE1	1:A:322:GLU:N	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:569:ALA:O	1:A:705:ILE:HA	2.13	0.48
1:A:102:ASP:OD2	1:A:800:ARG:NE	2.36	0.47
1:A:590:HIS:CE1	1:A:676:PHE:CD2	3.03	0.47
1:A:686:THR:HB	1:A:698:LEU:O	2.15	0.47
1:A:454:LYS:H	1:A:454:LYS:HE2	1.79	0.47
1:A:603:ALA:CB	1:A:615:ILE:HD11	2.44	0.47
1:A:30:PRO:O	1:A:31:ASP:HB2	2.14	0.47
1:A:579:LYS:H	1:A:582:ASN:HD21	1.61	0.47
1:A:591:THR:O	1:A:592:HIS:HB3	2.15	0.47
1:A:749:GLN:OE1	1:A:781:CYS:HB2	2.15	0.47
1:A:453:VAL:HG13	1:A:454:LYS:HD3	1.97	0.47
1:A:271:ALA:HB3	1:A:272:PRO:HD3	1.96	0.47
1:A:429:LEU:O	1:A:430:MET:HB2	2.15	0.47
1:A:571:VAL:CG1	1:A:674:VAL:HG23	2.43	0.46
1:A:282:LEU:HD23	1:A:282:LEU:HA	1.78	0.46
1:A:73:ASN:HA	1:A:398:LYS:CE	2.45	0.46
1:A:573:LYS:O	1:A:576:LYS:NZ	2.41	0.46
1:A:690:ASN:ND2	1:A:691:PRO:HD2	2.30	0.46
1:A:579:LYS:H	1:A:582:ASN:ND2	2.14	0.46
1:A:319:GLY:O	1:A:324:LYS:HB2	2.15	0.46
1:A:693:GLU:HG2	1:A:694:TRP:H	1.81	0.46
1:A:453:VAL:CG1	1:A:454:LYS:HD3	2.46	0.46
1:A:587:LYS:HA	1:A:621:GLU:O	2.16	0.46
1:A:590:HIS:HD2	1:A:624:ALA:HB2	1.81	0.46
1:A:658:TYR:CD1	1:A:667:CYS:HB2	2.51	0.46
1:A:257:ARG:HA	1:A:302:ALA:O	2.16	0.45
1:A:294:ARG:HG3	1:A:310:GLU:OE2	2.16	0.45
1:A:767:SER:CB	4:A:1001:HOH:O	2.55	0.45
1:A:130:TYR:CE2	1:A:147:THR:HG22	2.51	0.45
1:A:306:PRO:HG2	1:A:334:TYR:HA	1.98	0.45
1:A:543:TYR:CZ	1:A:545:ASN:HB3	2.51	0.45
1:A:596:ILE:HA	1:A:600:VAL:HB	1.98	0.45
1:A:599:TRP:C	1:A:602:PRO:HD2	2.37	0.45
1:A:682:VAL:HG13	1:A:683:PHE:N	2.30	0.45
1:A:244:ASN:ND2	4:A:1030:HOH:O	2.50	0.45
1:A:793:MET:HG2	1:A:810:ARG:NH1	2.31	0.45
1:A:284:TRP:CZ3	1:A:285:ASP:O	2.70	0.45
1:A:248:PHE:O	1:A:375:ARG:NH1	2.49	0.45
1:A:607:SER:OG	1:A:612:ASN:HA	2.17	0.44
1:A:620:GLY:O	1:A:632:LYS:HD2	2.17	0.44
