



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:39 AM GMT

PDB ID : 2XUM
Title : FACTOR INHIBITING HIF (FIH) Q239H MUTANT IN COMPLEX WITH
ZN(II), NOG AND ASP-SUBSTRATE PEPTIDE (20-MER)
Authors : Chowdhury, R.; Mcdonough, M.A.; Schofield, C.J.
Deposited on : 2010-10-19
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
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

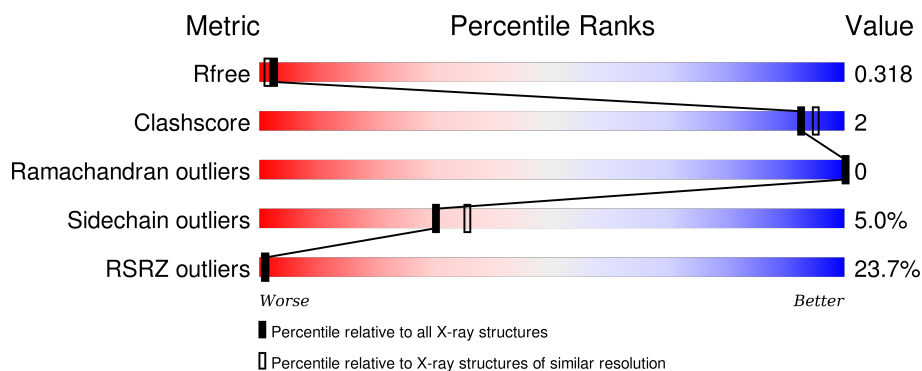
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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}	91344	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (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 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	349	<div> <div>22%</div> <div>89%</div> <div>10%</div> </div>
2	S	20	<div> <div>45%</div> <div>80%</div> <div>10%</div> <div>10%</div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 3191 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 HYPOXIA-INDUCIBLE FACTOR 1-ALPHA INHIBITOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	349	Total	C	N	O	S	0	5	0
			2873	1838	489	534	12			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	239	HIS	GLN	ENGINEERED MUTATION	UNP Q9NWT6

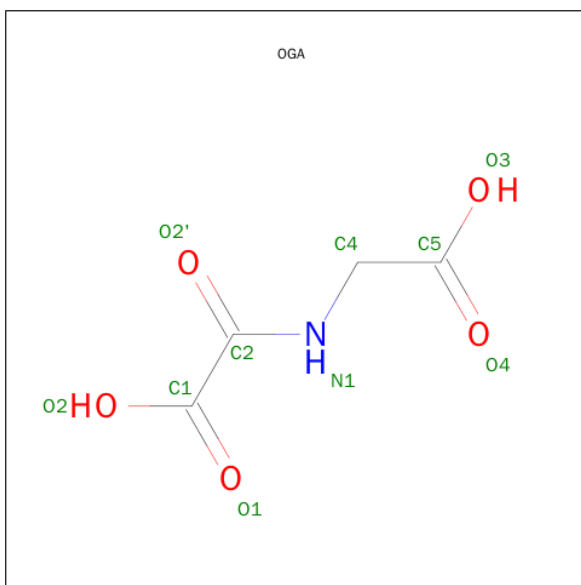
- Molecule 2 is a protein called ASP-SUBSTRATE PEPTIDE 2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	S	18	Total	C	N	O	0	0	0
			138	86	23	29			

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		

- Molecule 4 is N-OXALYLGLYCINE (three-letter code: OGA) (formula: C₄H₅NO₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			10	4	1	5		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

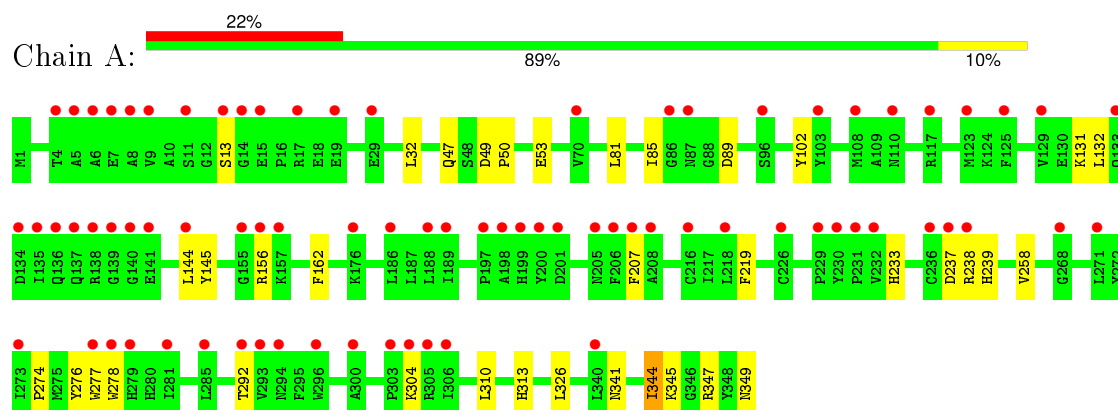
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	147	Total 147	O 147	0	0
6	S	7	Total 7	O 7	0	0

