



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 12:34 AM GMT

PDB ID : 2AX1
Title : Hepatitis C Virus NS5b RNA Polymerase in complex with a covalent inhibitor (5ee)
Authors : Powers, J.P.; Piper, D.E.; Li, Y.; Mayorga, V.; Anzola, J.; Chen, J.M.; Jaen, J.C.; Lee, G.; Liu, J.; Peterson, M.G.; Tonn, G.R.; Ye, Q.; Walker, N.P.; Wang, Z.
Deposited on : 2005-09-02
Resolution : 2.10 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

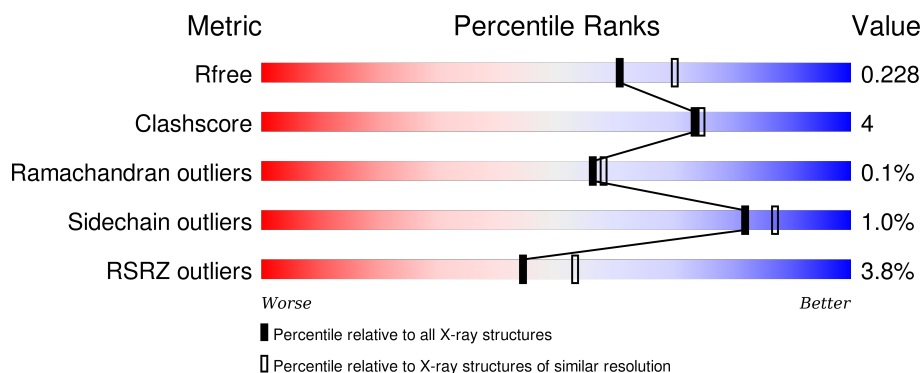
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	580	<div> <div>3%</div> <div>84%</div> <div>11%</div> <div>.</div> </div>
1	B	580	<div> <div>4%</div> <div>87%</div> <div>10%</div> <div>.</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9587 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 Genome polyprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	554	Total	C	N	O	S	0	0	0
			4315	2722	764	798	31			
1	B	561	Total	C	N	O	S	0	0	0
			4359	2749	771	808	31			

There are 42 discrepancies between the modelled and reference sequences:

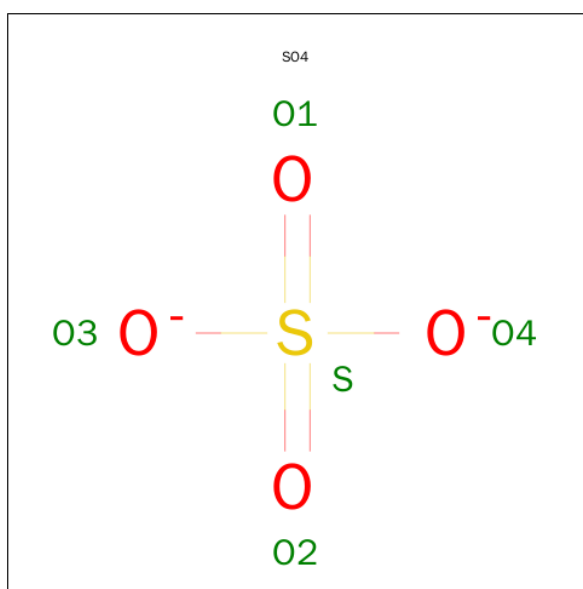
Chain	Residue	Modelled	Actual	Comment	Reference
A	499	ALA	VAL	ENGINEERED	UNP P26663
A	506	ASN	SER	ENGINEERED	UNP P26663
A	514	ARG	GLN	ENGINEERED	UNP P26663
A	520	ILE	THR	ENGINEERED	UNP P26663
A	540	ALA	PRO	ENGINEERED	UNP P26663
A	543	GLY	SER	ENGINEERED	UNP P26663
A	549	SER	GLY	ENGINEERED	UNP P26663
A	552	THR	VAL	ENGINEERED	UNP P26663
A	563	GLY	SER	ENGINEERED	UNP P26663
A	564	VAL	LEU	ENGINEERED	UNP P26663
A	566	HIS	ARG	ENGINEERED	UNP P26663
A	571	HIS	-	EXPRESSION TAG	UNP P26663
A	572	HIS	-	EXPRESSION TAG	UNP P26663
A	573	HIS	-	EXPRESSION TAG	UNP P26663
A	574	HIS	-	EXPRESSION TAG	UNP P26663
A	575	HIS	-	EXPRESSION TAG	UNP P26663
A	576	HIS	-	EXPRESSION TAG	UNP P26663
A	577	HIS	-	EXPRESSION TAG	UNP P26663
A	578	HIS	-	EXPRESSION TAG	UNP P26663
A	579	HIS	-	EXPRESSION TAG	UNP P26663
A	580	HIS	-	EXPRESSION TAG	UNP P26663
B	499	ALA	VAL	ENGINEERED	UNP P26663
B	506	ASN	SER	ENGINEERED	UNP P26663
B	514	ARG	GLN	ENGINEERED	UNP P26663
B	520	ILE	THR	ENGINEERED	UNP P26663

