



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 24, 2024 – 01:36 PM EDT

PDB ID : 6FR6
Title : HA1.7 Human T-Cell Receptor specific for Influenza virus epitope
PKYVKQNTLKLAT presented by Human Leukocyte Antigen HLA-DR0101
Authors : Rizkallah, P.J.; Cole, D.K.
Deposited on : 2018-02-15
Resolution : 2.98 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	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
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)	:	2.37.1

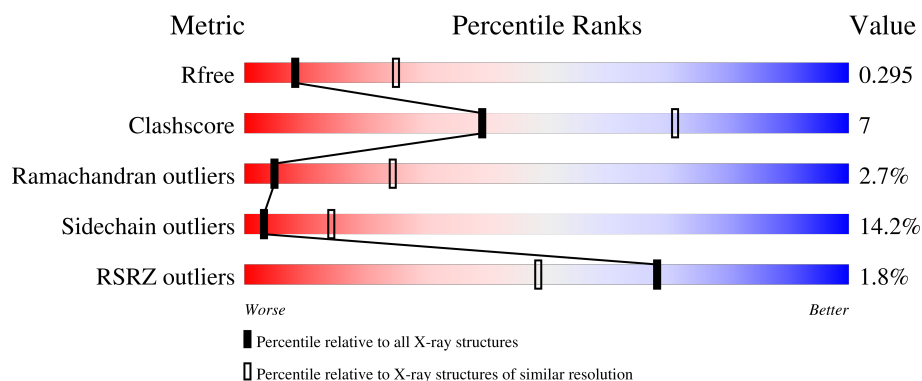
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.98 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	2754 (3.00-2.96)
Clashscore	141614	3103 (3.00-2.96)
Ramachandran outliers	138981	2993 (3.00-2.96)
Sidechain outliers	138945	2996 (3.00-2.96)
RSRZ outliers	127900	2644 (3.00-2.96)

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	202	
2	B	241	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3555 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 Human T-Cell Receptor Alpha Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	202	Total	C	N	O	S	0	2	0
			1588	1003	261	315	9			

- Molecule 2 is a protein called Human T-cell Receptor Beta Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	241	Total	C	N	O	S	0	0	0
			1938	1227	332	370	9			

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

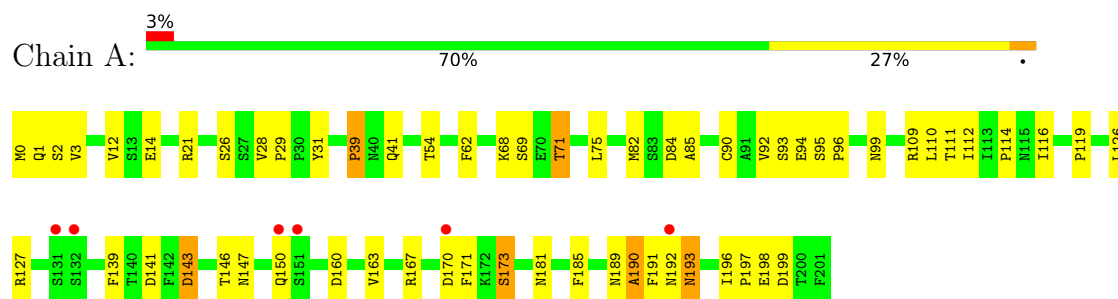
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	13	Total 13	O 13	0	0
4	B	6	Total 6	O 6	0	0

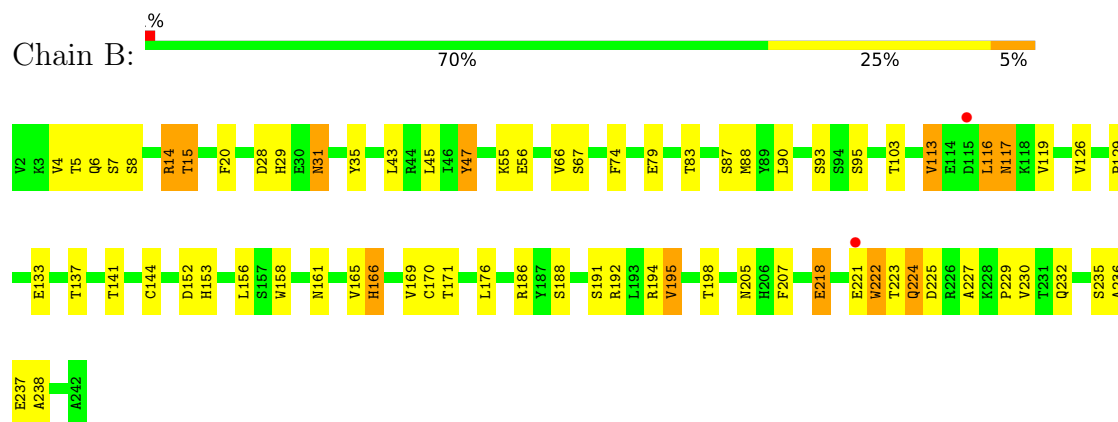
3 Residue-property plots

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: Human T-Cell Receptor Alpha Chain