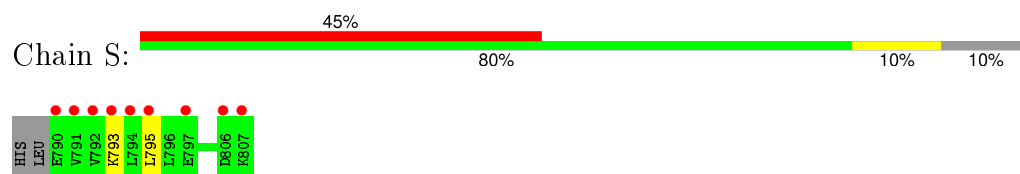
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 ($\text{RSRZ} > 2$). 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: HYPOXIA-INDUCIBLE FACTOR 1-ALPHA INHIBITOR



• Molecule 2: ASP-SUBSTRATE PEPTIDE 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	86.35Å 86.35Å 144.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	74.12 – 2.20 42.07 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.1 (74.12-2.20) 99.1 (42.07-2.20)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.31 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.201 , 0.222 0.305 , 0.318	Depositor DCC
R_{free} test set	1427 reflections (5.32%)	DCC
Wilson B-factor (Å ²)	50.5	Xtriage
Anisotropy	0.326	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 41.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 28291 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	3191	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.66% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: ZN, OGA, 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	0.39	0/2971	0.53	1/4033 (0.0%)
2	S	0.36	0/138	0.55	0/185
All	All	0.39	0/3109	0.53	1/4218 (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	A	347	ARG	NE-CZ-NH2	-5.66	117.47	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	2873	0	2763	12	0
2	S	138	0	137	0	0
3	A	1	0	0	0	0
4	A	10	0	3	0	0
5	A	15	0	0	0	0
6	A	147	0	0	1	0
6	S	7	0	0	0	0
All	All	3191	0	2903	12	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 2.

All (12) 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:344:ILE:HD12	1:A:349:ASN:HB3	1.81	0.61
1:A:81:LEU:HD22	1:A:85:ILE:HD12	1.88	0.56
1:A:237:ASP:O	1:A:238:ARG:HB2	2.10	0.51
1:A:274:PRO:HB2	1:A:277:TRP:CD1	2.46	0.50
1:A:219:PHE:HB2	1:A:278:TRP:HB2	1.94	0.49
1:A:276:TYR:CD2	1:A:313:HIS:HB2	2.50	0.47
1:A:207:PHE:CZ	1:A:292:THR:HG21	2.51	0.45
1:A:233:HIS:HE1	6:A:2132:HOH:O	2.01	0.43
1:A:49:ASP:HA	1:A:50:PRO:HD2	1.88	0.43
1:A:131:LYS:HG2	1:A:144:LEU:HD11	2.01	0.42
1:A:341:ASN:HB3	1:A:345:LYS:HE2	2.01	0.42
1:A:102:TYR:HB3	1:A:239:HIS:CE1	2.56	0.41

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	352/349 (101%)	346 (98%)	6 (2%)	0	100	100
2	S	16/20 (80%)	15 (94%)	1 (6%)	0	100	100
All	All	368/369 (100%)	361 (98%)	7 (2%)	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	308/304 (101%)	294 (96%)	14 (4%)	34	41
2	S	15/17 (88%)	13 (87%)	2 (13%)	5	4
All	All	323/321 (101%)	307 (95%)	16 (5%)	30	35

