



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2024 – 02:48 PM EST

PDB ID : 5RAO  
Title : PanDDA analysis group deposition – Crystal Structure of JMJD1B in complex with FM001084a  
Authors : Snee, M.; Nowak, R.; Johansson, C.; Burgess-Brown, N.A.; Arrowsmith, C.H.; Bountra, C.; Edwards, A.M.; Oppermann, U.  
Deposited on : 2020-03-16  
Resolution : 1.59 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)  
Xtrriage (Phenix) : 1.13  
EDS : 2.36  
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) : 2.36

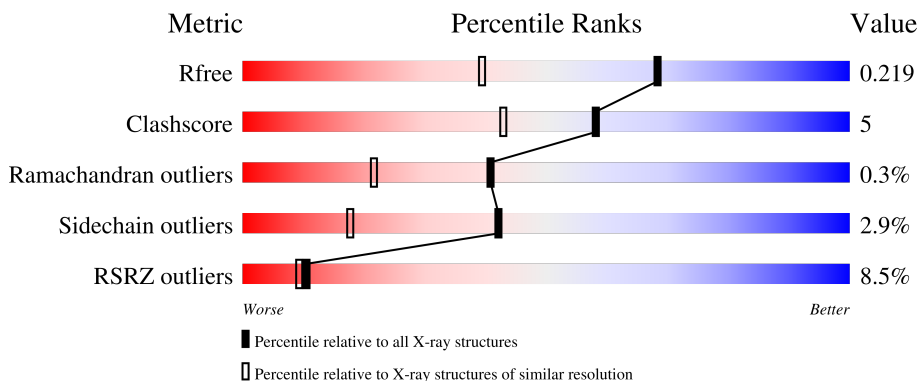
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.59 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	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

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	372	
1	B	372	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	S3S	A	1801	-	X	X	-
2	S3S	B	1801	-	X	-	-

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 6305 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 Lysine-specific demethylase 3B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	340	2768	1752	483	516	17	0	5	0
1	B	344	2798	1774	492	517	15	0	2	0

There are 50 discrepancies between the modelled and reference sequences:

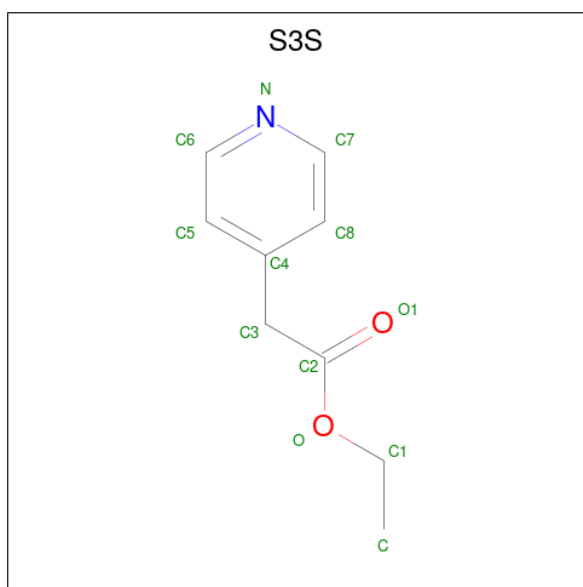
Chain	Residue	Modelled	Actual	Comment	Reference
A	1357	MET	-	initiating methionine	UNP Q7LBC6
A	1358	HIS	-	expression tag	UNP Q7LBC6
A	1359	HIS	-	expression tag	UNP Q7LBC6
A	1360	HIS	-	expression tag	UNP Q7LBC6
A	1361	HIS	-	expression tag	UNP Q7LBC6
A	1362	HIS	-	expression tag	UNP Q7LBC6
A	1363	HIS	-	expression tag	UNP Q7LBC6
A	1364	SER	-	expression tag	UNP Q7LBC6
A	1365	SER	-	expression tag	UNP Q7LBC6
A	1366	GLY	-	expression tag	UNP Q7LBC6
A	1367	VAL	-	expression tag	UNP Q7LBC6
A	1368	ASP	-	expression tag	UNP Q7LBC6
A	1369	LEU	-	expression tag	UNP Q7LBC6
A	1370	GLY	-	expression tag	UNP Q7LBC6
A	1371	THR	-	expression tag	UNP Q7LBC6
A	1372	GLU	-	expression tag	UNP Q7LBC6
A	1373	ASN	-	expression tag	UNP Q7LBC6
A	1374	LEU	-	expression tag	UNP Q7LBC6
A	1375	TYR	-	expression tag	UNP Q7LBC6
A	1376	PHE	-	expression tag	UNP Q7LBC6
A	1377	GLN	-	expression tag	UNP Q7LBC6
A	1378	SER	-	expression tag	UNP Q7LBC6
A	1379	MET	-	expression tag	UNP Q7LBC6
A	1601	GLU	GLN	conflict	UNP Q7LBC6
A	1606	HIS	GLY	conflict	UNP Q7LBC6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1357	MET	-	initiating methionine	UNP Q7LBC6
B	1358	HIS	-	expression tag	UNP Q7LBC6
B	1359	HIS	-	expression tag	UNP Q7LBC6
B	1360	HIS	-	expression tag	UNP Q7LBC6
B	1361	HIS	-	expression tag	UNP Q7LBC6
B	1362	HIS	-	expression tag	UNP Q7LBC6
B	1363	HIS	-	expression tag	UNP Q7LBC6
B	1364	SER	-	expression tag	UNP Q7LBC6
B	1365	SER	-	expression tag	UNP Q7LBC6
B	1366	GLY	-	expression tag	UNP Q7LBC6
B	1367	VAL	-	expression tag	UNP Q7LBC6
B	1368	ASP	-	expression tag	UNP Q7LBC6
B	1369	LEU	-	expression tag	UNP Q7LBC6
B	1370	GLY	-	expression tag	UNP Q7LBC6
B	1371	THR	-	expression tag	UNP Q7LBC6
B	1372	GLU	-	expression tag	UNP Q7LBC6
B	1373	ASN	-	expression tag	UNP Q7LBC6
B	1374	LEU	-	expression tag	UNP Q7LBC6
B	1375	TYR	-	expression tag	UNP Q7LBC6
B	1376	PHE	-	expression tag	UNP Q7LBC6
B	1377	GLN	-	expression tag	UNP Q7LBC6
B	1378	SER	-	expression tag	UNP Q7LBC6
B	1379	MET	-	expression tag	UNP Q7LBC6
B	1601	GLU	GLN	conflict	UNP Q7LBC6
B	1606	HIS	GLY	conflict	UNP Q7LBC6

- Molecule 2 is ethyl 2-pyridin-4-ylethanoate (three-letter code: S3S) (formula: C<sub>9</sub>H<sub>11</sub>NO<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			12	9	1	2		
2	B	1	Total	C	N	O	0	0
			12	9	1	2		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	4	Total	Cl	0	0
			4	4		
3	B	1	Total	Cl	0	0
			1	1		

- Molecule 4 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mn	0	0
			1	1		
4	B	1	Total	Mn	0	0
			1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	378	Total	O	0	0
			378	378		

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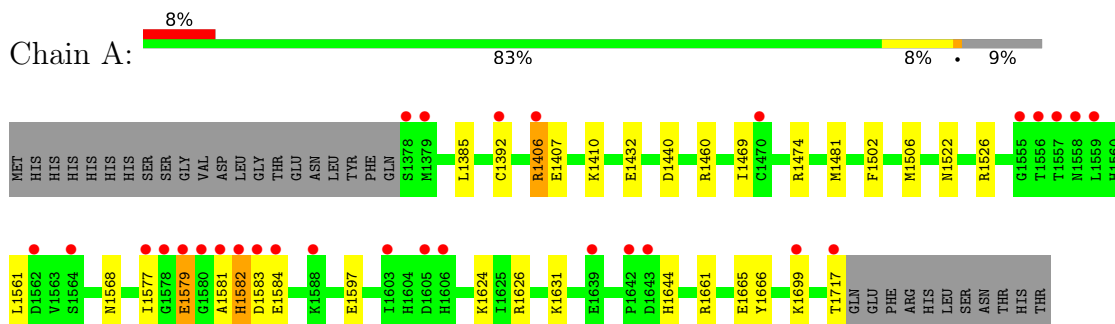
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
5	B	330	Total 330	O 330	0	0

