



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 02:09 PM UTC

PDB ID : 6HKG / pdb_00006hkg
Title : Structure of FISW84 Fab Fragment
Authors : Benton, D.J.; Rosenthal, P.B.
Deposited on : 2018-09-06
Resolution : 1.87 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
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

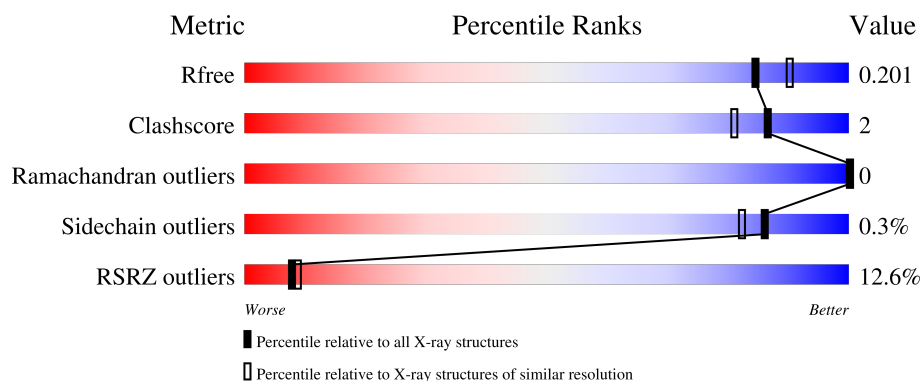
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.87 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	1220 (1.88-1.88)
Clashscore	190562	1234 (1.88-1.88)
Ramachandran outliers	187476	1222 (1.88-1.88)
Sidechain outliers	187428	1222 (1.88-1.88)
RSRZ outliers	180081	1220 (1.88-1.88)

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	217	4% 94% 6%
2	B	214	3% 94% 6%
3	C	194	25% 96% .
4	D	159	22% 95% 5%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6550 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 FISW84 Fab Fragment Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	217	Total	C	N	O	S	0	9	0
			1682	1060	288	322	12			

- Molecule 2 is a protein called FISW84 Fab Fragment Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	214	Total	C	N	O	S	0	13	0
			1734	1074	297	354	9			

- Molecule 3 is a protein called FISW84 Fab Fragment Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	194	Total	C	N	O	S	0	5	0
			1455	919	250	276	10			

- Molecule 4 is a protein called FISW84 Fab Fragment Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	159	Total	C	N	O	S	0	8	0
			1242	775	209	251	7			

- Molecule 5 is SULFATE ION (CCD ID: 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	B	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		

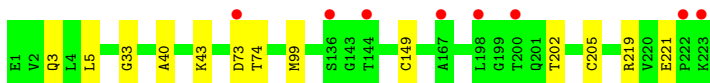
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	120	Total	O	0	0
			120	120		
6	B	149	Total	O	0	0
			149	149		
6	C	76	Total	O	0	0
			76	76		
6	D	62	Total	O	0	0
			62	62		

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.

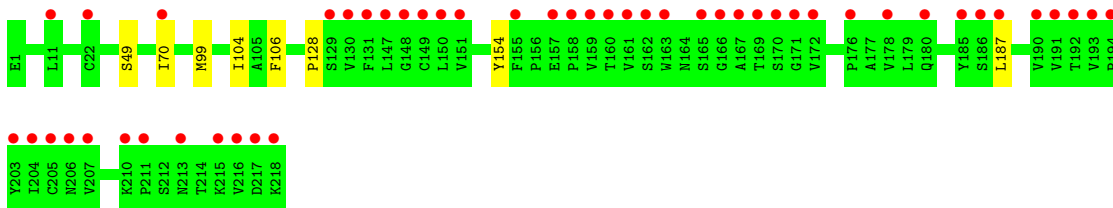
- Molecule 1: FISW84 Fab Fragment Heavy Chain



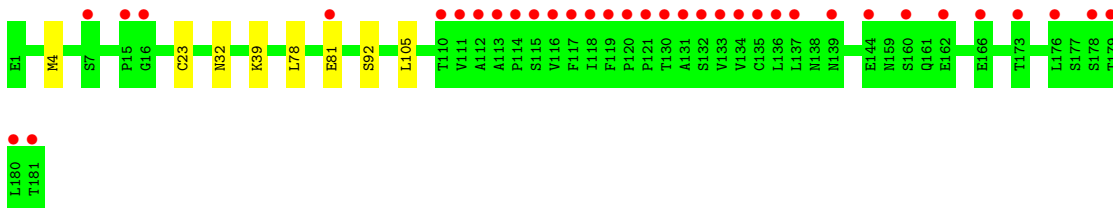
- Molecule 2: FISW84 Fab Fragment Light Chain