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Chain	Residue	Modelled	Actual	Comment	Reference
B	540	ALA	PRO	ENGINEERED	UNP P26663
B	543	GLY	SER	ENGINEERED	UNP P26663
B	549	SER	GLY	ENGINEERED	UNP P26663
B	552	THR	VAL	ENGINEERED	UNP P26663
B	563	GLY	SER	ENGINEERED	UNP P26663
B	564	VAL	LEU	ENGINEERED	UNP P26663
B	566	HIS	ARG	ENGINEERED	UNP P26663
B	571	HIS	-	EXPRESSION TAG	UNP P26663
B	572	HIS	-	EXPRESSION TAG	UNP P26663
B	573	HIS	-	EXPRESSION TAG	UNP P26663
B	574	HIS	-	EXPRESSION TAG	UNP P26663
B	575	HIS	-	EXPRESSION TAG	UNP P26663
B	576	HIS	-	EXPRESSION TAG	UNP P26663
B	577	HIS	-	EXPRESSION TAG	UNP P26663
B	578	HIS	-	EXPRESSION TAG	UNP P26663
B	579	HIS	-	EXPRESSION TAG	UNP P26663
B	580	HIS	-	EXPRESSION TAG	UNP P26663

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



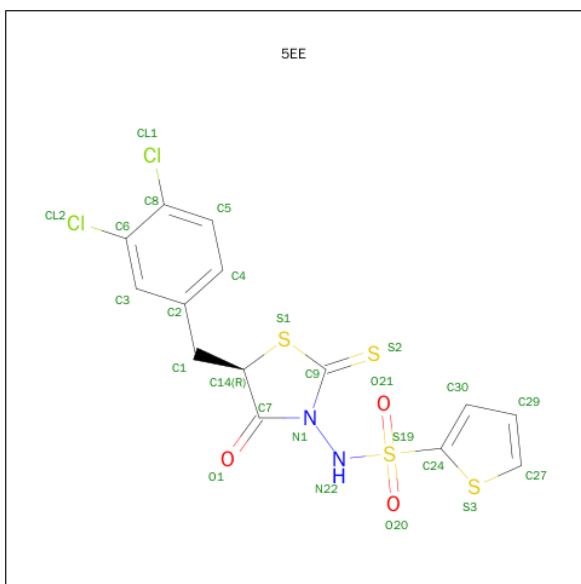
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is 5R-(3,4-DICHLOROPHENYLMETHYL)-3-(2-THIOPHENESULFO NYLAMINO)-4-OXO-2-THIONOTHIAZOLIDINE (three-letter code: 5EE) (formula: C₁₄H₁₀Cl₂N₂O₃S₄).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	S	0	0
			25	14	2	2	3	4		
3	B	1	Total	C	Cl	N	O	S	0	0
			25	14	2	2	3	4		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	397	Total	O	0	0
			397	397		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	426	Total 426	O 426	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	87.01Å 86.77Å 162.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.10 29.72 – 2.10	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-2.10) 92.9 (29.72-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.80 (at 2.10Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.202 , 0.229 0.201 , 0.228	Depositor DCC
R_{free} test set	6784 reflections (10.06%)	DCC
Wilson B-factor (Å ²)	30.6	Xtriage
Anisotropy	0.298	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 49.7	EDS
Estimated twinning fraction	0.014 for k,h,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 67443 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9587	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.12% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: 5EE, SO4

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	0.33	0/4409	0.57	0/5980
1	B	0.33	0/4453	0.56	0/6040
All	All	0.33	0/8862	0.57	0/12020

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	A	4315	0	4335	40	0
1	B	4359	0	4379	32	0
2	A	20	0	0	0	0
2	B	20	0	0	0	0
3	A	25	0	9	0	0
3	B	25	0	9	0	0
4	A	397	0	0	3	0
4	B	426	0	0	0	0
All	All	9587	0	8732	71	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.

