



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 09:58 AM EDT

PDB ID : 3VRZ / pdb_00003vrz
Title : Crystal structure of HCK complexed with a pyrrolo-pyrimidine inhibitor 1-[4-(4-amino-7-cyclopentyl-7H-pyrrolo[2,3-d]pyrimidin-5-yl)phenyl]-3-benzylurea
Authors : Kuratani, M.; Tomabechei, Y.; Handa, N.; Yokoyama, S.
Deposited on : 2012-04-21
Resolution : 2.22 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

<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>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

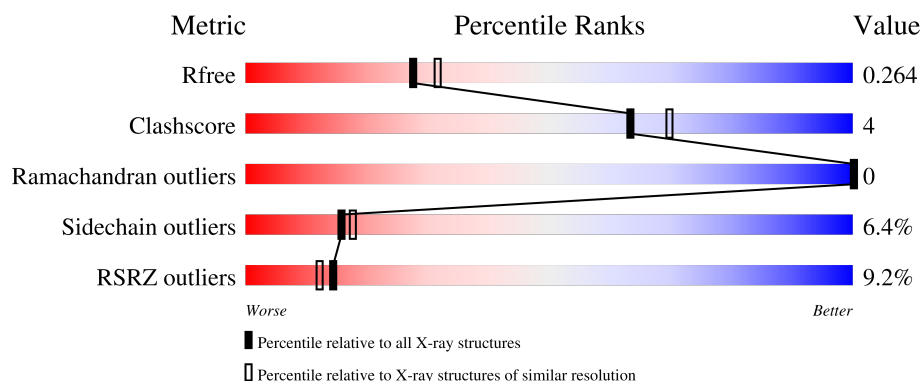
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.22 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}	180053	7682 (2.24-2.20)
Clashscore	190562	8402 (2.24-2.20)
Ramachandran outliers	187476	8303 (2.24-2.20)
Sidechain outliers	187428	8304 (2.24-2.20)
RSRZ outliers	180081	7683 (2.24-2.20)

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 ≥ 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	454	10% 82% 11% • 5%
1	B	454	7% 81% 13% • 5%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7258 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 Tyrosine-protein kinase HCK.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	430	Total	C	N	O	P	S	0	0	0
			3468	2217	583	647	1	20			
1	B	431	Total	C	N	O	P	S	0	0	0
			3479	2226	584	648	1	20			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	78	GLY	-	expression tag	UNP P08631
A	79	ALA	-	expression tag	UNP P08631
A	80	MET	-	expression tag	UNP P08631
A	81	GLY	-	expression tag	UNP P08631
A	82	SER	-	expression tag	UNP P08631
A	83	GLY	-	expression tag	UNP P08631
A	84	ILE	-	expression tag	UNP P08631
A	85	ARG	-	expression tag	UNP P08631
A	528	GLU	GLN	engineered mutation	UNP P08631
A	529	GLU	GLN	engineered mutation	UNP P08631
A	530	ILE	GLN	engineered mutation	UNP P08631
B	78	GLY	-	expression tag	UNP P08631
B	79	ALA	-	expression tag	UNP P08631
B	80	MET	-	expression tag	UNP P08631
B	81	GLY	-	expression tag	UNP P08631
B	82	SER	-	expression tag	UNP P08631
B	83	GLY	-	expression tag	UNP P08631
B	84	ILE	-	expression tag	UNP P08631
B	85	ARG	-	expression tag	UNP P08631
B	528	GLU	GLN	engineered mutation	UNP P08631
B	529	GLU	GLN	engineered mutation	UNP P08631
B	530	ILE	GLN	engineered mutation	UNP P08631

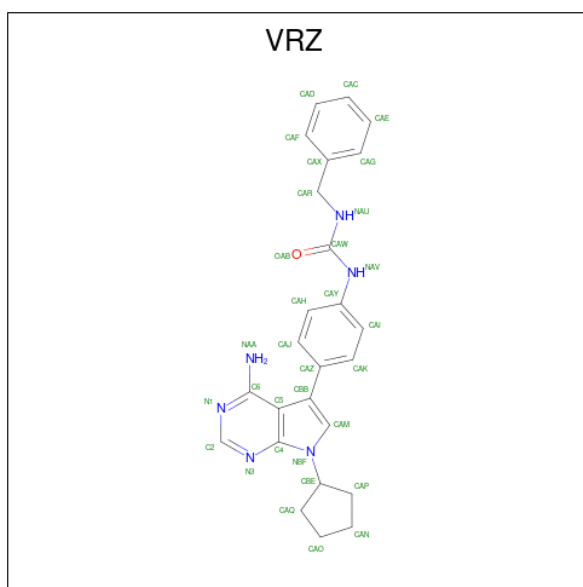
- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Ca 1 1	0	0
2	B	1	Total Ca 1 1	0	0

