



Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 05:00 PM GMT

PDB ID : 3V8W
Title : Crystal Structure of Interleukin-2 Inducible T-cell Kinase Itk Catalytic Domain with ThienopyrazolyindoleInhibitor 469
Authors : McLean, L.R.; Zhang, Y.
Deposited on : 2011-12-23
Resolution : 2.27 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

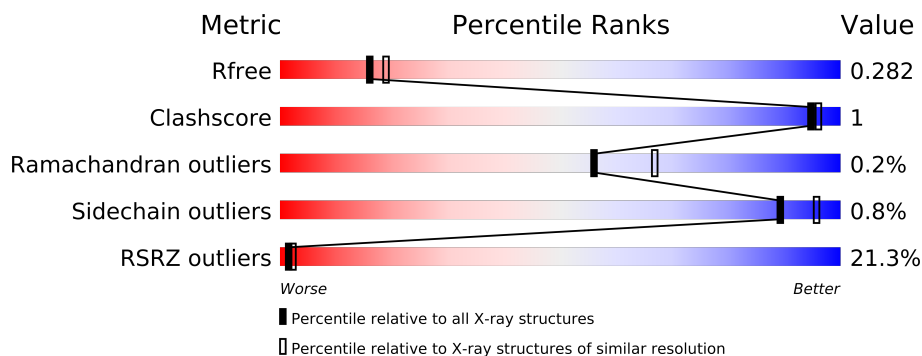
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance



The reported resolution of this entry is 2.27 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}	66092	3861 (2.30-2.26)
Clashscore	79885	4801 (2.30-2.26)
Ramachandran outliers	78287	4729 (2.30-2.26)
Sidechain outliers	78261	4728 (2.30-2.26)
RSRZ outliers	66119	3864 (2.30-2.26)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	266	
1	B	266	

2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 3792 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

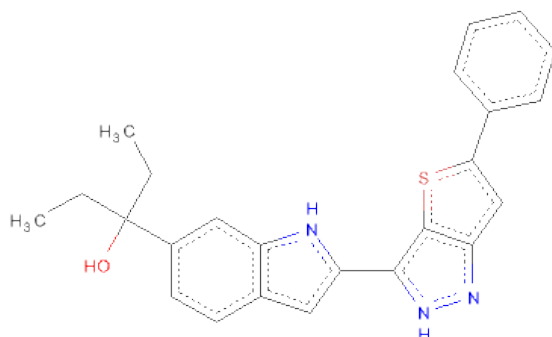
- Molecule 1 is a protein called Tyrosine-protein kinase ITK/TSK.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	243	Total	C	N	O	S	0	0	0
			1841	1179	311	336	15			
1	B	242	Total	C	N	O	S	0	0	0
			1839	1181	307	336	15			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	355	GLY	-	EXPRESSION TAG	UNP Q08881
A	356	SER	-	EXPRESSION TAG	UNP Q08881
B	355	GLY	-	EXPRESSION TAG	UNP Q08881
B	356	SER	-	EXPRESSION TAG	UNP Q08881

- Molecule 2 is 3-[2-(5-PHENYL-2H-THIENO[3,2-C]PYRAZOL-3-YL)-1H-INDOL-6-YL]PENTAN-3-OL (three-letter code: 0G2) (formula: C₂₄H₂₃N₃OS).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			29	24	3	1	1		
2	B	1	Total	C	N	O	S	0	0
			29	24	3	1	1		

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



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

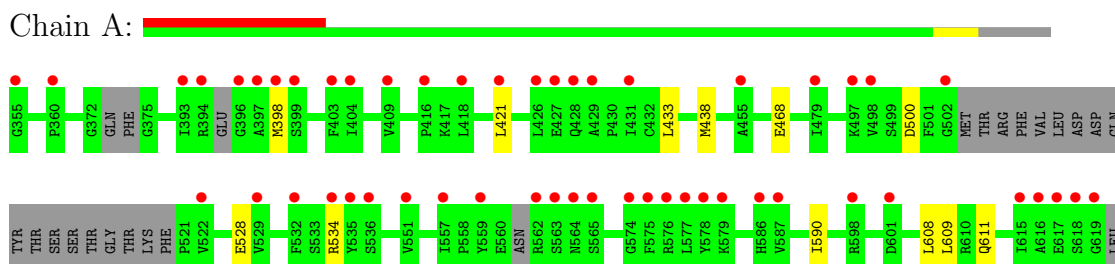
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	22	Total	O	0	0
			22	22		
4	B	27	Total	O	0	0
			27	27		

