

wwPDB X-ray Structure Validation Summary Report (i)

Apr 8, 2024 – 12:21 PM EDT

PDB ID	:	8SBH
Title	:	YeiE effector binding domain from E. coli
Authors	:	Momany, C.; Nune, M.; Brondani, J.C.; Afful, D.; Neidle, E.
Deposited on		
Resolution	:	1.93 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) 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 (1)) were used in the production of this report:

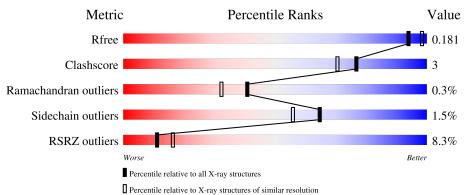
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 1.93 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	$\begin{array}{c} \textbf{Whole archive} \\ (\#\textbf{Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	130704	4310 (1.96-1.92)
Clashscore	141614	1023 (1.94-1.94)
Ramachandran outliers	138981	1007 (1.94-1.94)
Sidechain outliers	138945	1007 (1.94-1.94)
RSRZ outliers	127900	4250 (1.96-1.92)

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 <=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	А	209	89%	6%	5%
1	В	209	86%	10%	5%



8SBH

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 6986 atoms, of which 3331 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.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace		
1	1 Δ	199	Total	С	Η	Ν	0	S	0	5	0
	A	199	3249	1027	1633	288	289	12	0		
1	р	199	Total	С	Η	Ν	0	S	0	2	0
	D	199	3210	1017	1612	284	287	10			

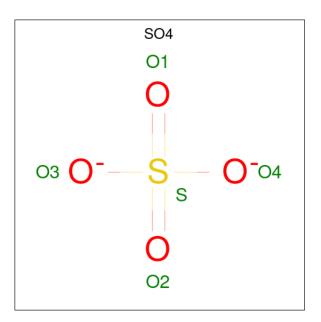
• Molecule 1 is a protein called Transcriptional regulator YeiE, LysR family.

Chain	Residue	Modelled	Actual	Comment	Reference
А	90	MET	-	initiating methionine	UNP P0ACR4
А	294	HIS	-	expression tag	UNP P0ACR4
А	295	HIS	-	expression tag	UNP P0ACR4
А	296	HIS	-	expression tag	UNP P0ACR4
А	297	HIS	-	expression tag	UNP P0ACR4
А	298	HIS	-	expression tag	UNP P0ACR4
В	90	MET	-	initiating methionine	UNP P0ACR4
В	294	HIS	-	expression tag	UNP P0ACR4
В	295	HIS	-	expression tag	UNP P0ACR4
В	296	HIS	-	expression tag	UNP P0ACR4
В	297	HIS	-	expression tag	UNP P0ACR4
В	298	HIS	-	expression tag	UNP P0ACR4

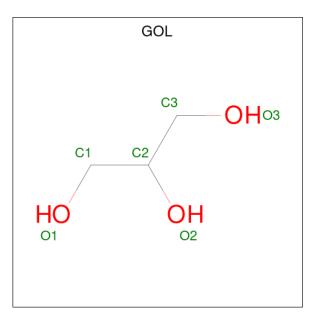
There are 12 discrepancies between the modelled and reference sequences:

• Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	В	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	В	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	А	1	Total	C 6	H 15	0 6	0	1
			1	0	10	0		



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	1	Total C H O 14 3 8 3	0	0
3	А	1	Total C H O 14 3 8 3	0	0
3	А	1	Total C H O 14 3 8 3	0	0
3	А	1	Total C H O 14 3 8 3	0	0
3	А	1	Total C H O 14 3 8 3	0	0
3	А	1	Total C H O 13 3 7 3	0	0
3	А	1	Total C H O 14 3 8 3	0	0
3	А	1	Total C H O 14 3 8 3	0	0
3	В	1	Total C H O 14 3 8 3	0	0

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• Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	В	1	Total Cl 1 1	0	0

• Molecule 5 is water.