1:A:179:GLY:HA2	1:A:199:SER:OG	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:HIS:ND1	1:A:611:ASP:OD1	2.43	0.44
1:A:621:GLU:OE2	1:A:635:LYS:CB	2.64	0.44
1:A:569:ALA:HB3	1:A:706:LEU:HB2	1.98	0.44
1:A:639:GLY:C	1:A:641:PRO:HD3	2.38	0.44
1:A:814:PRO:HD2	1:A:818:ILE:CD1	2.48	0.44
1:A:49:ILE:HD11	1:A:57:MET:HG2	1.99	0.44
1:A:454:LYS:H	1:A:454:LYS:HD3	1.82	0.44
1:A:693:GLU:HG2	1:A:694:TRP:N	2.33	0.44
1:A:666:ARG:HG2	1:A:694:TRP:CZ2	2.53	0.43
1:A:90:LYS:N	4:A:1010:HOH:O	2.21	0.43
1:A:682:VAL:HG13	1:A:683:PHE:H	1.84	0.43
1:A:693:GLU:HA	1:A:696:LYS:HE3	2.00	0.43
1:A:18:LYS:HG2	1:A:425:HIS:CE1	2.54	0.43
1:A:550:HIS:N	1:A:551:PRO:HD2	2.33	0.43
1:A:182:ILE:O	1:A:184:GLN:NE2	2.50	0.43
1:A:282:LEU:HD21	1:A:299:PHE:HB2	2.01	0.43
1:A:284:TRP:CZ3	1:A:292:ILE:HD11	2.53	0.43
1:A:592:HIS:NE2	1:A:595:ASP:HB2	2.33	0.42
1:A:194:MET:HG3	1:A:224:GLN:NE2	2.35	0.42
1:A:637:CYS:HA	1:A:658:TYR:HD2	1.84	0.42
1:A:323:LYS:HA	1:A:326:LYS:HG3	2.01	0.42
1:A:82:TYR:CE2	1:A:391:ALA:HB2	2.55	0.42
1:A:84:LEU:CD2	1:A:824:LYS:HE2	2.49	0.42
1:A:602:PRO:O	1:A:606:ILE:HG12	2.20	0.42
1:A:86:ARG:HB2	1:A:232:TRP:CD1	2.54	0.41
1:A:197:HIS:CE1	1:A:199:SER:HB2	2.54	0.41
1:A:18:LYS:HB2	1:A:18:LYS:HE2	1.52	0.41
1:A:333:TYR:CG	1:A:342:CYS:HB2	2.56	0.41
1:A:443:SER:OG	1:A:816:GLU:OE2	2.37	0.41
1:A:462:LEU:HD23	1:A:462:LEU:HA	1.82	0.41
1:A:644:PRO:HD2	1:A:647:SER:HB3	1.99	0.41
1:A:693:GLU:CA	1:A:696:LYS:HE3	2.51	0.41
1:A:786:ASP:OD2	4:A:1011:HOH:O	2.21	0.41
1:A:454:LYS:H	1:A:454:LYS:CE	2.33	0.40
1:A:86:ARG:HG3	1:A:232:TRP:CE2	2.56	0.40
1:A:616:GLU:O	1:A:632:LYS:HE3	2.22	0.40
1:A:701:GLU:O	1:A:701:GLU:HG3	2.22	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	809/854 (95%)	762 (94%)	45 (6%)	2 (0%)	47	55