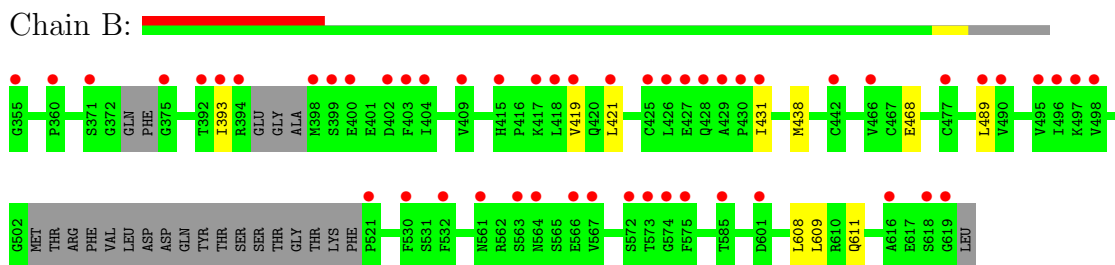
3 Residue-property plots

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 ($RSRZ > 2$). 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: Tyrosine-protein kinase ITK/TSK



- Molecule 1: Tyrosine-protein kinase ITK/TSK



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	146.08Å 69.29Å 68.58Å 90.00° 108.04° 90.00°	Depositor
Resolution (Å)	38.50 – 2.27 38.50 – 2.27	Depositor EDS
% Data completeness (in resolution range)	99.7 (38.50-2.27) 99.7 (38.50-2.27)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.12 (at 2.27Å)	Xtriage
Refinement program	BUSTER 2.9.1	Depositor
R, R_{free}	0.251 , 0.268 0.266 , 0.282	Depositor DCC
R_{free} test set	1518 reflections (5.04%)	DCC
Wilson B-factor (Å ²)	45.7	Xtriage
Anisotropy	0.297	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 37.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 30182 reflections (0.003%)	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	3792	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.95% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 0G2, 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	0.38	0/1879	0.56	0/2542
1	B	0.38	0/1879	0.55	0/2546
All	All	0.38	0/3758	0.56	0/5088

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1841	0	1739	5	0
1	B	1839	0	1754	5	0
2	A	29	0	23	1	0
2	B	29	0	23	1	0
3	B	5	0	0	0	0
4	A	22	0	0	0	0
4	B	27	0	0	0	0
All	All	3792	0	3539	10	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including

hydrogens) of the entry. The overall clashscore for this entry is 1.

All (10) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:438:MET:H	2:B:702:OG2:H17	1.43	0.67
1:B:393:ILE:HG12	1:B:431:ILE:HG13	1.78	0.65
1:A:438:MET:H	2:A:701:OG2:H17	1.48	0.59
1:A:468:GLU:HG3	1:A:609:LEU:HD11	1.91	0.53
1:B:468:GLU:HG3	1:B:609:LEU:HD11	1.96	0.47
1:B:419:VAL:HG21	1:B:489:LEU:HD12	1.96	0.46
1:A:528:GLU:HB3	1:A:534:ARG:HB2	2.01	0.43
1:A:421:LEU:HD11	1:A:433:LEU:HB3	2.01	0.42
1:B:608:LEU:HA	1:B:611:GLN:HE21	1.84	0.41
1:A:608:LEU:HA	1:A:611:GLN:HE21	1.85	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	233/266 (88%)	226 (97%)	6 (3%)	1 (0%)	43	51
1	B	234/266 (88%)	228 (97%)	6 (3%)	0	100	100
All	All	467/532 (88%)	454 (97%)	12 (3%)	1 (0%)	56	67