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Cl 1 1	0	0
3	B	1	Total Cl 1 1	0	0

- Molecule 4 is 1-[4-(4-amino-7-cyclopentyl-7H-pyrrolo[2,3-d]pyrimidin-5-yl)phenyl]-3-benzylurea (CCD ID: VRZ) (formula: C₂₅H₂₆N₆O).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 32 25 6 1	0	0
4	B	1	Total C N O 32 25 6 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	97	Total O 97 97	0	0

Continued on next page...

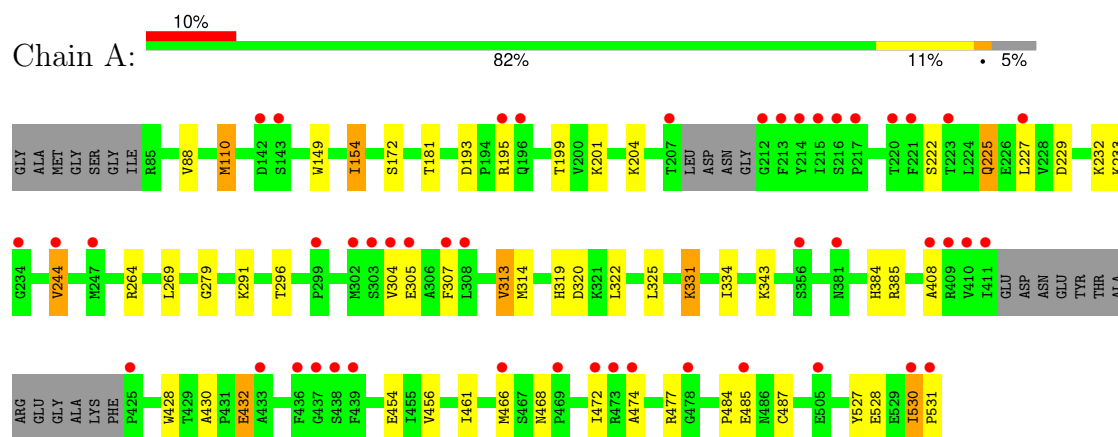
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	146	Total 146	O 146	0	0

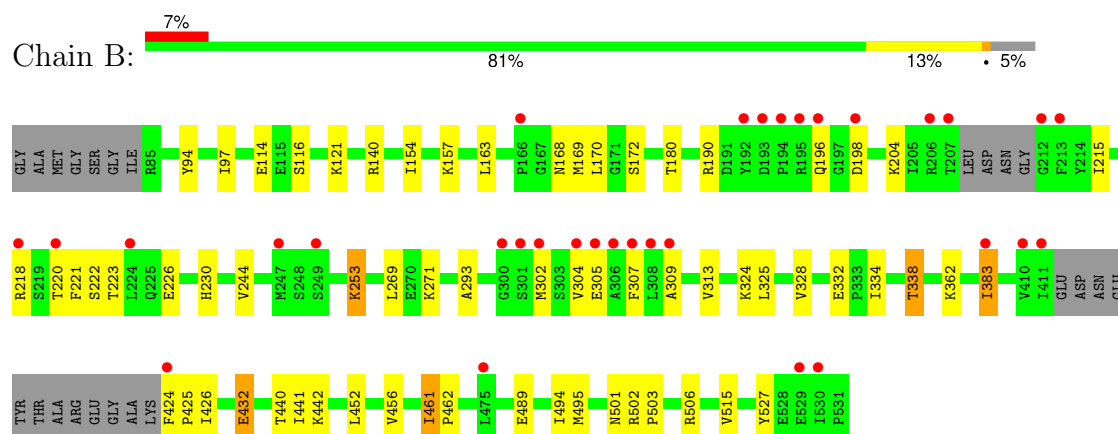
3 Residue-property plots [i](#)

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: Tyrosine-protein kinase HCK