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	SER
1	A	32	LEU
1	A	47	GLN
1	A	53	GLU
1	A	89	ASP
1	A	132	LEU
1	A	145	TYR
1	A	156	ARG
1	A	162	PHE
1	A	258	VAL
1	A	304	LYS
1	A	310	LEU
1	A	326	LEU
1	A	344	ILE
2	S	793	LYS
2	S	795	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	82	GLN
1	A	147	GLN
1	A	203	GLN
2	S	798	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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 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	OGA	A	601	3	3,9,9	0.50	0	3,11,11	0.66	0
5	SO4	A	602	-	4,4,4	0.20	0	6,6,6	0.08	0
5	SO4	A	603	-	4,4,4	0.17	0	6,6,6	0.14	0
5	SO4	A	604	-	4,4,4	0.19	0	6,6,6	0.16	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
4	OGA	A	601	3	-	0/3/9/9	0/0/0/0
5	SO4	A	602	-	-	0/0/0/0	0/0/0/0
5	SO4	A	603	-	-	0/0/0/0	0/0/0/0
5	SO4	A	604	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

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

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	349/349 (100%)	1.30	78 (22%) 1 1	44, 49, 55, 63	0
2	S	18/20 (90%)	1.94	9 (50%) 0 0	41, 45, 48, 49	0
All	All	367/369 (99%)	1.34	87 (23%) 1 1	41, 49, 55, 63	0

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	139	GLY	6.7
1	A	6	ALA	6.5
1	A	137	GLN	6.4
1	A	305	ARG	6.1
1	A	136	GLN	5.3
2	S	790	GLU	5.0
1	A	135	ILE	4.9
1	A	133	GLN	4.8
1	A	15	GLU	4.7
2	S	791	VAL	4.6
1	A	304	LYS	4.6
1	A	103	TYR	4.3
1	A	140	GLY	4.3
1	A	236	CYS	4.3
1	A	138	ARG	4.2
1	A	9	VAL	4.2
1	A	87[A]	ASN	4.1
1	A	134	ASP	3.8
2	S	794	LEU	3.6
1	A	17	ARG	3.6
2	S	806	ASP	3.5
1	A	86	GLY	3.5
1	A	176	LYS	3.4
1	A	11	SER	3.4

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Mol	Chain	Res	Type	RSRZ
2	S	792	VAL	3.3
1	A	123	MET	3.2
1	A	277	TRP	3.2
1	A	186	LEU	3.1
1	A	207	PHE	3.1
1	A	141	GLU	3.1
1	A	96	SER	3.0
1	A	273	ILE	3.0
1	A	278	TRP	3.0
1	A	200	TYR	3.0
1	A	4	THR	3.0
1	A	188	LEU	2.9
1	A	218	LEU	2.8
1	A	237	ASP	2.8
2	S	793	LYS	2.8
1	A	271	LEU	2.7
1	A	281	ILE	2.7
1	A	199	HIS	2.7
2	S	795	LEU	2.6
1	A	229	PRO	2.6
1	A	29	GLU	2.6
1	A	232	VAL	2.6
1	A	279	HIS	2.6
1	A	285	LEU	2.6
1	A	5	ALA	2.6
1	A	110	ASN	2.6
1	A	306	ILE	2.5
1	A	7	GLU	2.5
1	A	216	CYS	2.5
1	A	117	ARG	2.5
1	A	230	TYR	2.4
1	A	13	SER	2.4
1	A	19	GLU	2.4
1	A	129	VAL	2.4
1	A	208	ALA	2.4
1	A	108	MET	2.3
1	A	8	ALA	2.3
1	A	238	ARG	2.3
1	A	156	ARG	2.3
1	A	157	LYS	2.2
2	S	797	GLU	2.2
1	A	70	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	205	ASN	2.2
1	A	201	ASP	2.2
1	A	198	ALA	2.2
1	A	14	GLY	2.2
2	S	807	LYS	2.1
1	A	197	PRO	2.1
1	A	292	THR	2.1
1	A	231	PRO	2.1
1	A	296	TRP	2.1
1	A	226	CYS	2.1
1	A	340	LEU	2.1
1	A	155	GLY	2.1
1	A	300	ALA	2.1
1	A	293	VAL	2.1
1	A	294	ASN	2.1
1	A	303	PRO	2.1
1	A	206	PHE	2.0
1	A	144	LEU	2.0
1	A	268	GLY	2.0
1	A	189	ILE	2.0
1	A	125	PHE	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 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(Å ²)	Q<0.9
4	OGA	A	601	10/10	0.97	0.26	-0.04	43,44,46,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	ZN	A	501	1/1	0.99	0.22	-0.58	44,44,44,44	0
5	SO4	A	603	5/5	0.97	0.13	-1.40	102,102,102,102	0
5	SO4	A	604	5/5	0.91	0.14	-	89,89,89,90	0
5	SO4	A	602	5/5	0.82	0.15	-	109,109,110,110	0

6.5 Other polymers [i](#)

There are no such residues in this entry.