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	398	MET

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	185/233 (79%)	183 (99%)	2 (1%)	84	92
1	B	190/233 (82%)	189 (100%)	1 (0%)	94	98
All	All	375/466 (80%)	372 (99%)	3 (1%)	89	96

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

Mol	Chain	Res	Type
1	A	500	ASP
1	A	590	ILE
1	B	421	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	592	ASN
1	A	611	GLN
1	B	611	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

3 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	$\# Z > 2$
2	0G2	A	701	-	33,33,33	2.58	9 (27%)	43,49,49	15.31	8 (18%)
3	SO4	B	701	-	4,4,4	0.18	0	6,6,6	0.06	0
2	0G2	B	702	-	33,33,33	2.58	10 (30%)	43,49,49	16.79	8 (18%)

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
2	0G2	A	701	-	-	0/16/20/20	0/1/5/5
3	SO4	B	701	-	-	0/0/0/0	0/0/0/0
2	0G2	B	702	-	-	0/16/20/20	0/1/5/5

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	0G2	CAR-CAP	-8.12	1.40	1.48
2	B	702	0G2	CAR-CAP	-8.05	1.40	1.48
2	A	701	0G2	NAK-NAL	-7.54	1.24	1.37
2	B	702	0G2	NAK-NAL	-7.47	1.24	1.37
2	B	702	0G2	CAB-CAA	-4.59	1.33	1.38
2	B	702	0G2	CAM-SAQ	-4.58	1.68	1.74
2	A	701	0G2	CAB-CAA	-4.58	1.34	1.38
2	A	701	0G2	CAM-SAQ	-4.49	1.68	1.74
2	A	701	0G2	CAJ-CAM	-3.25	1.38	1.43
2	B	702	0G2	CAJ-CAM	-3.14	1.38	1.43
2	A	701	0G2	CAA-NAC	-2.93	1.33	1.36
2	B	702	0G2	CAA-NAC	-2.79	1.33	1.36
2	B	702	0G2	CAP-SAQ	-2.65	1.68	1.72
2	A	701	0G2	CAO-CAN	-2.49	1.35	1.41
2	B	702	0G2	CAO-CAN	-2.46	1.35	1.41
2	A	701	0G2	CAP-SAQ	-2.34	1.69	1.72
2	B	702	0G2	CAB-CAE	-2.16	1.33	1.41
2	A	701	0G2	CAB-CAE	-2.14	1.33	1.41
2	B	702	0G2	CAS-CAH	2.05	1.55	1.52

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	702	0G2	CAJ-CAA-NAC	109.12	125.27	120.34
2	A	701	0G2	CAJ-CAA-NAC	99.40	124.83	120.34
2	B	702	0G2	CAP-SAQ-CAM	10.36	96.09	91.39
2	A	701	0G2	CAP-SAQ-CAM	9.71	95.79	91.39
2	B	702	0G2	CAA-CAJ-NAK	5.53	128.90	121.45
2	A	701	0G2	CAA-CAJ-NAK	5.33	128.63	121.45
2	A	701	0G2	CAO-CAN-CAM	4.43	113.35	110.48
2	B	702	0G2	CAO-CAN-CAM	4.37	113.31	110.48
2	B	702	0G2	CAN-CAM-SAQ	-3.96	107.13	112.00
2	A	701	0G2	CAN-CAM-SAQ	-3.85	107.26	112.00
2	B	702	0G2	CAA-CAB-CAE	3.12	108.72	106.17
2	A	701	0G2	CAA-CAB-CAE	3.01	108.62	106.17
2	B	702	0G2	CAO-CAP-SAQ	-2.97	107.40	110.73
2	A	701	0G2	CAO-CAP-SAQ	-2.76	107.64	110.73
2	A	701	0G2	CAR-CAP-SAQ	2.66	123.14	116.58
2	B	702	0G2	CAR-CAP-SAQ	2.58	122.96	116.58

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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	243/266 (91%)	1.25	52 (21%) 1 2	36, 52, 77, 88	0
1	B	242/266 (90%)	1.25	52 (21%) 1 2	35, 51, 74, 92	0
All	All	485/532 (91%)	1.25	104 (21%) 1 2	35, 52, 76, 92	0