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	287	LEU
1	A	696	LYS

### 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	703/731 (96%)	677 (96%)	26 (4%)	34	43

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70	ASP
1	A	71	HIS
1	A	86	ARG
1	A	93	LYS
1	A	157	SER
1	A	158	GLN
1	A	212	LYS
1	A	311	THR
1	A	326	LYS

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Mol	Chain	Res	Type
1	A	432	ASP
1	A	445	ILE
1	A	454	LYS
1	A	488	LYS
1	A	504	SER
1	A	565	LYS
1	A	573	LYS
1	A	574	SER
1	A	576	LYS
1	A	631	SER
1	A	650	CYS
1	A	673	ASP
1	A	689	LYS
1	A	700	SER
1	A	754	ARG
1	A	771	GLN
1	A	824	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	168	GLN
1	A	590	HIS
1	A	608	ASN
1	A	685	ASN
1	A	825	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules 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 monosaccharides in this entry.

## 5.6 Ligand geometry

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	1PE	A	902	-	15,15,15	0.52	0	14,14,14	0.32	0
2	QDX	A	901	-	55,61,61	5.17	25 (45%)	67,91,91	3.35	26 (38%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	1PE	A	902	-	-	7/13/13/13	-
2	QDX	A	901	-	-	18/30/80/80	0/7/7/7

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	901	QDX	C31-C27	19.26	1.70	1.39
2	A	901	QDX	C02-N01	-11.72	1.33	1.47
2	A	901	QDX	C34-C37	-10.57	1.23	1.39
2	A	901	QDX	C32-C28	10.48	1.58	1.35
2	A	901	QDX	C08-N04	9.08	1.49	1.35
2	A	901	QDX	C34-C30	-8.84	1.22	1.38
2	A	901	QDX	C33-C36	-8.70	1.24	1.45
2	A	901	QDX	C01-C02	-8.64	1.36	1.52
2	A	901	QDX	C35-C31	7.83	1.53	1.38
2	A	901	QDX	C03-N07	6.80	1.46	1.34
2	A	901	QDX	C17-N08	6.30	1.47	1.33
2	A	901	QDX	C33-C29	-5.95	1.21	1.36
2	A	901	QDX	C10-N06	5.82	1.47	1.34
2	A	901	QDX	C28-C26	5.71	1.53	1.40
2	A	901	QDX	O10-C36	5.37	1.41	1.24
2	A	901	QDX	C08-N05	4.91	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	901	QDX	O08-C30	-4.47	1.31	1.38
2	A	901	QDX	C21-C25	3.85	1.55	1.49
2	A	901	QDX	C03-N01	3.69	1.42	1.35
2	A	901	QDX	O03-C10	3.50	1.41	1.35
2	A	901	QDX	C26-C25	3.48	1.50	1.39
2	A	901	QDX	C05-N04	2.36	1.50	1.45
2	A	901	QDX	C18-C17	2.34	1.55	1.50
2	A	901	QDX	C35-C37	-2.33	1.34	1.38
2	A	901	QDX	C27-C25	-2.18	1.41	1.47

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	901	QDX	C29-C33-C36	10.30	129.85	120.76
2	A	901	QDX	O08-C30-C27	-9.65	112.39	121.56
2	A	901	QDX	C30-O08-C29	8.10	134.86	119.70
2	A	901	QDX	C35-C37-C34	7.80	128.72	120.17
2	A	901	QDX	C31-C27-C30	-6.88	109.19	118.21
2	A	901	QDX	C28-C26-C25	6.23	137.32	123.96
2	A	901	QDX	C33-C29-C26	6.11	131.53	122.90
2	A	901	QDX	O03-C10-N06	5.80	119.64	110.61
2	A	901	QDX	C01-C02-N01	5.63	110.20	103.83
2	A	901	QDX	C31-C35-C37	-5.14	114.24	119.88
2	A	901	QDX	O08-C29-C26	-4.78	115.09	120.49
2	A	901	QDX	C30-C34-C37	4.22	125.90	119.05
2	A	901	QDX	C35-C31-C27	-4.12	114.25	120.94
2	A	901	QDX	N01-C03-N02	-3.84	120.08	125.42
2	A	901	QDX	C28-C26-C29	-3.41	107.93	115.62
2	A	901	QDX	C25-C26-C29	-3.40	114.75	119.29
2	A	901	QDX	C34-C30-C27	3.32	127.71	121.35
2	A	901	QDX	C31-C27-C25	3.29	129.86	123.28
2	A	901	QDX	C28-C32-C36	-3.11	116.93	121.23
2	A	901	QDX	O04-C10-N06	-2.91	120.50	124.96
2	A	901	QDX	O08-C30-C34	2.74	119.91	115.79
2	A	901	QDX	C23-C21-C25	-2.67	119.62	123.33
2	A	901	QDX	N05-C08-N04	-2.51	118.72	122.64
2	A	901	QDX	C32-C28-C26	-2.42	117.11	121.49
2	A	901	QDX	O03-C10-O04	-2.29	119.86	124.25
2	A	901	QDX	O08-C29-C33	-2.15	113.38	116.61

