



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 09:32 PM UTC

PDB ID : 8Z7K / pdb_00008z7k
Title : Crystal structure of Hemolysin co-regulated protein 1 (Hcp1) VariantB from Burkholderia pseudomallei
Authors : Lebedev, A.A.; Charoenwattanasatien, R.; Tandhavanant, S.; Chantratita, N.
Deposited on : 2024-04-20
Resolution : 1.58 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

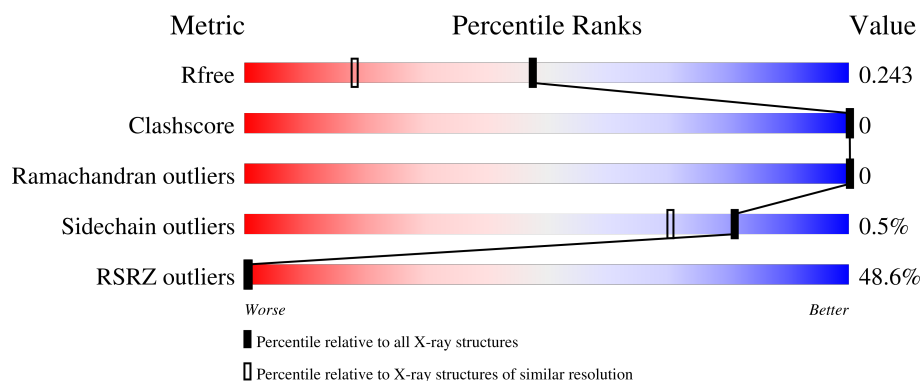
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.58 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	1094 (1.58-1.58)
Clashscore	190562	1105 (1.58-1.58)
Ramachandran outliers	187476	1082 (1.58-1.58)
Sidechain outliers	187428	1081 (1.58-1.58)
RSRZ outliers	180081	1094 (1.58-1.58)

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	178	37% 77% 22%
1	B	178	40% 81% 19%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4475 atoms, of which 2118 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 Hcp family type VI secretion system effector.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	138	Total	C	H	N	O	S	0	4	0
			2133	701	1045	176	205	6			
1	B	144	Total	C	H	N	O	S	0	2	0
			2192	720	1073	182	211	6			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	MET	-	initiating methionine	UNP G4XEK9
A	-6	ALA	-	expression tag	UNP G4XEK9
A	-5	ALA	-	expression tag	UNP G4XEK9
A	-4	HIS	-	expression tag	UNP G4XEK9
A	-3	HIS	-	expression tag	UNP G4XEK9
A	-2	HIS	-	expression tag	UNP G4XEK9
A	-1	HIS	-	expression tag	UNP G4XEK9
A	0	HIS	-	expression tag	UNP G4XEK9
A	1	HIS	-	expression tag	UNP G4XEK9
A	14	THR	GLN	engineered mutation	UNP G4XEK9
A	90	TYR	HIS	engineered mutation	UNP G4XEK9
A	91	SER	ARG	engineered mutation	UNP G4XEK9
A	94	ALA	THR	engineered mutation	UNP G4XEK9
A	96	LYS	THR	engineered mutation	UNP G4XEK9
A	97	GLU	-	insertion	UNP G4XEK9
A	168	LYS	THR	engineered mutation	UNP G4XEK9
B	-7	MET	-	initiating methionine	UNP G4XEK9
B	-6	ALA	-	expression tag	UNP G4XEK9
B	-5	ALA	-	expression tag	UNP G4XEK9
B	-4	HIS	-	expression tag	UNP G4XEK9
B	-3	HIS	-	expression tag	UNP G4XEK9
B	-2	HIS	-	expression tag	UNP G4XEK9
B	-1	HIS	-	expression tag	UNP G4XEK9
B	0	HIS	-	expression tag	UNP G4XEK9
B	1	HIS	-	expression tag	UNP G4XEK9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	14	THR	GLN	engineered mutation	UNP G4XEK9
B	90	TYR	HIS	engineered mutation	UNP G4XEK9
B	91	SER	ARG	engineered mutation	UNP G4XEK9
B	94	ALA	THR	engineered mutation	UNP G4XEK9
B	96	LYS	THR	engineered mutation	UNP G4XEK9
B	97	GLU	-	insertion	UNP G4XEK9
B	168	LYS	THR	engineered mutation	UNP G4XEK9