• Molecule 1: Tyrosine-protein kinase HCK



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	73.64Å 96.49Å 180.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.14 – 2.22 49.14 – 2.22	Depositor EDS
% Data completeness (in resolution range)	91.9 (49.14-2.22) 92.0 (49.14-2.22)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.40 (at 2.22Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.239 , 0.267 0.234 , 0.264	Depositor DCC
R_{free} test set	2000 reflections (3.36%)	wwPDB-VP
Wilson B-factor (Å ²)	38.3	Xtriage
Anisotropy	0.661	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 34.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7258	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 36.97 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.6065e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: VRZ, PTR, CA, CL

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	0.34	0/3533	0.75	0/4767
1	B	0.35	0/3545	0.75	1/4784 (0.0%)
All	All	0.34	0/7078	0.75	1/9551 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	215	ILE	N-CA-C	-5.25	106.69	111.67

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	3468	0	3430	26	0
1	B	3479	0	3438	29	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	32	0	26	2	0
4	B	32	0	26	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	97	0	0	0	0
5	B	146	0	0	2	0
All	All	7258	0	6920	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 4.

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:A:385:ARG:HD2	1:A:408:ALA:HB1	1.59	0.83
1:B:304:VAL:HG13	1:B:334:ILE:HD11	1.69	0.75
1:B:440:THR:HG23	1:B:442:LYS:H	1.60	0.66
1:B:223:THR:H	1:B:226:GLU:HG3	1.62	0.64
1:A:313:VAL:HG12	1:A:314:MET:HE2	1.83	0.61
1:B:94:TYR:CE1	1:B:253:LYS:HE3	2.36	0.60
1:A:319:HIS:HB3	1:A:322:LEU:HG	1.83	0.60
1:B:163:LEU:O	1:B:190:ARG:NH1	2.36	0.59
1:B:432:GLU:OE2	1:B:506:ARG:NH1	2.31	0.58
1:B:180:THR:OG1	1:B:204:LYS:NZ	2.37	0.55
1:B:97:ILE:HG12	1:B:253:LYS:HE2	1.91	0.53
1:B:293:ALA:HB3	1:B:338:THR:HG22	1.92	0.52
1:B:424:PHE:HB3	1:B:425:PRO:HD3	1.92	0.52
1:A:264:ARG:NH2	1:A:331:LYS:O	2.40	0.52
1:B:253:LYS:NZ	5:B:726:HOH:O	2.42	0.51
1:B:172:SER:HA	1:B:244:VAL:O	2.11	0.51
1:B:440:THR:HG23	1:B:442:LYS:N	2.25	0.50
1:B:302:MET:HG3	1:B:307:PHE:HD1	1.76	0.50
1:B:221:PHE:HB3	1:B:226:GLU:HB2	1.93	0.50
1:B:302:MET:HG3	1:B:307:PHE:CD1	2.47	0.50
1:B:221:PHE:HZ	1:B:230:HIS:CD2	2.30	0.50
1:A:181:THR:OG1	1:A:204:LYS:NZ	2.45	0.49
1:B:362:LYS:NZ	5:B:815:HOH:O	2.45	0.49
1:A:172:SER:HA	1:A:244:VAL:O	2.12	0.49
1:A:428:TRP:NE1	1:A:454:GLU:OE1	2.40	0.48
1:A:430:ALA:HB1	1:A:432:GLU:OE2	2.13	0.48
1:A:456:VAL:HG11	1:A:487:CYS:HB2	1.96	0.48
1:A:484:PRO:HG2	1:A:487:CYS:HB2	1.96	0.47
1:B:222:SER:OG	1:B:226:GLU:OE2	2.32	0.47
1:A:307:PHE:CZ	4:A:603:VRZ:H23	2.50	0.46
1:B:309:ALA:O	1:B:313:VAL:HG23	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:168:ASN:HB2	1:B:190:ARG:NH1	2.31	0.46
1:A:314:MET:HG3	4:A:603:VRZ:H21	1.99	0.46
1:B:452:LEU:HD23	1:B:495:MET:HG2	1.99	0.45
1:A:468:ASN:O	1:A:472:ILE:HG13	2.17	0.45
1:A:530:ILE:HA	1:A:531:PRO:HD2	1.63	0.44
1:A:384:HIS:O	1:A:385:ARG:HB3	2.18	0.44
1:A:225:GLN:NE2	1:A:229:ASP:OD2	2.50	0.44
1:B:114:GLU:HB2	1:B:121:LYS:HB3	2.00	0.44
1:A:232:LYS:HE2	1:A:232:LYS:HB3	1.84	0.43
1:A:530:ILE:HD12	1:A:531:PRO:HD2	2.00	0.43
1:B:461:ILE:HG13	1:B:462:PRO:HD2	2.01	0.43
1:B:494:ILE:HD11	1:B:515:VAL:HG11	2.02	0.42
1:B:502:ARG:HA	1:B:503:PRO:HD3	1.92	0.42
1:A:474:ALA:HA	1:A:477:ARG:HD2	2.02	0.42
1:B:383:ILE:HD11	1:B:441:ILE:N	2.34	0.41
1:A:279:GLY:HA3	1:A:296:THR:O	2.20	0.41
1:A:88:VAL:HG23	1:A:110:MET:HG3	2.02	0.41
1:A:154:ILE:HD12	1:A:154:ILE:HA	1.87	0.41
1:A:149:TRP:HZ2	1:A:225:GLN:HG2	1.85	0.41
1:A:201:LYS:HD3	1:A:528:GLU:CD	2.45	0.41
1:A:466:MET:HB3	1:A:466:MET:HE2	1.81	0.41
1:B:223:THR:OG1	1:B:226:GLU:HG2	2.21	0.41
1:A:334:ILE:H	1:A:334:ILE:HG12	1.74	0.40
1:B:157:LYS:HA	1:B:157:LYS:HD2	1.89	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	423/454 (93%)	408 (96%)	15 (4%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	424/454 (93%)	412 (97%)	12 (3%)	0	100	100
All	All	847/908 (93%)	820 (97%)	27 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	374/393 (95%)	351 (94%)	23 (6%)	17	19
1	B	375/393 (95%)	350 (93%)	25 (7%)	15	16
All	All	749/786 (95%)	701 (94%)	48 (6%)	16	18

