



Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 06:47 am BST

PDB ID : 6HKG
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 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)
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

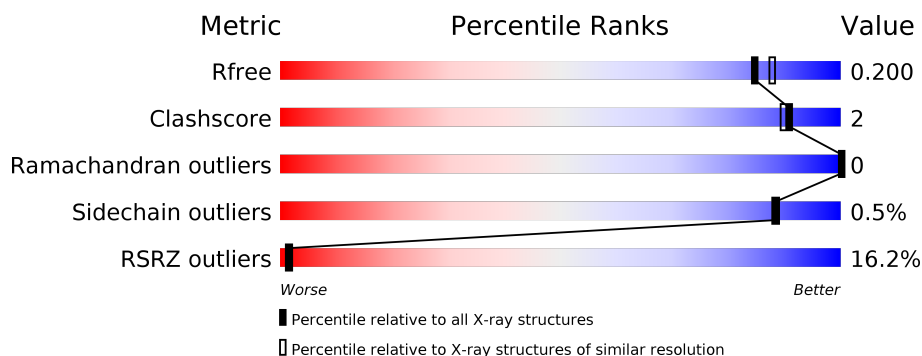
1 Overall quality at a glance

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}	130704	9470 (1.90-1.86)
Clashscore	141614	10282 (1.90-1.86)
Ramachandran outliers	138981	10152 (1.90-1.86)
Sidechain outliers	138945	10152 (1.90-1.86)
RSRZ outliers	127900	9303 (1.90-1.86)

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 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	<div> <div>7%</div> <div> <div></div> <div>95%</div> <div>5%</div> </div> </div>
2	B	214	<div> <div>5%</div> <div> <div></div> <div>95%</div> <div>5%</div> </div> </div>
3	C	194	<div> <div>32%</div> <div> <div></div> <div>95%</div> <div>• •</div> </div> </div>
4	D	159	<div> <div>25%</div> <div> <div></div> <div>96%</div> <div>•</div> </div> </div>

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 (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	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		

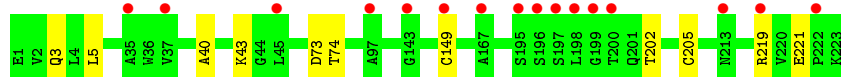
- Molecule 6 is water.

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		

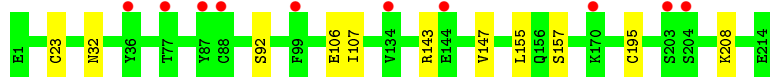
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

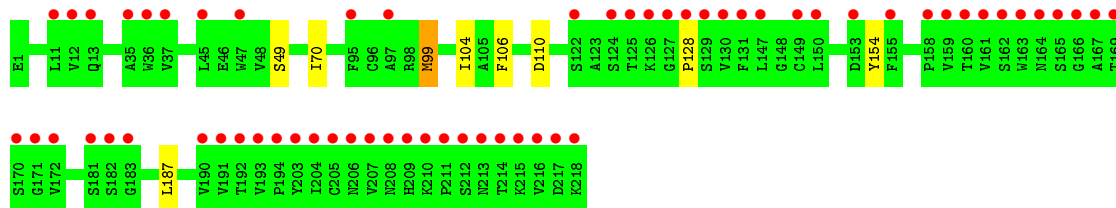
- Molecule 1: FISW84 Fab Fragment Heavy Chain



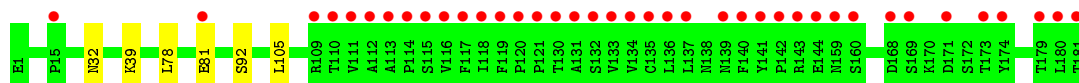
- Molecule 2: FISW84 Fab Fragment Light Chain