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

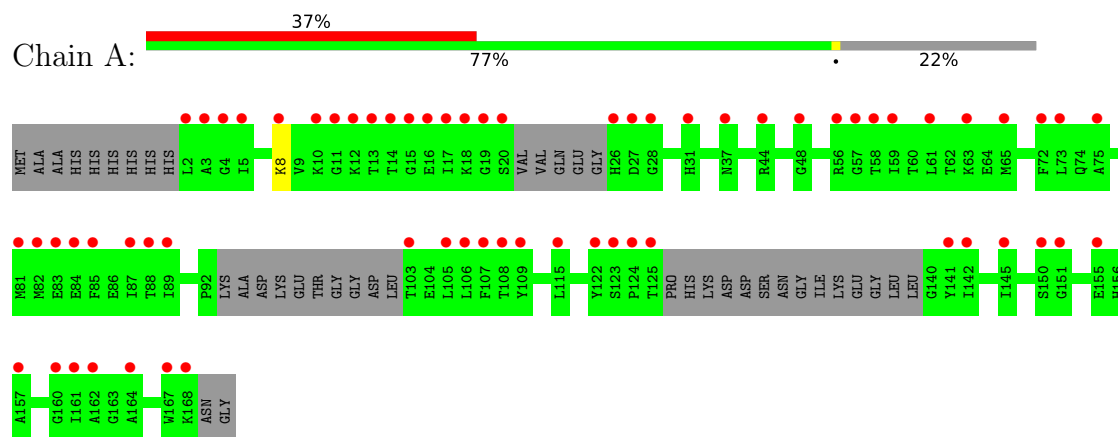
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	66	Total	O	0	0
			66	66		
3	B	64	Total	O	0	0
			64	64		

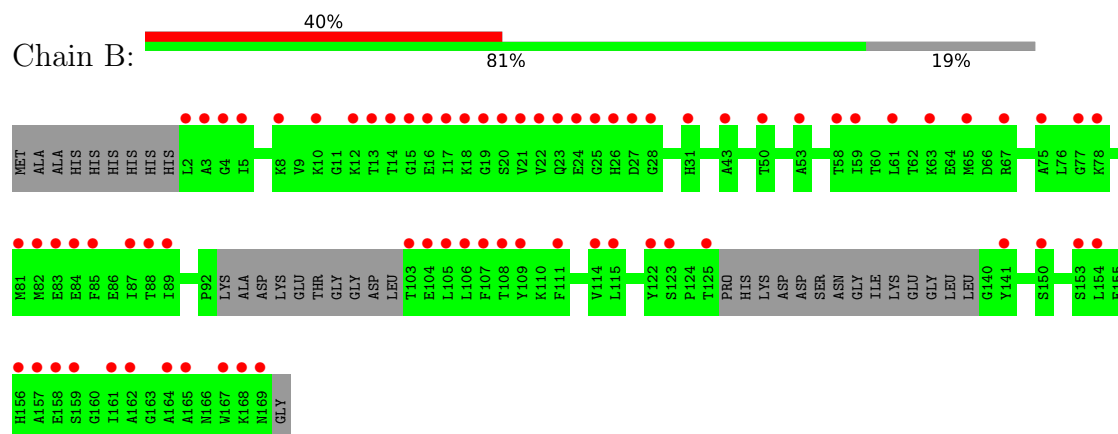
3 Residue-property plots [i](#)