The worst 5 of 71 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:200:ARG:HD3	1:A:384:LEU:HD11	1.66	0.77
1:B:461:GLN:HG2	1:B:541:ALA:HB3	1.69	0.74
1:A:445:CYS:SG	1:A:454:ILE:HD12	2.28	0.73
1:B:82:LEU:HD13	1:B:249:ALA:HB2	1.74	0.70
1:B:280:ARG:HD2	1:B:291:ASN:OD1	1.93	0.69

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	550/580 (95%)	538 (98%)	12 (2%)	0	100	100
1	B	557/580 (96%)	546 (98%)	10 (2%)	1 (0%)	52	53
All	All	1107/1160 (95%)	1084 (98%)	22 (2%)	1 (0%)	56	58

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	151	LYS

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	471/492 (96%)	467 (99%)	4 (1%)	86	91
1	B	475/492 (96%)	470 (99%)	5 (1%)	80	85
All	All	946/984 (96%)	937 (99%)	9 (1%)	82	87

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	150	GLU
1	B	461	GLN
1	B	366	CYS
1	A	184	GLN
1	B	184	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	506	ASN
1	B	35	ASN
1	B	330	GLN
1	A	475	HIS
1	B	273	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

10 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	5EE	A	1001	1	23,27,27	1.54	3 (13%)	26,40,40	1.61	4 (15%)
2	SO4	A	1101	-	4,4,4	1.11	0	6,6,6	0.10	0
2	SO4	A	1102	-	4,4,4	1.21	0	6,6,6	0.10	0
2	SO4	A	1103	-	4,4,4	1.13	0	6,6,6	0.05	0
2	SO4	A	1108	-	4,4,4	1.19	0	6,6,6	0.09	0
3	5EE	B	1002	1	23,27,27	1.61	3 (13%)	26,40,40	1.27	3 (11%)
2	SO4	B	1104	-	4,4,4	1.15	0	6,6,6	0.13	0
2	SO4	B	1105	-	4,4,4	1.23	0	6,6,6	0.07	0
2	SO4	B	1106	-	4,4,4	1.25	0	6,6,6	0.07	0
2	SO4	B	1107	-	4,4,4	1.22	0	6,6,6	0.07	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	5EE	A	1001	1	-	0/7/31/31	0/3/3/3
2	SO4	A	1101	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1102	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1103	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1108	-	-	0/0/0/0	0/0/0/0
3	5EE	B	1002	1	-	0/7/31/31	0/3/3/3
2	SO4	B	1104	-	-	0/0/0/0	0/0/0/0
2	SO4	B	1105	-	-	0/0/0/0	0/0/0/0
2	SO4	B	1106	-	-	0/0/0/0	0/0/0/0
2	SO4	B	1107	-	-	0/0/0/0	0/0/0/0

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1001	5EE	C24-S19	-3.76	1.70	1.76
3	B	1002	5EE	C24-S19	-3.62	1.70	1.76
3	B	1002	5EE	C8-C6	2.65	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1001	5EE	C8-C6	2.83	1.46	1.39
3	A	1001	5EE	S19-N22	4.36	1.74	1.65

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1001	5EE	C7-C14-S1	-5.77	100.55	105.99
3	B	1002	5EE	C7-C14-S1	-3.81	102.40	105.99
3	A	1001	5EE	O1-C7-N1	-2.67	121.45	124.33
3	B	1002	5EE	O1-C7-N1	-2.53	121.60	124.33
3	A	1001	5EE	C1-C14-S1	-2.29	110.60	113.00

There are no chirality outliers.

There are no torsion outliers.

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, 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	554/580 (95%)	0.16	20 (3%)	46 55	19, 29, 43, 51	0
1	B	561/580 (96%)	0.12	22 (3%)	43 52	16, 28, 44, 55	0
All	All	1115/1160 (96%)	0.14	42 (3%)	44 53	16, 29, 44, 55	0

The worst 5 of 42 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	402	HIS	6.2
1	A	402	HIS	6.1
1	B	149	PRO	5.8
1	B	150	GLU	5.1
1	B	152	GLY	4.4

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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
3	5EE	A	1001	25/25	0.87	0.15	1.96	43,45,49,49	0
2	SO4	A	1102	5/5	0.92	0.15	0.93	58,58,58,58	0
3	5EE	B	1002	25/25	0.87	0.14	0.62	41,45,47,48	0
2	SO4	A	1103	5/5	0.96	0.20	0.09	55,55,56,56	0
2	SO4	B	1106	5/5	0.89	0.20	-0.15	82,82,82,82	0
2	SO4	B	1104	5/5	0.98	0.08	-0.91	40,40,40,40	0
2	SO4	A	1101	5/5	0.98	0.08	-0.98	50,51,51,51	0
2	SO4	B	1105	5/5	0.99	0.08	-1.33	36,36,36,37	0
2	SO4	A	1108	5/5	0.91	0.35	-	90,91,91,91	0
2	SO4	B	1107	5/5	0.88	0.22	-	94,94,94,94	0

6.5 Other polymers [i](#)

There are no such residues in this entry.