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	110	MET
1	A	154	ILE
1	A	193	ASP
1	A	195	ARG
1	A	199	THR
1	A	222	SER
1	A	225	GLN
1	A	227	LEU
1	A	233	LYS
1	A	244	VAL
1	A	269	LEU
1	A	291	LYS
1	A	304	VAL
1	A	305	GLU
1	A	313	VAL
1	A	320	ASP
1	A	325	LEU
1	A	331	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	343	LYS
1	A	432	GLU
1	A	461	ILE
1	A	485	GLU
1	A	530	ILE
1	B	116	SER
1	B	140	ARG
1	B	154	ILE
1	B	169	MET
1	B	170	LEU
1	B	196	GLN
1	B	198	ASP
1	B	218	ARG
1	B	220	THR
1	B	253	LYS
1	B	269	LEU
1	B	271	LYS
1	B	305	GLU
1	B	324	LYS
1	B	325	LEU
1	B	328	VAL
1	B	332	GLU
1	B	338	THR
1	B	383	ILE
1	B	426	ILE
1	B	432	GLU
1	B	456	VAL
1	B	461	ILE
1	B	489	GLU
1	B	501	ASN

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	196	GLN
1	A	318	GLN
1	A	468	ASN
1	B	235	ASN
1	B	252	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	PTR	A	527	1,2	15,16,17	1.19	1 (6%)	17,22,24	0.51	0
1	PTR	B	527	1,2	15,16,17	1.22	1 (6%)	17,22,24	0.45	0

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
1	PTR	A	527	1,2	-	1/10/11/13	0/1/1/1
1	PTR	B	527	1,2	-	1/10/11/13	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	527	PTR	OH-CZ	-4.61	1.30	1.40
1	A	527	PTR	OH-CZ	-4.44	1.30	1.40

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	527	PTR	C-CA-CB-CG
1	A	527	PTR	C-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 for Mogul analysis.