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: Hcp family type VI secretion system effector



- Molecule 1: Hcp family type VI secretion system effector



4 Data and refinement statistics

Property	Value	Source
Space group	P 6	Depositor
Cell constants a, b, c, α , β , γ	82.72Å 82.72Å 64.07Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.76 – 1.58 47.76 – 1.58	Depositor EDS
% Data completeness (in resolution range)	95.9 (47.76-1.58) 95.9 (47.76-1.58)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.17 (at 1.58Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.225 , 0.243 0.224 , 0.243	Depositor DCC
R_{free} test set	1558 reflections (4.56%)	wwPDB-VP
Wilson B-factor (Å ²)	27.1	Xtriage
Anisotropy	0.584	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.22 , 60.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.052 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	4475	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.13% 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	0.67	0/1128	1.06	0/1514
1	B	0.68	0/1149	1.05	0/1545
All	All	0.68	0/2277	1.05	0/3059

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

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	1088	1045	1054	0	0
1	B	1119	1073	1091	0	0
2	A	10	0	0	0	0
2	B	10	0	0	0	0
3	A	66	0	0	0	0
3	B	64	0	0	0	0
All	All	2357	2118	2145	0	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 0.

There are no clashes within the asymmetric unit.

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	134/178 (75%)	132 (98%)	2 (2%)	0	100	100
1	B	140/178 (79%)	136 (97%)	4 (3%)	0	100	100
All	All	274/356 (77%)	268 (98%)	6 (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	113/145 (78%)	112 (99%)	1 (1%)	70	52
1	B	115/145 (79%)	115 (100%)	0	100	100
All	All	228/290 (79%)	227 (100%)	1 (0%)	81	75

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	LYS

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

Mol	Chain	Res	Type
1	A	46	GLN
1	B	46	GLN
1	B	121	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

4 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	SO4	B	202	-	4,4,4	0.33	0	6,6,6	0.28	0
2	SO4	A	202	-	4,4,4	0.39	0	6,6,6	0.19	0
2	SO4	B	201	-	4,4,4	0.32	0	6,6,6	0.08	0
2	SO4	A	201	-	4,4,4	0.28	0	6,6,6	0.06	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	138/178 (77%)	2.49	65 (47%) 0 1	8, 16, 29, 44	138 (100%)
1	B	144/178 (80%)	2.54	72 (50%) 0 0	10, 16, 31, 54	144 (100%)
All	All	282/356 (79%)	2.52	137 (48%) 0 1	8, 16, 31, 54	282 (100%)

All (137) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	19	GLY	11.3
1	B	4	GLY	10.3
1	B	21	VAL	9.5
1	A	27	ASP	9.3
1	B	27	ASP	9.1
1	A	19	GLY	8.8
1	B	25	GLY	8.6
1	B	28	GLY	8.6
1	A	105	LEU	7.7
1	B	22	VAL	7.7
1	A	106	LEU	7.6
1	B	105	LEU	7.5
1	A	157	ALA	7.5
1	A	28	GLY	7.3
1	A	5	ILE	7.2
1	B	103	THR	7.2
1	A	125	THR	7.0
1	A	103	THR	6.8
1	B	3	ALA	6.8
1	A	162	ALA	6.6
1	A	20	SER	6.4
1	B	24	GLU	6.4
1	A	161	ILE	6.4
1	A	107	PHE	6.3