All (104) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	429	ALA	9.1
1	A	397	ALA	6.5
1	A	393	ILE	6.1
1	A	398	MET	6.0
1	B	572	SER	6.0
1	B	426	LEU	5.6
1	A	532	PHE	5.4
1	B	427	GLU	5.2
1	B	393	ILE	4.9
1	B	402	ASP	4.8
1	B	573	THR	4.7
1	B	355	GLY	4.5
1	A	426	LEU	4.4
1	B	400	GLU	4.2
1	A	396	GLY	4.1
1	B	618	SER	4.1
1	A	428	GLN	4.0
1	B	575	PHE	4.0
1	A	427	GLU	4.0
1	B	619	GLY	3.8
1	B	431	ILE	3.8
1	A	403	PHE	3.7
1	A	616	ALA	3.6
1	B	497	LYS	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	535	TYR	3.6
1	B	430	PRO	3.4
1	A	421	LEU	3.3
1	A	455	ALA	3.2
1	B	404	ILE	3.2
1	A	575	PHE	3.2
1	B	495	VAL	3.2
1	B	601	ASP	3.2
1	B	564	ASN	3.2
1	B	498	VAL	3.2
1	A	399	SER	3.1
1	A	502	GLY	3.1
1	B	428	GLN	3.1
1	A	577	LEU	3.0
1	A	404	ILE	3.0
1	A	355	GLY	3.0
1	A	429	ALA	2.9
1	A	574	GLY	2.9
1	A	534	ARG	2.9
1	A	576	ARG	2.9
1	A	360	PRO	2.8
1	B	616	ALA	2.8
1	A	409	VAL	2.8
1	A	618	SER	2.8
1	B	418	LEU	2.8
1	B	371	SER	2.8
1	A	579	LYS	2.7
1	B	403	PHE	2.7
1	B	496	ILE	2.7
1	B	425	CYS	2.6
1	B	477	CYS	2.6
1	B	360	PRO	2.6
1	A	586	HIS	2.5
1	B	394	ARG	2.5
1	B	398	MET	2.5
1	B	561	ASN	2.5
1	A	522	VAL	2.5
1	A	619	GLY	2.5
1	A	418	LEU	2.4
1	B	532	PHE	2.4
1	A	536	SER	2.4
1	A	479	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	521	PRO	2.4
1	A	578	TYR	2.4
1	A	562	ARG	2.4
1	B	585	THR	2.4
1	B	489	LEU	2.4
1	A	551	VAL	2.4
1	B	466	VAL	2.4
1	A	559	TYR	2.3
1	A	431	ILE	2.3
1	B	392	THR	2.3
1	A	563	SER	2.3
1	A	565	SER	2.3
1	A	529	VAL	2.3
1	B	421	LEU	2.3
1	A	498	VAL	2.3
1	A	587	VAL	2.3
1	B	567	VAL	2.3
1	B	530	PHE	2.3
1	A	617	GLU	2.3
1	B	563	SER	2.3
1	A	598	ARG	2.2
1	A	557	ILE	2.2
1	A	601	ASP	2.2
1	A	497	LYS	2.2
1	A	564	ASN	2.2
1	B	490	VAL	2.2
1	A	394	ARG	2.2
1	B	566	GLU	2.2
1	A	615	ILE	2.2
1	A	416	PRO	2.2
1	B	574	GLY	2.2
1	B	415	HIS	2.2
1	B	409	VAL	2.2
1	B	419	VAL	2.2
1	B	442	CYS	2.2
1	B	417	LYS	2.1
1	B	399	SER	2.1
1	B	375	GLY	2.1

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

There are no carbohydrates in this entry.

6.4 Ligands

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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	OG2	B	702	29/29	0.15	-1.39	24,41,71,80	0
2	OG2	A	701	29/29	0.14	-1.57	25,39,75,121	0
3	SO4	B	701	5/5	0.12	-2.77	52,56,57,57	0

6.5 Other polymers

There are no such residues in this entry.