- Molecule 3: FISW84 Fab Fragment Heavy Chain



- Molecule 4: FISW84 Fab Fragment Light Chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	130.16Å 130.16Å 167.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.75 – 1.87 29.75 – 1.87	Depositor EDS
% Data completeness (in resolution range)	99.7 (29.75-1.87) 99.6 (29.75-1.87)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.31 (at 1.87Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.183 , 0.200 0.184 , 0.201	Depositor DCC
R_{free} test set	5869 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	39.3	Xtriage
Anisotropy	0.156	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 47.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6550	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.59% 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, 0.333 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: 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	0/1719	0.53	0/2335
2	B	0.32	0/1770	0.53	0/2406
3	C	0.28	0/1485	0.48	0/2015
4	D	0.30	0/1268	0.54	0/1732
All	All	0.31	0/6242	0.52	0/8488

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	1682	0	1648	9	0
2	B	1734	0	1662	7	0
3	C	1455	0	1374	6	0
4	D	1242	0	1164	4	0
5	A	10	0	0	0	0
5	B	10	0	0	0	0
5	C	10	0	0	0	0
6	A	120	0	0	0	0
6	B	149	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	C	76	0	0	0	0
6	D	62	0	0	0	0
All	All	6550	0	5848	25	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 (25) 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:3[A]:GLN:HG2	1:A:5:LEU:HG	1.80	0.62
4:D:4:MET:HE3	4:D:23[A]:CYS:SG	2.43	0.59
2:B:143:ARG:NH1	6:B:402:HOH:O	2.37	0.57
1:A:40:ALA:HB3	1:A:43[B]:LYS:HD2	1.87	0.56
2:B:147:VAL:HG13	2:B:195[B]:CYS:SG	2.47	0.54
2:B:32:ASN:HB2	2:B:92:SER:HB2	1.89	0.54
1:A:219:ARG:NH1	1:A:221:GLU:OE1	2.43	0.52
3:C:99:MET:HG3	3:C:106:PHE:CD1	2.46	0.50
4:D:78:LEU:HD21	4:D:105:LEU:HD13	1.93	0.50
2:B:208:LYS:NZ	6:B:401:HOH:O	2.31	0.49
1:A:3[A]:GLN:OE1	1:A:5:LEU:HD11	2.13	0.48
4:D:32:ASN:HB2	4:D:92:SER:HB2	1.98	0.46
1:A:202:THR:HG23	1:A:219:ARG:HE	1.82	0.44
1:A:33:GLY:C	1:A:99:MET:HG2	2.43	0.43
2:B:155:LEU:HG	3:C:104:ILE:HD11	2.00	0.43
3:C:154:TYR:OH	3:C:187:LEU:HD23	2.20	0.42
3:C:49:SER:OG	3:C:70[B]:ILE:HD11	2.20	0.41
1:A:149[B]:CYS:SG	1:A:205[B]:CYS:SG	3.13	0.41
1:A:43[A]:LYS:HE3	1:A:43[A]:LYS:HB3	1.94	0.41
3:C:128:PRO:HB3	3:C:154:TYR:HB3	2.01	0.41
2:B:106:GLU:HG2	2:B:107:ILE:N	2.34	0.41
1:A:73:ASP:OD1	1:A:74:THR:N	2.54	0.40
4:D:39:LYS:HE2	4:D:81[B]:GLU:O	2.21	0.40
3:C:187:LEU:C	3:C:187:LEU:HD12	2.46	0.40
2:B:135[B]:CYS:HG	2:B:195[B]:CYS:HG	1.63	0.40

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	222/217 (102%)	218 (98%)	4 (2%)	0	100	100
2	B	225/214 (105%)	220 (98%)	5 (2%)	0	100	100
3	C	191/194 (98%)	189 (99%)	2 (1%)	0	100	100
4	D	162/159 (102%)	159 (98%)	3 (2%)	0	100	100
All	All	800/784 (102%)	786 (98%)	14 (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	187/179 (104%)	187 (100%)	0	100	100
2	B	197/184 (107%)	194 (98%)	3 (2%)	57	46
3	C	152/161 (94%)	152 (100%)	0	100	100
4	D	137/137 (100%)	137 (100%)	0	100	100
All	All	673/661 (102%)	670 (100%)	3 (0%)	86	79

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	23[A]	CYS
2	B	23[B]	CYS
2	B	157	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	84	ASN
2	B	37	GLN
3	C	39	GLN
4	D	38	GLN
4	D	79	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 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	$\# Z > 2$
5	SO4	B	302	-	4,4,4	0.26	0	6,6,6	0.08	0
5	SO4	A	302	-	4,4,4	0.20	0	6,6,6	0.41	0
5	SO4	B	301	-	4,4,4	0.28	0	6,6,6	0.36	0
5	SO4	C	302	-	4,4,4	0.28	0	6,6,6	0.12	0
5	SO4	C	301	-	4,4,4	0.23	0	6,6,6	0.26	0
5	SO4	A	301	-	4,4,4	0.23	0	6,6,6	0.19	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	C	3
4	D	1
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	144:GLU	C	159:ASN	N	19.15
1	A	136:SER	C	143:GLY	N	11.96
1	C	194:PRO	C	203:TYR	N	11.68
1	C	131:PHE	C	147:LEU	N	11.17
1	C	167:ALA	C	169:THR	N	3.87