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Mol	Chain	Res	Type	RSRZ
1	A	167	TRP	5.9
1	B	20	SER	5.8
1	B	107	PHE	5.8
1	A	3	ALA	5.8
1	B	122	TYR	5.7
1	B	5	ILE	5.3
1	B	161	ILE	5.3
1	A	122	TYR	5.2
1	B	167	TRP	5.2
1	B	31	HIS	4.8
1	B	13	THR	4.7
1	B	67	ARG	4.6
1	B	63	LYS	4.6
1	B	169	ASN	4.5
1	A	87	ILE	4.4
1	A	26	HIS	4.3
1	A	81[A]	MET	4.3
1	A	16	GLU	4.3
1	B	18	LYS	4.2
1	A	83	GLU	4.1
1	A	63	LYS	4.1
1	B	162	ALA	4.0
1	A	4	GLY	4.0
1	B	59	ILE	4.0
1	B	125	THR	3.9
1	A	65	MET	3.9
1	A	59	ILE	3.9
1	B	81[A]	MET	3.8
1	B	89	ILE	3.7
1	A	31	HIS	3.7
1	A	155[A]	GLU	3.6
1	B	26	HIS	3.6
1	A	13	THR	3.5
1	B	159	SER	3.5
1	B	61	LEU	3.5
1	B	141	TYR	3.4
1	A	2	LEU	3.4
1	B	123	SER	3.3
1	A	168	LYS	3.3
1	B	14	THR	3.3
1	B	168	LYS	3.2
1	B	83	GLU	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	150	SER	3.2
1	B	16	GLU	3.2
1	B	23	GLN	3.2
1	A	89	ILE	3.2
1	B	12	LYS	3.2
1	A	124	PRO	3.2
1	A	10	LYS	3.1
1	B	87	ILE	3.1
1	A	141	TYR	3.1
1	A	75	ALA	3.1
1	B	157	ALA	3.1
1	B	85	PHE	3.0
1	B	84	GLU	3.0
1	B	156	HIS	3.0
1	A	142	ILE	3.0
1	A	72	PHE	3.0
1	A	58	THR	3.0
1	A	61	LEU	2.9
1	B	43	ALA	2.9
1	A	160	GLY	2.9
1	B	88	THR	2.9
1	B	104	GLU	2.9
1	A	8	LYS	2.8
1	A	11	GLY	2.8
1	A	15	GLY	2.8
1	A	164	ALA	2.8
1	B	58	THR	2.8
1	A	109	TYR	2.8
1	B	158	GLU	2.7
1	A	82[A]	MET	2.7
1	A	85	PHE	2.7
1	A	108	THR	2.7
1	A	84	GLU	2.7
1	B	115	LEU	2.6
1	A	18	LYS	2.6
1	B	17	ILE	2.6
1	B	65	MET	2.6
1	A	151	GLY	2.6
1	B	8	LYS	2.5
1	A	37	ASN	2.5
1	B	2	LEU	2.5
1	B	15	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	153	SER	2.5
1	A	115	LEU	2.5
1	B	165	ALA	2.4
1	A	123	SER	2.4
1	B	154	LEU	2.4
1	B	164	ALA	2.4
1	B	109	TYR	2.4
1	A	48	GLY	2.4
1	B	108	THR	2.3
1	B	106	LEU	2.3
1	B	111	PHE	2.3
1	A	17	ILE	2.3
1	A	145	ILE	2.3
1	A	44	ARG	2.2
1	A	88	THR	2.2
1	B	78	LYS	2.2
1	A	56	ARG	2.2
1	A	12	LYS	2.2
1	A	57	GLY	2.2
1	B	75	ALA	2.2
1	B	50	THR	2.2
1	A	150	SER	2.1
1	B	82[A]	MET	2.1
1	A	73	LEU	2.1
1	B	114	VAL	2.1
1	B	53	ALA	2.1
1	B	10	LYS	2.0
1	B	77	GLY	2.0
1	A	14	THR	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 ⓘ

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(Å ²)	Q<0.9
2	SO4	A	201	5/5	0.88	0.11	51,55,63,65	5
2	SO4	A	202	5/5	0.92	0.17	68,73,78,80	5
2	SO4	B	201	5/5	0.93	0.09	50,50,60,63	5
2	SO4	B	202	5/5	0.94	0.12	41,42,50,50	5

6.5 Other polymers [i](#)

There are no such residues in this entry.