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	901	QDX	N06-C10-O03-C09
2	A	901	QDX	O04-C10-O03-C09
2	A	901	QDX	C21-C25-C27-C31
2	A	901	QDX	C26-C25-C27-C31
2	A	901	QDX	O05-C17-C18-C19
2	A	901	QDX	N08-C17-C18-C19
2	A	901	QDX	O05-C17-C18-C20
2	A	901	QDX	N08-C17-C18-C20
2	A	901	QDX	C14-C15-C16-N08
2	A	901	QDX	N06-C11-C12-C13
2	A	901	QDX	O03-C10-N06-C11
3	A	902	1PE	OH7-C16-C26-OH6
3	A	902	1PE	C13-C23-OH3-C22
2	A	901	QDX	O04-C10-N06-C11
2	A	901	QDX	C13-C14-C15-C16
3	A	902	1PE	OH6-C15-C25-OH5
2	A	901	QDX	C11-C12-C13-C14
2	A	901	QDX	C22-C23-C24-O06
3	A	902	1PE	OH2-C12-C22-OH3
2	A	901	QDX	C22-C23-C24-O07
3	A	902	1PE	C16-C26-OH6-C15
2	A	901	QDX	C21-C23-C24-O06
2	A	901	QDX	C21-C23-C24-O07
3	A	902	1PE	OH4-C13-C23-OH3
3	A	902	1PE	OH5-C14-C24-OH4

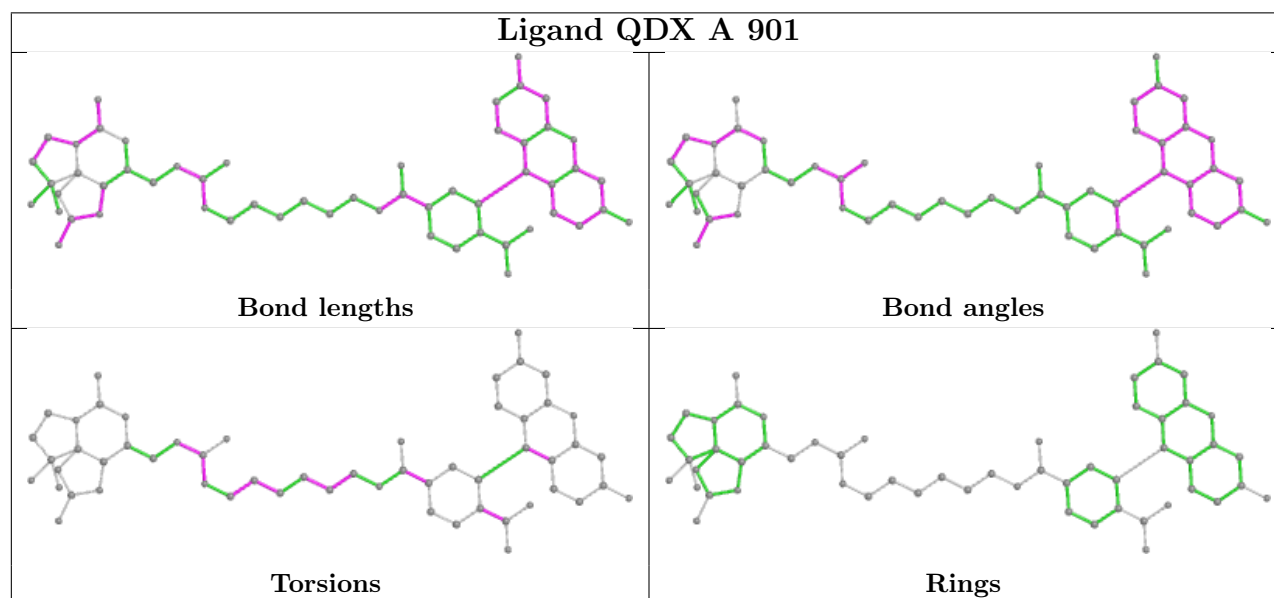
There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	902	1PE	3	0
2	A	901	QDX	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 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	819/854 (95%)	0.05	36 (4%) 34 32	45, 65, 120, 157	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	290	GLY	7.1
1	A	697	ASP	5.9
1	A	174	LYS	5.7
1	A	691	PRO	4.7
1	A	649	ARG	4.4
1	A	648	THR	4.0
1	A	466	VAL	3.7
1	A	641	PRO	3.6
1	A	644	PRO	3.6
1	A	638	ILE	3.6
1	A	688	GLY	3.5
1	A	173	GLY	3.4
1	A	172	GLY	3.3
1	A	650	CYS	3.1
1	A	643	ASN	3.1
1	A	31	ASP	3.0
1	A	694	TRP	3.0
1	A	629	THR	2.9
1	A	577	ASP	2.8
1	A	287	LEU	2.7
1	A	696	LYS	2.7
1	A	571	VAL	2.5
1	A	576	LYS	2.4
1	A	471	LYS	2.4
1	A	621	GLU	2.3
1	A	574	SER	2.3
1	A	285	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	714	PRO	2.2
1	A	698	LEU	2.2
1	A	286	GLY	2.2
1	A	712	ARG	2.1
1	A	284	TRP	2.1
1	A	655	LYS	2.1
1	A	149	VAL	2.1
1	A	223	THR	2.1
1	A	630	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](#)