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
4	VRZ	B	603	-	36,36,36	1.07	4 (11%)	47,50,50	1.83	9 (19%)
4	VRZ	A	603	-	36,36,36	0.96	4 (11%)	47,50,50	2.12	13 (27%)

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
4	VRZ	B	603	-	-	0/17/24/24	0/5/5/5
4	VRZ	A	603	-	-	0/17/24/24	0/5/5/5

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	603	VRZ	CAM-CBB	3.14	1.40	1.37
4	A	603	VRZ	C5-CBB	-2.57	1.40	1.46
4	B	603	VRZ	C5-C6	-2.52	1.39	1.42
4	B	603	VRZ	C5-CBB	-2.50	1.40	1.46
4	A	603	VRZ	CAM-NBF	-2.28	1.34	1.38
4	A	603	VRZ	CAM-CBB	2.21	1.39	1.37
4	A	603	VRZ	C5-C6	-2.21	1.39	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	603	VRZ	CAM-NBF	-2.13	1.34	1.38

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	603	VRZ	C5-C4-N3	-7.13	119.40	126.97
4	B	603	VRZ	C5-C4-N3	-6.64	119.93	126.97
4	B	603	VRZ	N1-C2-N3	-5.06	120.92	128.58
4	A	603	VRZ	N1-C2-N3	-4.97	121.06	128.58
4	A	603	VRZ	NAV-CAW-NAU	4.06	120.61	113.83
4	A	603	VRZ	CBB-CAM-NBF	-3.93	108.90	110.54
4	A	603	VRZ	C6-C5-C4	3.68	118.50	115.74
4	B	603	VRZ	C2-N3-C4	3.63	120.69	111.83
4	A	603	VRZ	C2-N3-C4	3.58	120.59	111.83
4	A	603	VRZ	CAK-CAZ-CBB	-3.13	117.06	120.98
4	B	603	VRZ	CBB-CAM-NBF	-2.79	109.37	110.54
4	A	603	VRZ	C4-NBF-CAM	2.76	109.22	108.08
4	A	603	VRZ	OAB-CAW-NAU	-2.75	117.75	122.47
4	A	603	VRZ	N3-C4-NBF	2.72	131.80	127.17
4	B	603	VRZ	NAV-CAW-NAU	2.68	118.31	113.83
4	A	603	VRZ	CAQ-CBE-NBF	-2.55	107.58	114.39
4	B	603	VRZ	C6-C5-C4	2.48	117.59	115.74
4	B	603	VRZ	CAX-CAR-NAU	2.35	118.02	113.07
4	A	603	VRZ	CAZ-CBB-CAM	-2.28	119.94	124.37
4	B	603	VRZ	N3-C4-NBF	2.21	130.92	127.17
4	B	603	VRZ	CAZ-CBB-CAM	-2.14	120.21	124.37
4	A	603	VRZ	CAJ-CAZ-CBB	2.08	123.59	120.98

There are no chirality outliers.

There are no torsion outliers.