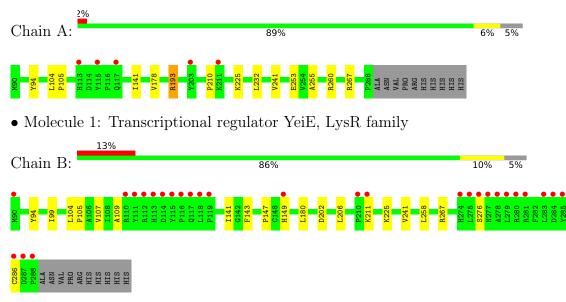
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	177	Total O 184 184	0	7
5	В	172	Total O 175 175	0	3



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: Transcriptional regulator YeiE, LysR family





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants	71.10Å 71.10Å 196.34Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	31.80 - 1.93	Depositor
Resolution (A)	31.80 - 1.93	EDS
% Data completeness	99.5 (31.80-1.93)	Depositor
(in resolution range)	94.9 (31.80-1.93)	EDS
R _{merge}	0.07	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.52 (at 1.94 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
D D.	0.166 , 0.181	Depositor
R, R_{free}	0.167 , 0.181	DCC
R_{free} test set	1119 reflections (2.89%)	wwPDB-VP
Wilson B-factor $(Å^2)$	21.6	Xtriage
Anisotropy	0.404	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.44 , 62.0	EDS
L-test for twinning ²	$ < L >=0.48, < L^2>=0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6986	wwPDB-VP
Average B, all atoms $(Å^2)$	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.97% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

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: GOL, CME, SO4, 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	А	0.27	0/1647	0.53	0/2236	
1	В	0.27	0/1627	0.53	0/2210	
All	All	0.27	0/3274	0.53	0/4446	

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 (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	А	1616	1633	1620	10	0
1	В	1598	1612	1611	11	0
2	А	5	0	0	0	0
2	В	10	0	0	0	0
3	А	60	78	80	0	0
3	В	6	8	8	0	0
4	В	1	0	0	0	0
5	А	184	0	0	2	0
5	В	175	0	0	0	0
All	All	3655	3331	3319	20	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 3.

The worst 5 of 20 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:180:LEU:HD21	1:B:258:LEU:HD21	1.73	0.70	
1:B:141:ILE:HD11	1:B:267:ARG:HD2	1.81	0.63	
1:A:178:VAL:HG22	1:A:255:ALA:O	2.05	0.56	
1:A:225:LYS:HD3	1:A:241:VAL:HG12	1.86	0.56	
1:B:147:PRO:O	1:B:149:HIS:CD2	2.63	0.51	

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	А	199/209~(95%)	193~(97%)	5(2%)	1 (0%)	29 17	
1	В	198/209~(95%)	194 (98%)	4(2%)	0	100 100	
All	All	397/418~(95%)	387~(98%)	9~(2%)	1 (0%)	41 32	

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	210	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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	А	175/180~(97%)	173~(99%)	2(1%)	73 67		
1	В	173/180~(96%)	170 (98%)	3(2%)	60 49		
All	All	348/360~(97%)	343~(99%)	5 (1%)	65 58		

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	94	TYR
1	А	193	ARG
1	В	94	TYR
1	В	211	LYS
1	В	276	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

3 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).

Mal	Mol Type	Chain	Res	Link	Bond lengths			Bond angles		
	туре	Unam	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	CME	А	148[B]	-	8,9,10	1.19	0	5,9,11	0.82	0
1	CME	А	148[A]	-	8,9,10	1.08	0	5,9,11	0.80	0
1	CME	В	148	1	8,9,10	0.95	0	5, 9, 11	0.53	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	CME	А	148[B]	-	-	3/5/8/10	-
1	CME	А	148[A]	-	-	1/5/8/10	-
1	CME	В	148	1	-	2/5/8/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	А	148[A]	CME	SD-CE-CZ-OH
1	А	148[B]	CME	SD-CE-CZ-OH
1	В	148	CME	N-CA-CB-SG
1	А	148[B]	CME	CE-SD-SG-CB
1	А	148[B]	CME	CA-CB-SG-SD

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 15 ligands modelled in this entry, 1 is monoatomic - leaving 14 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).

Mal	Mol Type Chain Res		Link	Bond lengths			Bond angles			
10101	туре	Chain	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GOL	А	302[B]	-	$5,\!5,\!5$	0.87	0	$5,\!5,\!5$	1.02	0
3	GOL	А	306	-	$5,\!5,\!5$	0.84	0	$5,\!5,\!5$	1.02	0
3	GOL	В	303	-	$5,\!5,\!5$	0.87	0	$5,\!5,\!5$	1.04	0
3	GOL	А	310	-	$5,\!5,\!5$	0.88	0	$5,\!5,\!5$	0.99	0