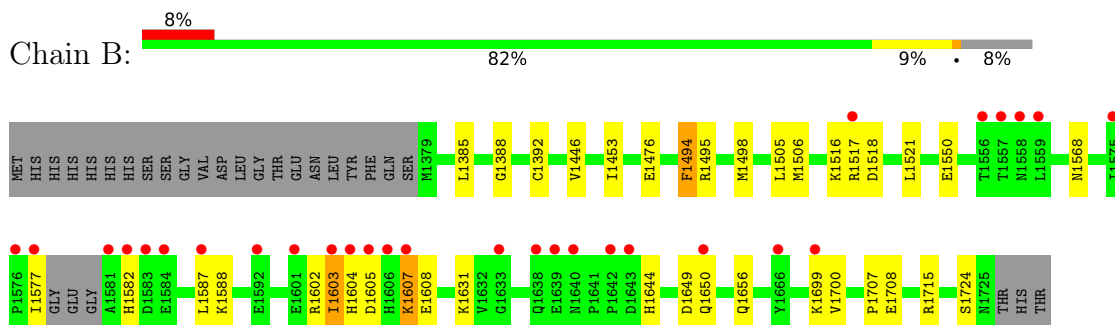
### 3 Residue-property plots [i](#)

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: Lysine-specific demethylase 3B



- Molecule 1: Lysine-specific demethylase 3B





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	57.54Å 93.61Å 93.44Å 90.00° 108.01° 90.00°	Depositor
Resolution (Å)	54.78 – 1.59 54.72 – 1.59	Depositor EDS
% Data completeness (in resolution range)	99.0 (54.78-1.59) 99.1 (54.72-1.59)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.56 (at 1.59Å)	Xtrriage
Refinement program	REFMAC 5.8.0238	Depositor
R, $R_{free}$	0.182 , 0.209 0.193 , 0.219	Depositor DCC
$R_{free}$ test set	6268 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	25.3	Xtrriage
Anisotropy	0.035	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 47.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.025 for h,-k,-h-l	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	6305	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.78% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: S3S, CL, MN

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	0.91	1/2841 (0.0%)	0.96	3/3854 (0.1%)
1	B	0.86	1/2872 (0.0%)	0.89	0/3895
All	All	0.89	2/5713 (0.0%)	0.93	3/7749 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1432	GLU	CD-OE1	6.34	1.32	1.25
1	B	1708	GLU	CD-OE2	5.05	1.31	1.25

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1460	ARG	NE-CZ-NH1	6.42	123.51	120.30
1	A	1481	MET	CG-SD-CE	-5.73	91.03	100.20
1	A	1626	ARG	NE-CZ-NH2	-5.09	117.76	120.30

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	2768	0	2650	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2798	0	2685	26	0
2	A	12	0	0	6	0
2	B	12	0	0	4	0
3	A	4	0	0	0	0
3	B	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	378	0	0	8	2
5	B	330	0	0	9	1
All	All	6305	0	5335	53	2

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 5.