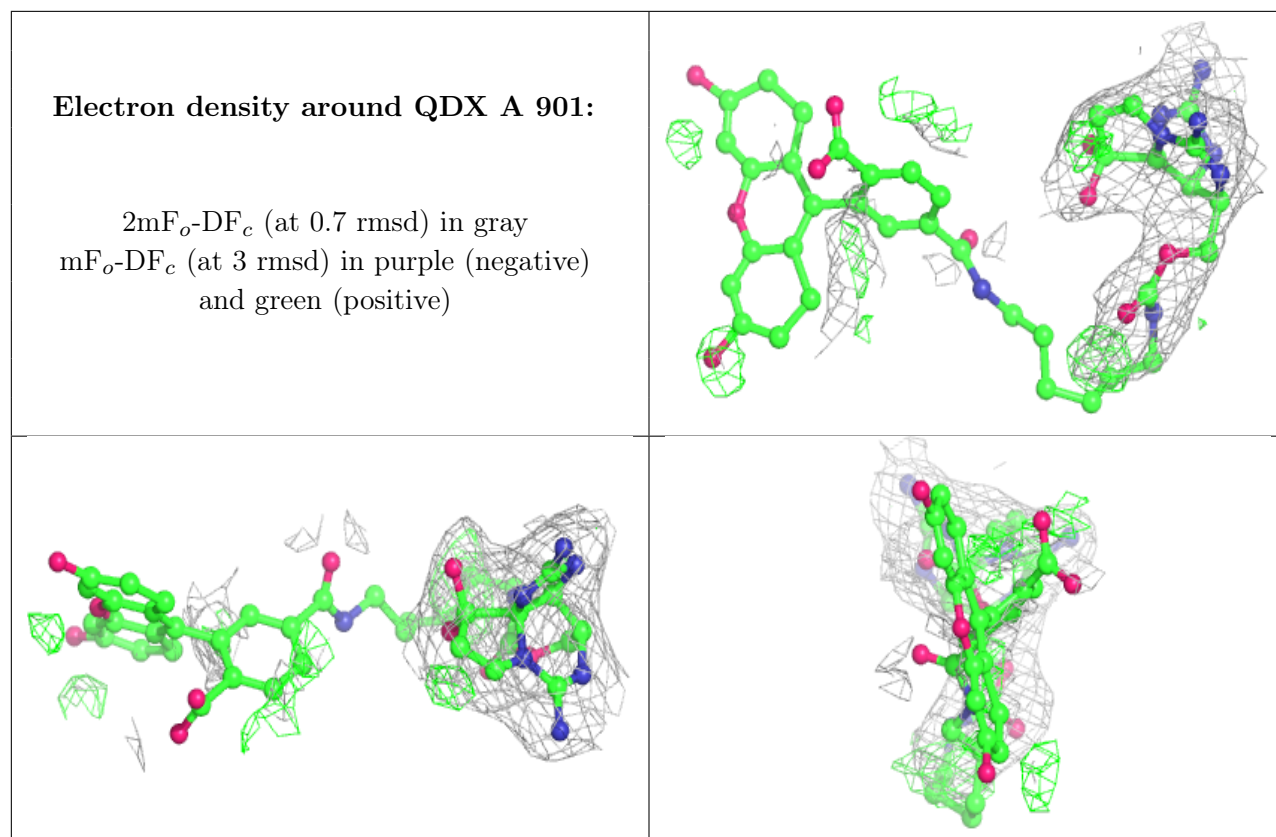
There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	1PE	A	902	16/16	0.84	0.17	75,102,112,115	0
2	QDX	A	901	55/55	0.94	0.12	53,75,85,87	33

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



## 6.5 Other polymers [i](#)

There are no such residues in this entry.