• Molecule 2: Human T-cell Receptor Beta Chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	70.00Å 50.24Å 73.17Å 90.00° 93.31° 90.00°	Depositor
Resolution (Å)	36.52 – 2.98 36.52 – 2.98	Depositor EDS
% Data completeness (in resolution range)	98.8 (36.52-2.98) 98.8 (36.52-2.98)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.55 (at 3.00Å)	Xtriage
Refinement program	REFMAC 5.8.0189	Depositor
R, R_{free}	0.201 , 0.299 0.204 , 0.295	Depositor DCC
R_{free} test set	502 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å ²)	53.5	Xtriage
Anisotropy	0.196	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 37.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.029 for l,-k,h	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	3555	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.61% 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

5.1 Standard geometry

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	0.86	0/1628	0.98	2/2209 (0.1%)
2	B	0.78	0/1988	0.98	3/2696 (0.1%)
All	All	0.82	0/3616	0.98	5/4905 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	B	0	4
All	All	0	5

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	21	ARG	NE-CZ-NH2	6.46	123.53	120.30
2	B	186	ARG	NE-CZ-NH1	6.04	123.32	120.30
2	B	152	ASP	CB-CG-OD1	6.03	123.72	118.30
1	A	21	ARG	NE-CZ-NH1	-5.70	117.45	120.30
2	B	116	LEU	CA-CB-CG	5.34	127.57	115.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	119	PRO	Peptide

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Mol	Chain	Res	Type	Group
2	B	113	VAL	Peptide
2	B	166	HIS	Peptide
2	B	221	GLU	Peptide
2	B	235	SER	Peptide

5.2 Too-close contacts ⓘ

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	1588	0	1526	25	0
2	B	1938	0	1865	27	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
4	A	13	0	0	0	0
4	B	6	0	0	1	0
All	All	3555	0	3391	51	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 7.

All (51) 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)
2:B:126:VAL:HG23	2:B:236:ALA:HB3	1.59	0.84
1:A:114:PRO:HG3	1:A:163:VAL:HG21	1.71	0.73
2:B:117:ASN:HD22	2:B:117:ASN:N	1.92	0.66
1:A:193:ASN:HD22	1:A:193:ASN:N	1.93	0.66
1:A:0:MET:HB3	1:A:94:GLU:HG3	1.79	0.64
2:B:171:THR:HG23	2:B:191:SER:HB2	1.84	0.59
2:B:31:ASN:N	2:B:31:ASN:OD1	2.36	0.59
2:B:47:TYR:CB	2:B:66:VAL:HG21	2.33	0.58
1:A:126:LEU:HD23	2:B:129:PRO:HA	1.86	0.57
2:B:207:PHE:O	2:B:238:ALA:N	2.37	0.57
1:A:62:PHE:HB3	1:A:75:LEU:HD11	1.87	0.56
2:B:79:GLU:N	2:B:79:GLU:OE1	2.39	0.56
2:B:43:LEU:HD21	2:B:90:LEU:CD2	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:THR:OG1	1:A:196:ILE:HD11	2.07	0.54
1:A:185:PHE:CE2	1:A:190:ALA:HB2	2.42	0.54
1:A:84:ASP:O	1:A:110:LEU:HD23	2.09	0.53
1:A:85:ALA:HB1	1:A:109[A]:ARG:NH1	2.25	0.52
2:B:47:TYR:HB3	2:B:66:VAL:HG21	1.92	0.51
1:A:111:THR:C	1:A:112:ILE:HD13	2.31	0.51
1:A:71:THR:O	1:A:71:THR:HG23	2.10	0.50
2:B:218:GLU:N	2:B:218:GLU:OE2	2.45	0.49
2:B:43:LEU:HD21	2:B:90:LEU:HD22	1.94	0.49
1:A:0:MET:HG2	1:A:92:VAL:HG13	1.95	0.48
1:A:26:SER:OG	1:A:28:VAL:O	2.31	0.48
2:B:144:CYS:HB2	2:B:158:TRP:CZ2	2.48	0.48
1:A:139:PHE:HB2	1:A:191:PHE:CE2	2.49	0.47
1:A:31:TYR:CG	1:A:96:PRO:HA	2.50	0.46
2:B:133:GLU:O	2:B:137:THR:OG1	2.31	0.46
2:B:156:LEU:C	2:B:156:LEU:HD23	2.37	0.45
1:A:0:MET:HG3	1:A:93:SER:CA	2.46	0.45
2:B:170:CYS:HB3	2:B:192:ARG:HD2	1.99	0.44
1:A:71:THR:O	1:A:71:THR:CG2	2.65	0.44
2:B:224:GLN:NE2	4:B:401:HOH:O	2.40	0.44
2:B:161:ASN:ND2	2:B:205:ASN:OD1	2.43	0.43
1:A:116:ILE:HG13	1:A:143:ASP:HA	1.99	0.43
2:B:117:ASN:N	2:B:117:ASN:ND2	2.62	0.43
2:B:6:GLN:O	2:B:7:SER:C	2.57	0.43
2:B:4:VAL:CG2	2:B:103:THR:HG22	2.49	0.43
1:A:0:MET:HG3	1:A:93:SER:C	2.39	0.43
2:B:4:VAL:HG23	2:B:103:THR:HG22	2.01	0.43
2:B:35:TYR:CZ	2:B:45:LEU:HD13	2.54	0.42
1:A:185:PHE:HA	1:A:189:ASN:HD22	1.85	0.42
2:B:194:ARG:O	2:B:195:VAL:HG13	2.19	0.42
2:B:87:SER:OG	2:B:88:MET:N	2.51	0.42
1:A:171:PHE:CE2	1:A:173:SER:HB3	2.54	0.41
1:A:0:MET:O	1:A:2:SER:N	2.53	0.41
1:A:82:MET:HE2	1:A:112:ILE:CG2	2.50	0.41
1:A:193:ASN:N	1:A:193:ASN:ND2	2.64	0.41
2:B:222:TRP:CZ2	2:B:229:PRO:HD3	2.56	0.41
1:A:12:VAL:O	1:A:112:ILE:HA	2.22	0.40
2:B:14:ARG:O	2:B:15:THR:C	2.60	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	202/202 (100%)	175 (87%)	18 (9%)	9 (4%)	2	13
2	B	239/241 (99%)	210 (88%)	26 (11%)	3 (1%)	12	43
All	All	441/443 (100%)	385 (87%)	44 (10%)	12 (3%)	5	24