All (53) 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:1568:ASN:HD21	2:B:1801:S3S:C	1.24	1.48
1:A:1568:ASN:HD21	2:A:1801:S3S:C	1.41	1.33
1:B:1568:ASN:ND2	2:B:1801:S3S:C	2.01	1.22
1:A:1624:LYS:NZ	5:A:1901:HOH:O	1.78	1.13
1:A:1568:ASN:ND2	2:A:1801:S3S:C	2.21	1.04
1:A:1407:GLU:HG2	5:A:2192:HOH:O	1.59	1.02
1:B:1517[B]:ARG:HG3	1:B:1517[B]:ARG:HH11	1.39	0.85
1:B:1516:LYS:HE3	5:B:1934:HOH:O	1.77	0.84
1:B:1715:ARG:HG3	5:B:2135:HOH:O	1.79	0.83
1:A:1582:HIS:CE1	5:A:2019:HOH:O	2.33	0.81
1:A:1406[A]:ARG:NH1	5:A:1903:HOH:O	2.14	0.79
1:A:1582:HIS:O	1:A:1582:HIS:CG	2.36	0.78
1:A:1631:LYS:HE2	1:A:1666:TYR:OH	1.84	0.78
1:B:1518:ASP:HB3	5:B:2139:HOH:O	1.86	0.75
1:B:1517[B]:ARG:HG3	1:B:1517[B]:ARG:NH1	1.95	0.75
1:B:1517[B]:ARG:HH11	1:B:1517[B]:ARG:CG	2.01	0.74
1:B:1644:HIS:NE2	1:B:1649:ASP:OD2	2.23	0.71
1:A:1385:LEU:HD12	1:A:1392[B]:CYS:SG	2.35	0.66
1:A:1407:GLU:O	1:A:1410:LYS:HG2	1.94	0.66
1:B:1385:LEU:HD12	1:B:1392:CYS:SG	2.36	0.65
1:A:1406[A]:ARG:NH2	5:A:1909:HOH:O	2.30	0.64
1:B:1446:VAL:HG22	1:B:1453:ILE:HD13	1.81	0.63
1:A:1597:GLU:OE1	5:A:1904:HOH:O	2.16	0.61
1:A:1699:LYS:HZ3	2:A:1801:S3S:C1	2.14	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1699:LYS:HD2	2:A:1801:S3S:C1	2.31	0.59
1:B:1656:GLN:OE1	5:B:1902:HOH:O	2.17	0.58
1:B:1518:ASP:OD1	5:B:1901:HOH:O	2.17	0.57
1:B:1506:MET:O	1:B:1516:LYS:HE2	2.05	0.57
1:A:1582:HIS:O	1:A:1582:HIS:ND1	2.38	0.55
1:A:1502:PHE:CE2	1:A:1506:MET:HE2	2.45	0.51
1:A:1661:ARG:HG3	1:A:1665:GLU:OE2	2.10	0.51
1:B:1494:PHE:CZ	1:B:1498:MET:HE3	2.47	0.49
1:B:1631:LYS:HG2	5:B:2147:HOH:O	2.12	0.49
1:B:1505:LEU:HD22	1:B:1700:VAL:HG11	1.94	0.49
1:B:1550:GLU:HG3	5:B:2096:HOH:O	2.13	0.48
2:B:1801:S3S:C1	2:B:1801:S3S:C8	2.93	0.47
1:A:1385:LEU:CD1	1:A:1392[B]:CYS:SG	3.04	0.44
1:B:1699:LYS:HD2	2:B:1801:S3S:C1	2.48	0.44
1:A:1583:ASP:O	1:A:1583:ASP:OD1	2.36	0.44
1:B:1388:GLY:N	5:B:1910:HOH:O	2.47	0.43
1:A:1469:ILE:HD12	1:A:1579:GLU:HB2	2.00	0.43
1:A:1699:LYS:HD2	2:A:1801:S3S:C	2.48	0.43
2:A:1801:S3S:C	2:A:1801:S3S:C5	2.97	0.42
1:B:1521:LEU:O	1:B:1707:PRO:HD3	2.20	0.42
1:B:1587:LEU:HD13	1:B:1603:ILE:HD11	2.02	0.42
1:B:1602:ARG:HH11	1:B:1608:GLU:HG2	1.83	0.42
1:A:1522:ASN:O	1:A:1526:ARG:NH1	2.53	0.41
1:B:1607:LYS:NZ	1:B:1607:LYS:HA	2.35	0.41
1:A:1440:ASP:HB2	5:A:2123:HOH:O	2.19	0.41
1:A:1474:ARG:NH2	5:A:1902:HOH:O	2.10	0.41
1:A:1561:LEU:C	1:A:1561:LEU:HD12	2.41	0.41
1:B:1476:GLU:OE2	5:B:1903:HOH:O	2.22	0.40
1:B:1494:PHE:CD1	1:B:1494:PHE:C	2.95	0.40

All (2) 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	Interatomic distance (Å)	Clash overlap (Å)
5:A:2208:HOH:O	5:A:2244:HOH:O[2_648]	1.82	0.38
5:A:2182:HOH:O	5:B:1920:HOH:O[2_557]	2.13	0.07

## 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	343/372 (92%)	335 (98%)	7 (2%)	1 (0%)	41	21
1	B	342/372 (92%)	329 (96%)	12 (4%)	1 (0%)	41	21
All	All	685/744 (92%)	664 (97%)	19 (3%)	2 (0%)	41	21