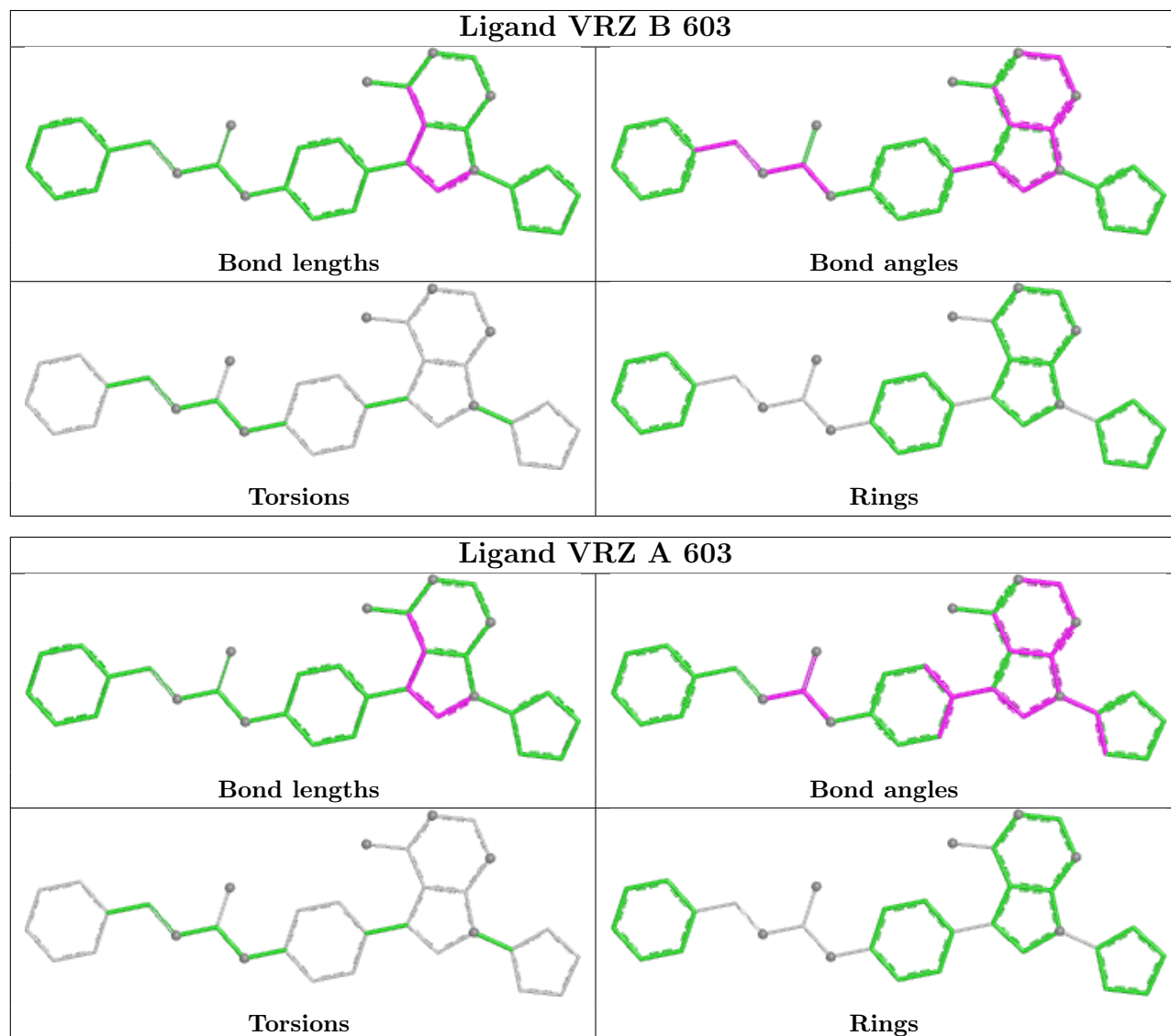
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	603	VRZ	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, 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	429/454 (94%)	0.76	47 (10%) 10 8	25, 46, 77, 92	1 (0%)
1	B	430/454 (94%)	0.50	32 (7%) 20 18	22, 42, 66, 91	1 (0%)
All	All	859/908 (94%)	0.63	79 (9%) 14 12	22, 44, 75, 92	2 (0%)

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	411	ILE	5.5
1	A	213	PHE	5.5
1	A	530	ILE	5.0
1	A	425	PRO	4.9
1	A	212	GLY	4.7
1	A	207	THR	4.7
1	B	424	PHE	4.5
1	B	410	VAL	4.4
1	B	411	ILE	3.9
1	A	304	VAL	3.7
1	B	307	PHE	3.7
1	A	410	VAL	3.7
1	A	469	PRO	3.6
1	B	529	GLU	3.6
1	A	215	ILE	3.5
1	A	436	PHE	3.4
1	B	207	THR	3.4
1	B	212	GLY	3.4
1	B	194	PRO	3.3
1	B	192	TYR	3.3
1	B	302	MET	3.3
1	A	473	ARG	3.3
1	B	530	ILE	3.3
1	A	214	TYR	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	195	ARG	3.2
1	B	196	GLN	3.2
1	A	217	PRO	3.1
1	A	466	MET	3.1
1	A	220	THR	3.1
1	B	213	PHE	3.0
1	B	300	GLY	2.9
1	A	302	MET	2.9
1	B	301	SER	2.9
1	A	305	GLU	2.8
1	B	308	LEU	2.8
1	B	305	GLU	2.7
1	A	433	ALA	2.7
1	B	195	ARG	2.7
1	A	244	VAL	2.6
1	A	531	PRO	2.6
1	A	143	SER	2.6
1	A	307	PHE	2.6
1	A	196	GLN	2.5
1	A	308	LEU	2.5
1	A	234	GLY	2.5
1	B	304	VAL	2.4
1	A	299	PRO	2.4
1	A	505	GLU	2.4
1	A	223	THR	2.4
1	A	472	ILE	2.4
1	B	220	THR	2.4
1	B	309	ALA	2.3
1	A	142	ASP	2.3
1	B	193	ASP	2.3
1	B	383	ILE	2.3
1	A	408	ALA	2.3
1	A	247	MET	2.2
1	B	306	ALA	2.2
1	A	485	GLU	2.2
1	A	303	SER	2.2
1	A	356	SER	2.2
1	A	438	SER	2.2
1	B	249	SER	2.2
1	A	409	ARG	2.1
1	A	227	LEU	2.1
1	B	198	ASP	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	221	PHE	2.1
1	A	216	SER	2.1
1	B	206	ARG	2.1
1	B	218	ARG	2.1
1	B	247	MET	2.1
1	A	437	GLY	2.1
1	B	224	LEU	2.1
1	B	475	LEU	2.1
1	B	166	PRO	2.1
1	A	478	GLY	2.1
1	A	474	ALA	2.0
1	A	439	PHE	2.0
1	A	381	ASN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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, 95th 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 ²)	Q<0.9
1	PTR	A	527	16/17	0.94	0.10	32,38,42,43	0
1	PTR	B	527	16/17	0.97	0.07	30,37,42,42	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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, 95th 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.