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1	GLN
1	A	160	ASP
1	A	167	ARG
1	A	170	ASP
1	A	190	ALA
2	B	227	ALA
1	A	39	PRO
1	A	141	ASP
2	B	74	PHE
2	B	230	VAL
1	A	29	PRO
1	A	197	PRO

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	182/180 (101%)	161 (88%)	21 (12%)	5	22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	215/215 (100%)	180 (84%)	35 (16%)	2	10
All	All	397/395 (100%)	341 (86%)	56 (14%)	3	14

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	VAL
1	A	14	GLU
1	A	39	PRO
1	A	41	GLN
1	A	54	THR
1	A	68	LYS
1	A	69	SER
1	A	71	THR
1	A	90	CYS
1	A	95	SER
1	A	99	ASN
1	A	127	ARG
1	A	143	ASP
1	A	147	ASN
1	A	150	GLN
1	A	173	SER
1	A	181	ASN
1	A	192	ASN
1	A	193	ASN
1	A	198	GLU
1	A	199	ASP
2	B	5	THR
2	B	8	SER
2	B	14	ARG
2	B	15	THR
2	B	20	PHE
2	B	28	ASP
2	B	29	HIS
2	B	31	ASN
2	B	47	TYR
2	B	55	LYS
2	B	56	GLU
2	B	67	SER
2	B	83	THR
2	B	93	SER
2	B	95	SER

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Mol	Chain	Res	Type
2	B	113	VAL
2	B	116	LEU
2	B	117	ASN
2	B	119	VAL
2	B	141	THR
2	B	153	HIS
2	B	165	VAL
2	B	166	HIS
2	B	169	VAL
2	B	176	LEU
2	B	188	SER
2	B	195	VAL
2	B	198	THR
2	B	218	GLU
2	B	222	TRP
2	B	223	THR
2	B	224	GLN
2	B	225	ASP
2	B	232	GLN
2	B	237	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	ASN
1	A	117	GLN
1	A	147	ASN
1	A	189	ASN
1	A	193	ASN
2	B	117	ASN
2	B	224	GLN
2	B	232	GLN

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 [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 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	SO4	B	301	-	4,4,4	0.35	0	6,6,6	0.24	0
3	SO4	A	301	-	4,4,4	0.37	0	6,6,6	0.12	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 [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	202/202 (100%)	-0.01	6 (2%) 50 31	26, 52, 97, 123	0
2	B	241/241 (100%)	-0.11	2 (0%) 86 71	28, 59, 95, 122	0
All	All	443/443 (100%)	-0.06	8 (1%) 68 48	26, 58, 97, 123	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	131	SER	4.5
2	B	115	ASP	3.9
1	A	192	ASN	2.9
1	A	150	GLN	2.6
1	A	132	SER	2.3
2	B	221	GLU	2.2
1	A	170	ASP	2.1
1	A	151	SER	2.1

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 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, 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(\AA^2)	Q<0.9
3	SO4	A	301	5/5	0.81	0.21	94,96,100,102	0
3	SO4	B	301	5/5	0.90	0.26	97,102,105,106	0

6.5 Other polymers [i](#)

There are no such residues in this entry.