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1581	ALA
1	B	1603	ILE

### 5.3.2 Protein sidechains [i](#)

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	299/331 (90%)	291 (97%)	8 (3%)	44	20
1	B	302/331 (91%)	292 (97%)	10 (3%)	38	14
All	All	601/662 (91%)	583 (97%)	18 (3%)	42	16

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1406[A]	ARG
1	A	1406[B]	ARG
1	A	1577	ILE
1	A	1579	GLU

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Mol	Chain	Res	Type
1	A	1582	HIS
1	A	1584	GLU
1	A	1644	HIS
1	A	1717	THR
1	B	1494	PHE
1	B	1495	ARG
1	B	1577	ILE
1	B	1582	HIS
1	B	1588	LYS
1	B	1604	HIS
1	B	1605	ASP
1	B	1607	LYS
1	B	1650	GLN
1	B	1724	SER

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	1568	ASN
1	A	1640	ASN
1	A	1650	GLN
1	B	1568	ASN
1	B	1656	GLN

### 5.3.3 RNA [i](#)

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 monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 7 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
2	S3S	B	1801	4	12,12,12	4.62	7 (58%)	14,14,14	3.52	8 (57%)
2	S3S	A	1801	4	12,12,12	4.10	5 (41%)	14,14,14	2.90	7 (50%)

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
2	S3S	B	1801	4	-	2/7/7/7	0/1/1/1
2	S3S	A	1801	4	-	2/7/7/7	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1801	S3S	C3-C4	-10.15	1.35	1.51
2	A	1801	S3S	C3-C4	-9.92	1.35	1.51
2	B	1801	S3S	C3-C2	-9.91	1.32	1.51
2	A	1801	S3S	C3-C2	-8.46	1.35	1.51
2	B	1801	S3S	C8-C7	-3.80	1.30	1.38
2	B	1801	S3S	O-C1	-3.60	1.35	1.46
2	B	1801	S3S	C5-C4	-3.44	1.31	1.38
2	A	1801	S3S	C5-C6	-3.21	1.32	1.38
2	A	1801	S3S	O-C1	-3.15	1.36	1.46
2	A	1801	S3S	C8-C4	-2.22	1.34	1.38
2	B	1801	S3S	C8-C4	-2.10	1.34	1.38
2	B	1801	S3S	C7-N	-2.04	1.27	1.33

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1801	S3S	C1-O-C2	6.60	135.91	116.73
2	B	1801	S3S	C3-C4-C8	-6.02	112.27	120.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1801	S3S	C8-C4-C5	5.29	126.48	118.17
2	A	1801	S3S	C3-C4-C5	-5.14	113.54	120.89
2	B	1801	S3S	C8-C4-C5	4.99	126.00	118.17
2	A	1801	S3S	C3-C4-C8	-4.59	114.32	120.89
2	B	1801	S3S	C6-C5-C4	-4.45	113.33	119.63
2	B	1801	S3S	C3-C4-C5	-4.44	114.54	120.89
2	A	1801	S3S	C6-C5-C4	-3.65	114.45	119.63
2	A	1801	S3S	C7-C8-C4	-3.53	114.62	119.63
2	B	1801	S3S	C7-C8-C4	-3.41	114.80	119.63
2	B	1801	S3S	O-C1-C	-3.07	97.12	108.42
2	A	1801	S3S	C1-O-C2	2.53	124.08	116.73
2	A	1801	S3S	O-C1-C	-2.16	100.48	108.42
2	B	1801	S3S	O-C2-C3	2.11	114.65	111.07

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1801	S3S	C3-C2-O-C1
2	A	1801	S3S	O1-C2-O-C1
2	B	1801	S3S	C3-C2-O-C1
2	B	1801	S3S	O1-C2-O-C1