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	217/217 (100%)	0.27	8 (3%) 45 49	17, 44, 79, 100	9 (4%)
2	B	214/214 (100%)	0.22	7 (3%) 49 54	17, 44, 66, 87	13 (6%)
3	C	194/194 (100%)	1.17	49 (25%) 1 1	19, 56, 129, 139	5 (2%)
4	D	159/159 (100%)	0.99	35 (22%) 2 2	16, 53, 124, 137	8 (5%)
All	All	784/784 (100%)	0.62	99 (12%) 8 9	16, 46, 120, 139	35 (4%)

All (99) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	130	THR	7.2
3	C	167	ALA	7.2
4	D	116	VAL	6.9
3	C	204	ILE	6.4
4	D	181	THR	6.1
3	C	192	THR	5.9
3	C	203	TYR	5.7
4	D	118	ILE	5.5
4	D	117	PHE	5.5
3	C	194	PRO	5.3
3	C	147	LEU	5.2
3	C	191	VAL	4.8
4	D	132	SER	4.8
4	D	119	PHE	4.8
3	C	218	LYS	4.8
3	C	169	THR	4.5
3	C	165	SER	4.3
3	C	150	LEU	4.2
3	C	131	PHE	4.2
4	D	136	LEU	4.1
3	C	205	CYS	4.1

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Mol	Chain	Res	Type	RSRZ
4	D	134	VAL	4.1
4	D	180	LEU	4.1
4	D	135[A]	CYS	4.0
3	C	217	ASP	3.8
4	D	133	VAL	3.8
4	D	114	PRO	3.7
3	C	149	CYS	3.6
3	C	166	GLY	3.6
4	D	15	PRO	3.6
3	C	187	LEU	3.6
4	D	121	PRO	3.5
3	C	193	VAL	3.5
4	D	120	PRO	3.4
1	A	200	THR	3.3
3	C	159	VAL	3.2
3	C	161	VAL	3.2
2	B	144	GLU	3.2
4	D	16	GLY	3.2
3	C	130	VAL	3.1
4	D	115	SER	3.1
4	D	144	GLU	3.1
4	D	111	VAL	3.0
3	C	210	LYS	3.0
1	A	136	SER	2.9
3	C	213	ASN	2.9
4	D	131	ALA	2.9
3	C	190	VAL	2.9
3	C	171	GLY	2.8
3	C	216	VAL	2.8
1	A	73	ASP	2.8
3	C	215	LYS	2.8
4	D	176	LEU	2.7
4	D	7	SER	2.7
4	D	160	SER	2.7
4	D	110	THR	2.7
3	C	172	VAL	2.7
2	B	124[A]	GLU	2.6
4	D	137	LEU	2.6
3	C	207	VAL	2.6
4	D	113	ALA	2.5
2	B	1	GLU	2.5
3	C	180	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
3	C	163	TRP	2.5
3	C	160	THR	2.5
4	D	173	THR	2.5
3	C	170	SER	2.4
1	A	222	PRO	2.4
3	C	129	SER	2.4
2	B	171	ASP	2.4
1	A	167	ALA	2.4
4	D	112	ALA	2.4
3	C	155	PHE	2.3
4	D	162	GLU	2.3
1	A	198	LEU	2.3
1	A	223	LYS	2.3
3	C	158	PRO	2.3
3	C	211	PRO	2.3
3	C	148	GLY	2.3
3	C	176	PRO	2.2
4	D	166	GLU	2.2
3	C	186	SER	2.2
4	D	179	THR	2.2
3	C	162	SER	2.2
3	C	151	VAL	2.2
1	A	144	THR	2.2
3	C	11	LEU	2.2
3	C	206	ASN	2.1
3	C	185	TYR	2.1
2	B	104	ARG	2.1
4	D	178	SER	2.1
3	C	157	GLU	2.1
3	C	70[A]	ILE	2.1
4	D	81[A]	GLU	2.0
4	D	139	ASN	2.0
2	B	135[A]	CYS	2.0
3	C	22[A]	CYS	2.0
2	B	24[A]	ARG	2.0
3	C	178	VAL	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

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($\text{\AA}^2$)	Q<0.9
5	SO4	C	302	5/5	0.85	0.11	116,117,122,124	0
5	SO4	B	302	5/5	0.88	0.08	107,110,115,116	0
5	SO4	A	301	5/5	0.90	0.11	89,91,102,103	0
5	SO4	A	302	5/5	0.91	0.14	71,73,82,84	0
5	SO4	C	301	5/5	0.94	0.09	63,64,74,74	0
5	SO4	B	301	5/5	0.94	0.08	64,73,76,78	0

6.5 Other polymers [i](#)

There are no such residues in this entry.