- 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) 99.7 (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 0.183 , 0.200	Depositor DCC
R_{free} test set	5869 reflections (4.97%)	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)	0.33 , 55.0	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	0.97	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	0.41	0/1719	0.60	0/2335
2	B	0.42	0/1770	0.60	0/2406
3	C	0.37	0/1485	0.58	1/2015 (0.0%)
4	D	0.37	0/1268	0.57	0/1732
All	All	0.40	0/6242	0.59	1/8488 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	110	ASP	CB-CG-OD1	5.13	122.92	118.30

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	1682	0	1648	8	0
2	B	1734	0	1662	6	0
3	C	1455	0	1374	5	0
4	D	1242	0	1164	3	0
5	A	10	0	0	0	0
5	B	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	10	0	0	0	0
6	A	120	0	0	0	0
6	B	149	0	0	2	0
6	C	76	0	0	0	0
6	D	62	0	0	0	0
All	All	6550	0	5848	21	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 (21) 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
2:B:208:LYS:NZ	6:B:401:HOH:O	2.31	0.60
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
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
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
2:B:106:GLU:HG2	2:B:107:ILE:N	2.34	0.41
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
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

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	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 [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	187/179 (104%)	187 (100%)	0	100	100
2	B	197/184 (107%)	194 (98%)	3 (2%)	65	59
3	C	152/161 (94%)	151 (99%)	1 (1%)	84	83
4	D	137/137 (100%)	137 (100%)	0	100	100
All	All	673/661 (102%)	669 (99%)	4 (1%)	88	86

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	23[A]	CYS
2	B	23[B]	CYS

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Mol	Chain	Res	Type
2	B	157	SER
3	C	99	MET

Some 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](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates 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	C	302	-	4,4,4	0.17	0	6,6,6	0.08	0
5	SO4	A	301	-	4,4,4	0.13	0	6,6,6	0.17	0
5	SO4	C	301	-	4,4,4	0.15	0	6,6,6	0.23	0
5	SO4	A	302	-	4,4,4	0.14	0	6,6,6	0.40	0
5	SO4	B	302	-	4,4,4	0.15	0	6,6,6	0.06	0
5	SO4	B	301	-	4,4,4	0.17	0	6,6,6	0.35	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
1	A	1
4	D	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%)	0.37	16 (7%)	14 15	30, 44, 79, 100	0
2	B	214/214 (100%)	0.16	10 (4%)	31 33	32, 45, 66, 87	0
3	C	194/194 (100%)	1.45	62 (31%)	0 0	31, 56, 129, 139	0
4	D	159/159 (100%)	1.26	39 (24%)	0 0	29, 54, 124, 137	0
All	All	784/784 (100%)	0.76	127 (16%)	1 1	29, 47, 120, 139	0

All (127) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	180	LEU	9.6
3	C	216	VAL	7.9
4	D	117	PHE	7.8
4	D	112	ALA	7.5
4	D	113	ALA	7.3
3	C	205	CYS	7.3
3	C	191	VAL	7.2
3	C	163	TRP	7.1
4	D	160	SER	7.0
4	D	120	PRO	6.6
4	D	115	SER	6.5
3	C	166	GLY	6.3
4	D	133	VAL	6.1
4	D	121	PRO	6.1
4	D	116	VAL	5.8
4	D	181	THR	5.6
3	C	208	ASN	5.5
1	A	200	THR	5.5
4	D	114	PRO	5.5
3	C	213	ASN	5.5
3	C	204	ILE	5.4