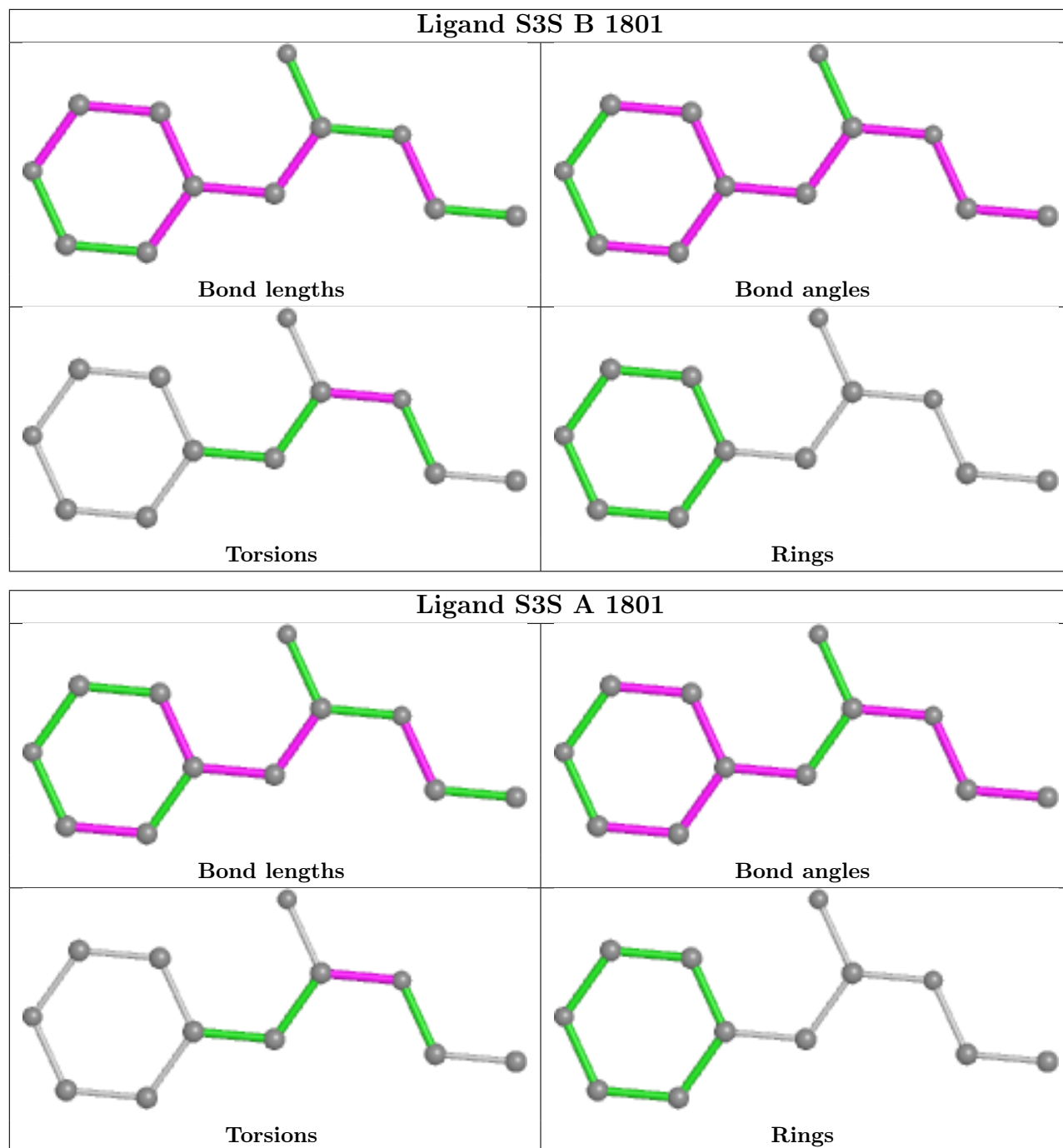
There are no ring outliers.

2 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1801	S3S	4	0
2	A	1801	S3S	6	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	340/372 (91%)	0.56	29 (8%)	10   9	16, 27, 61, 105	20 (5%)
1	B	344/372 (92%)	0.43	29 (8%)	11   9	18, 31, 62, 143	9 (2%)
All	All	684/744 (91%)	0.50	58 (8%)	10   9	16, 29, 62, 143	29 (4%)