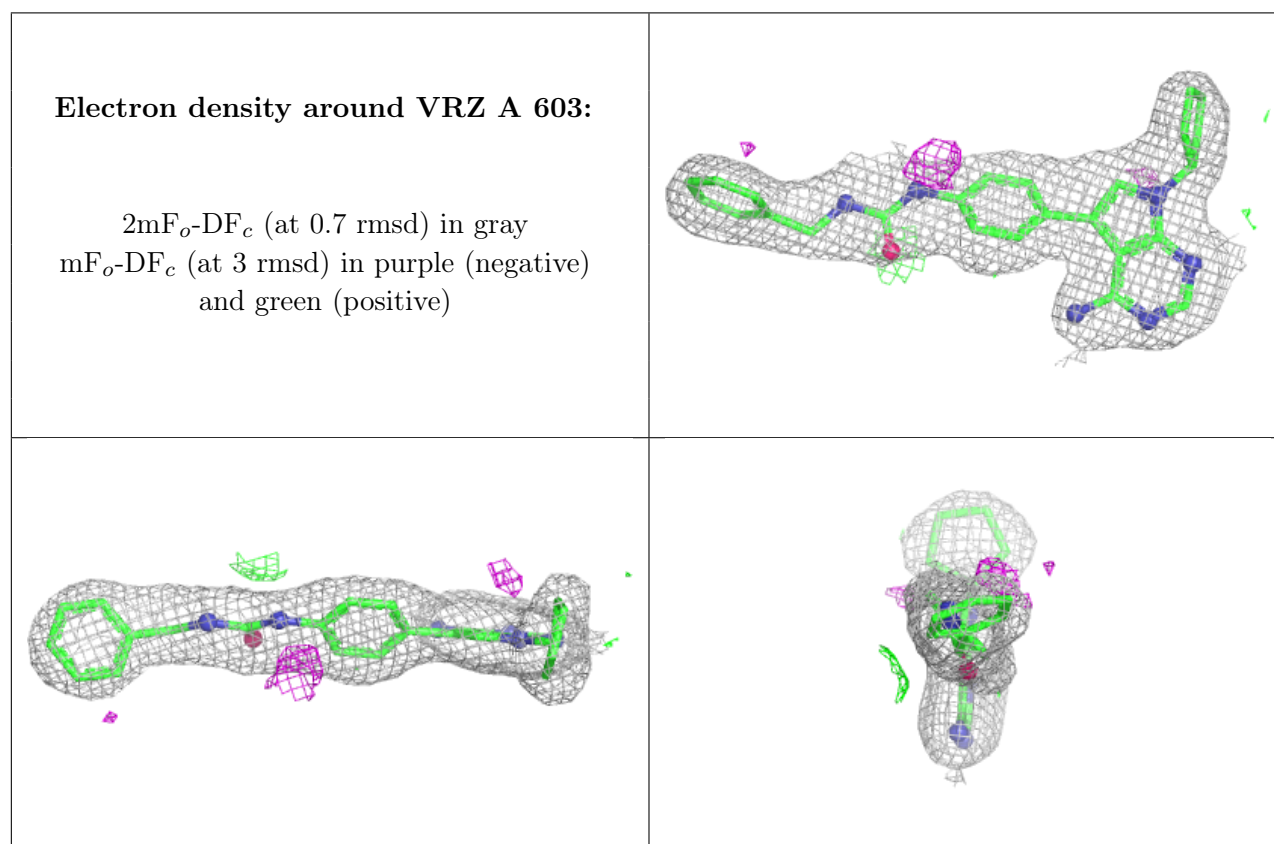
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	CL	A	602	1/1	0.87	0.18	71,71,71,71	0
2	CA	A	601	1/1	0.90	0.12	41,41,41,41	0
2	CA	B	601	1/1	0.91	0.14	45,45,45,45	0