Mol	Turne	Chain	Res	Link	В	ond leng	gths	B	ond ang	gles
IVIOI	Type	Unam	nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
2	SO4	А	301	-	$4,\!4,\!4$	0.16	0	$6,\!6,\!6$	0.06	0
2	SO4	В	301	-	$4,\!4,\!4$	0.17	0	$6,\!6,\!6$	0.07	0
3	GOL	А	307	-	$5,\!5,\!5$	0.85	0	$5,\!5,\!5$	1.00	0
3	GOL	А	303	-	$5,\!5,\!5$	0.84	0	$5,\!5,\!5$	0.91	0
3	GOL	А	304	-	$5,\!5,\!5$	0.85	0	$5,\!5,\!5$	1.02	0
3	GOL	А	309	-	$5,\!5,\!5$	0.84	0	$5,\!5,\!5$	0.93	0
3	GOL	А	305	-	$5,\!5,\!5$	0.92	0	$5,\!5,\!5$	1.03	0
2	SO4	В	302	-	$4,\!4,\!4$	0.14	0	$6,\!6,\!6$	0.05	0
3	GOL	А	302[A]	-	$5,\!5,\!5$	0.82	0	$5,\!5,\!5$	1.03	0
3	GOL	А	308	-	$5,\!5,\!5$	0.79	0	$5,\!5,\!5$	1.10	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
3	GOL	А	302[B]	-	-	2/4/4/4	-
3	GOL	А	306	-	-	0/4/4/4	-
3	GOL	В	303	-	-	3/4/4/4	-
3	GOL	А	310	-	-	2/4/4/4	-
3	GOL	А	307	-	-	2/4/4/4	-
3	GOL	А	309	-	-	0/4/4/4	-
3	GOL	А	303	-	-	2/4/4/4	-
3	GOL	А	304	-	-	2/4/4/4	-
3	GOL	А	305	-	-	2/4/4/4	-
3	GOL	А	302[A]	-	-	2/4/4/4	-
3	GOL	А	308	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

 $5~{\rm of}~19$ torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	А	302[A]	GOL	O1-C1-C2-C3
3	А	302[B]	GOL	O1-C1-C2-C3
3	А	303	GOL	O1-C1-C2-C3
3	А	304	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
3	А	305	GOL	C1-C2-C3-O3

There are no ring outliers.

No monomer is involved in short contacts.

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 (i)

6.1 Protein, DNA and RNA chains (i)

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^{th} 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	$\langle RSRZ \rangle$	#RSRZ>2	$OWAB(Å^2)$	Q<0.9
1	А	198/209~(94%)	-0.01	5 (2%) 57 64	14, 26, 54, 72	0
1	В	198/209~(94%)	0.50	28 (14%) 2 4	14, 26, 87, 109	0
All	All	396/418~(94%)	0.25	33 (8%) 11 16	14, 26, 75, 109	0

The worst 5 of 33 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	118	LEU	7.1
1	В	117	GLN	6.1
1	В	275	LEU	5.1
1	В	210	PRO	5.1
1	В	285	TYR	4.8

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, 95^{th} 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	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q<0.9
1	CME	А	148[A]	10/11	0.84	0.20	$35,\!45,\!58,\!58$	15
1	CME	А	148[B]	10/11	0.84	0.20	35,45,58,58	15
1	CME	В	148	10/11	0.85	0.21	37,57,87,95	0

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^{th} 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	$\operatorname{B-factors}(\operatorname{\AA}^2)$	Q<0.9
3	GOL	В	303	6/6	0.80	0.25	47,63,76,76	0
3	GOL	А	307	6/6	0.81	0.47	51,68,81,81	0
3	GOL	А	309	6/6	0.82	0.25	40,48,56,68	0
3	GOL	А	304	6/6	0.84	0.28	41,49,66,66	0
3	GOL	А	308	6/6	0.85	0.19	$30,\!37,\!56,\!56$	0
3	GOL	А	310	6/6	0.87	0.27	$28,\!60,\!72,\!77$	0
3	GOL	А	302[A]	6/6	0.88	0.24	$23,\!28,\!35,\!35$	13
3	GOL	А	302[B]	6/6	0.88	0.24	$24,\!31,\!36,\!38$	14
3	GOL	А	305	6/6	0.92	0.15	40,49,59,63	0
3	GOL	А	303	6/6	0.95	0.15	$32,\!41,\!52,\!62$	0
3	GOL	А	306	6/6	0.96	0.11	$29,\!39,\!45,\!52$	0
2	SO4	В	302	5/5	0.99	0.10	$20,\!24,\!31,\!32$	0
2	SO4	А	301	5/5	0.99	0.09	19,20,21,24	0
2	SO4	В	301	5/5	0.99	0.08	26,29,31,34	0
4	CL	В	304	1/1	0.99	0.08	$25,\!25,\!25,\!25$	0

6.5 Other polymers (i)

There are no such residues in this entry.