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1577	ILE	25.7
1	A	1578	GLY	15.1
1	A	1580	GLY	15.1
1	B	1581	ALA	14.6
1	A	1392[A]	CYS	11.9
1	B	1605	ASP	10.6
1	B	1577	ILE	10.1
1	A	1581	ALA	10.1
1	B	1517[A]	ARG	9.9
1	A	1406[A]	ARG	8.9
1	A	1559	LEU	8.2
1	A	1582	HIS	7.1
1	A	1579	GLU	7.1
1	A	1564[A]	SER	7.0
1	A	1557	THR	6.8
1	B	1603	ILE	6.7
1	A	1556	THR	6.5
1	B	1582	HIS	6.2
1	B	1587	LEU	6.2
1	B	1604	HIS	6.0
1	A	1379[A]	MET	5.9
1	B	1606	HIS	5.7
1	A	1378	SER	4.9
1	A	1699	LYS	4.8

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Mol	Chain	Res	Type	RSRZ
1	A	1555	GLY	4.6
1	B	1601	GLU	4.4
1	B	1559	LEU	4.4
1	B	1557	THR	4.3
1	A	1558	ASN	4.2
1	A	1562	ASP	4.2
1	B	1556	THR	4.1
1	B	1575	ILE	4.0
1	A	1642	PRO	3.9
1	B	1583	ASP	3.9
1	A	1606	HIS	3.6
1	A	1588[A]	LYS	3.5
1	B	1576	PRO	3.5
1	B	1607	LYS	3.3
1	A	1639	GLU	3.2
1	A	1717	THR	3.0
1	A	1603	ILE	3.0
1	B	1558	ASN	2.8
1	A	1605	ASP	2.7
1	B	1640	ASN	2.7
1	B	1642	PRO	2.6
1	B	1638	GLN	2.6
1	A	1583	ASP	2.6
1	B	1666	TYR	2.5
1	A	1470	CYS	2.4
1	A	1584	GLU	2.4
1	B	1592	GLU	2.3
1	B	1584	GLU	2.3
1	B	1699	LYS	2.2
1	B	1633	GLY	2.2
1	B	1643	ASP	2.2
1	A	1643	ASP	2.1
1	B	1650	GLN	2.1
1	B	1639	GLU	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](#)

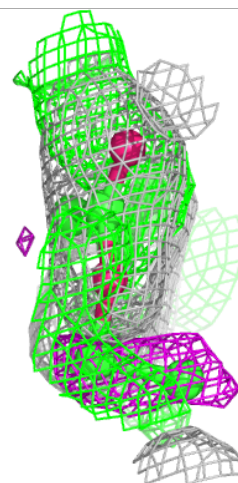
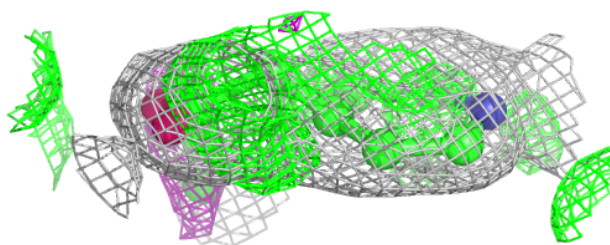
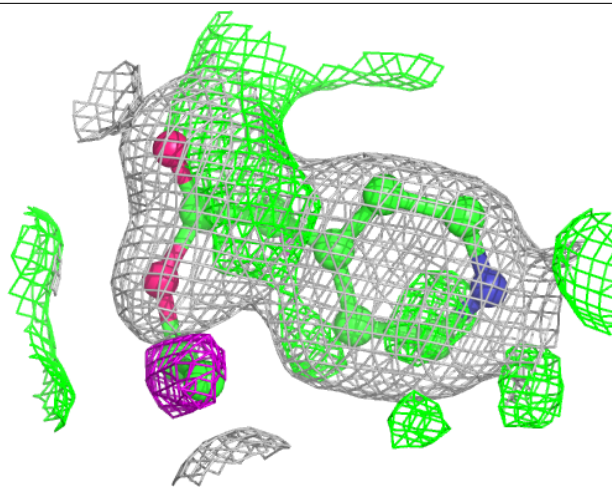
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