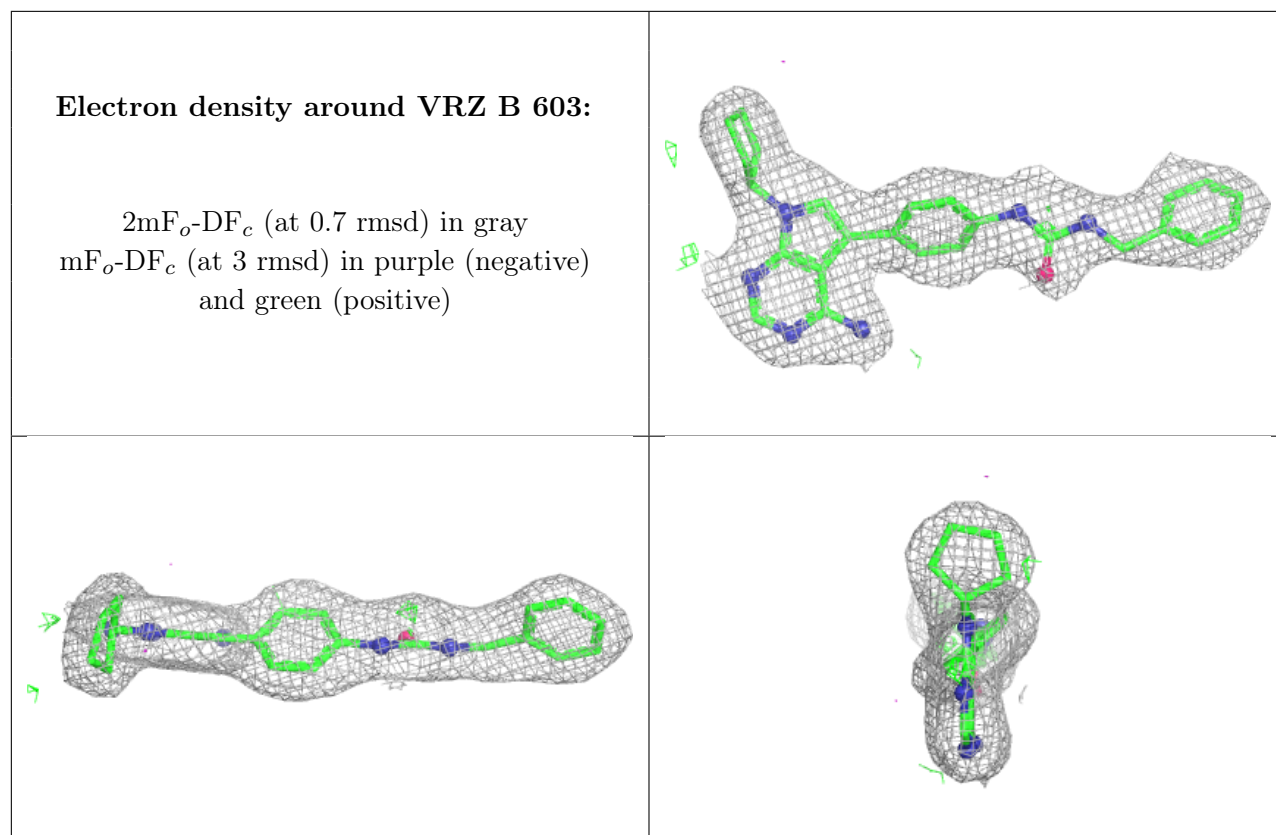
Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	CL	B	602	1/1	0.92	0.14	70,70,70,70	0
4	VRZ	A	603	32/32	0.94	0.10	24,33,56,62	0
4	VRZ	B	603	32/32	0.96	0.08	19,27,50,54	0

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.