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Mol	Chain	Res	Type	RSRZ
4	D	110	THR	5.4
4	D	111	VAL	5.4
4	D	135[A]	CYS	5.4
3	C	212	SER	5.3
3	C	211	PRO	5.1
3	C	172	VAL	5.1
4	D	119	PHE	5.0
3	C	209	HIS	5.0
1	A	198	LEU	4.8
3	C	153	ASP	4.8
4	D	131	ALA	4.7
3	C	147	LEU	4.7
3	C	194	PRO	4.7
4	D	159	ASN	4.7
3	C	192	THR	4.5
4	D	179	THR	4.5
3	C	214	THR	4.5
3	C	210	LYS	4.4
3	C	155	PHE	4.4
3	C	130	VAL	4.3
4	D	140	PHE	4.3
4	D	132	SER	4.3
3	C	170	SER	4.2
3	C	181	SER	4.2
3	C	165	SER	4.1
3	C	159	VAL	4.0
3	C	167	ALA	4.0
3	C	160	THR	4.0
3	C	162	SER	3.9
3	C	193	VAL	3.8
3	C	206	ASN	3.8
1	A	199	GLY	3.7
4	D	136	LEU	3.7
3	C	207	VAL	3.5
3	C	124	SER	3.5
3	C	131	PHE	3.5
3	C	11	LEU	3.5
4	D	137	LEU	3.4
3	C	35	ALA	3.4
3	C	13	GLN	3.4
3	C	161	VAL	3.4
3	C	171	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
3	C	129	SER	3.3
1	A	37	VAL	3.3
4	D	171	ASP	3.3
1	A	45	LEU	3.3
3	C	37	VAL	3.2
4	D	141	TYR	3.2
4	D	118	ILE	3.1
1	A	196	SER	3.1
3	C	169	THR	3.1
3	C	127	GLY	3.1
3	C	203	TYR	3.1
3	C	215	LYS	3.0
3	C	128	PRO	3.0
3	C	164	ASN	3.0
3	C	125	THR	3.0
3	C	97	ALA	2.9
1	A	143	GLY	2.9
4	D	144	GLU	2.9
2	B	170	LYS	2.9
3	C	122	SER	2.9
3	C	183	GLY	2.9
4	D	143	ARG	2.8
4	D	139	ASN	2.8
1	A	197	SER	2.8
4	D	15	PRO	2.7
2	B	99	PHE	2.7
3	C	36	TRP	2.7
4	D	174	TYR	2.7
2	B	134	VAL	2.7
1	A	149[A]	CYS	2.6
2	B	204	SER	2.5
2	B	88[A]	CYS	2.5
3	C	150	LEU	2.4
1	A	167	ALA	2.4
1	A	213	ASN	2.4
4	D	130	THR	2.4
4	D	109	ARG	2.4
4	D	142	PRO	2.4
2	B	87	TYR	2.4
3	C	149	CYS	2.4
1	A	97	ALA	2.3
2	B	77	THR	2.3

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Mol	Chain	Res	Type	RSRZ
3	C	47	TRP	2.3
4	D	169	SER	2.3
3	C	182	SER	2.3
1	A	219	ARG	2.3
3	C	12	VAL	2.2
3	C	217	ASP	2.2
4	D	134	VAL	2.2
1	A	222	PRO	2.2
3	C	126	LYS	2.2
3	C	218	LYS	2.2
1	A	195	SER	2.1
3	C	158	PRO	2.1
3	C	45	LEU	2.1
2	B	144	GLU	2.1
3	C	190	VAL	2.1
1	A	35	ALA	2.1
3	C	95	PHE	2.1
2	B	36	TYR	2.0
4	D	81[A]	GLU	2.0
4	D	168	ASP	2.0
2	B	203	SER	2.0
4	D	173	THR	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. 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(Å ²)	Q<0.9
5	SO4	C	302	5/5	0.90	0.22	116,117,122,124	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	SO4	A	301	5/5	0.94	0.18	89,91,102,103	0
5	SO4	B	302	5/5	0.95	0.41	107,110,115,116	0
5	SO4	C	301	5/5	0.96	0.09	63,64,74,74	0
5	SO4	B	301	5/5	0.96	0.10	64,73,76,78	0
5	SO4	A	302	5/5	0.98	0.13	71,73,82,84	0

6.5 Other polymers [i](#)

There are no such residues in this entry.