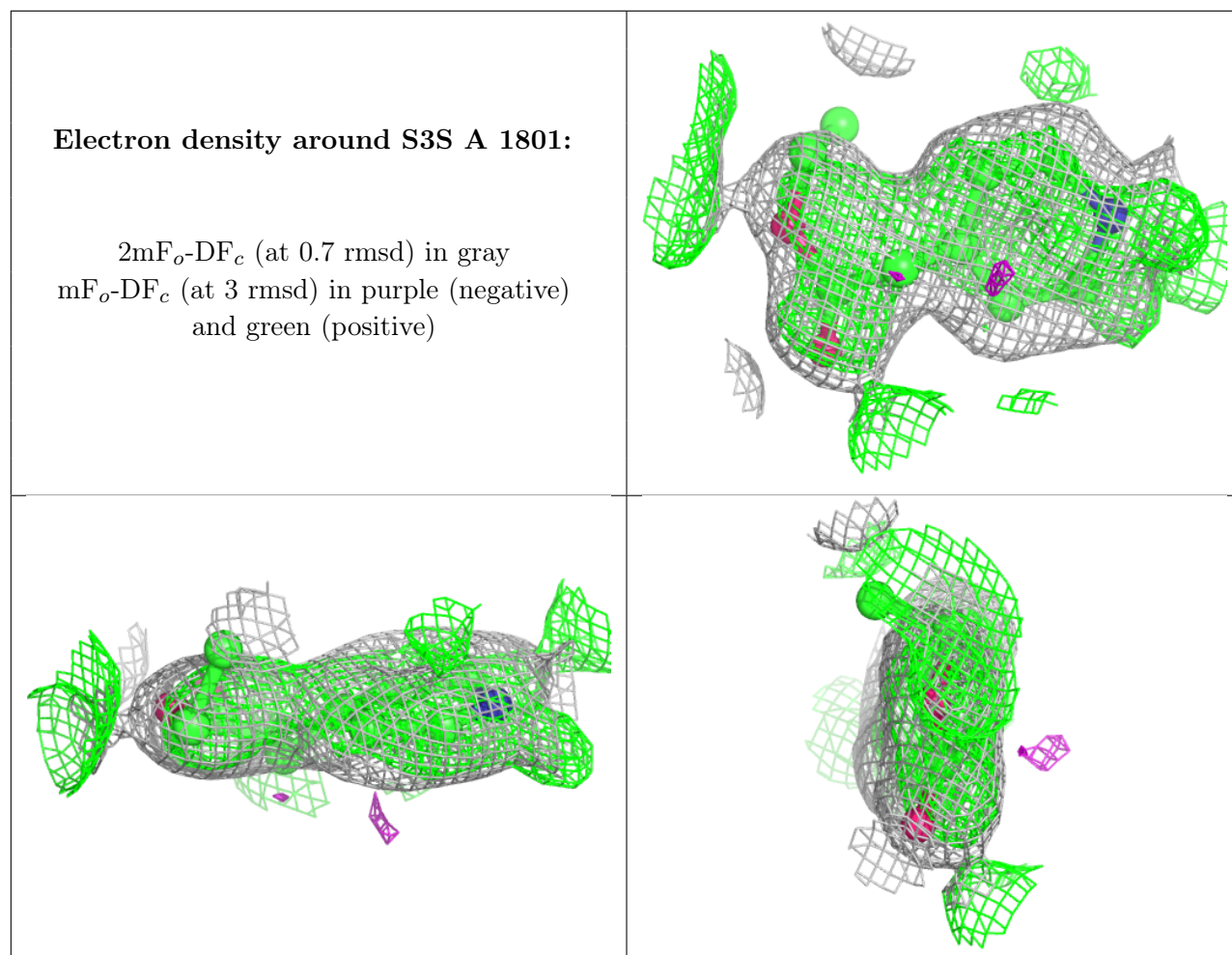
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	S3S	B	1801	12/12	0.85	0.26	21,25,37,37	12
2	S3S	A	1801	12/12	0.87	0.36	15,19,34,35	12
3	CL	A	1805	1/1	0.94	0.10	49,49,49,49	0
3	CL	B	1802	1/1	0.98	0.06	40,40,40,40	0
3	CL	A	1803	1/1	0.99	0.06	38,38,38,38	0
3	CL	A	1804	1/1	0.99	0.05	34,34,34,34	0
4	MN	B	1803	1/1	0.99	0.09	23,23,23,23	0
4	MN	A	1806	1/1	1.00	0.10	21,21,21,21	0
3	CL	A	1802	1/1	1.00	0.11	24,24,24,24	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.

**Electron density around S3S B 1801:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.