



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 13, 2020 – 04:54 PM BST

PDB ID : 4JBL
Title : Crystal structure of O-Acetyl Serine Sulfhydrylase from *Entamoeba histolytica* in complex with Methionine
Authors : Raj, I.; Gourinath, S.
Deposited on : 2013-02-19
Resolution : 2.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 : 2.14.4.dev1
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) : 2.14.4.dev1

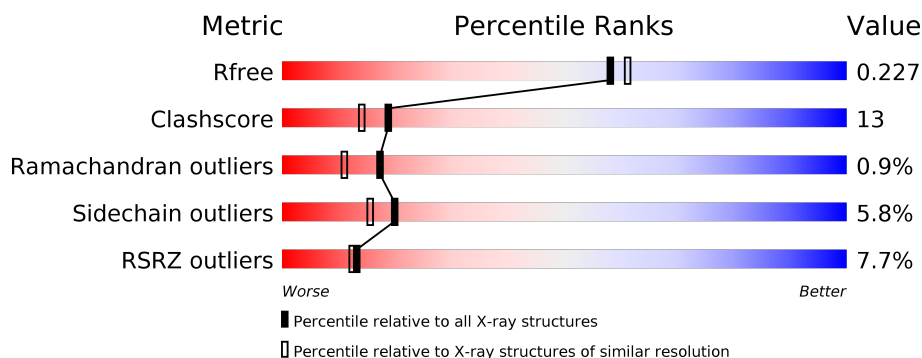
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	339	<div> <div>2%</div> <div> <div></div> <div>83%</div> <div>13%</div> <div>.</div> </div> </div>
1	B	339	<div> <div>13%</div> <div> <div></div> <div>77%</div> <div>18%</div> <div>..</div> </div> </div>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 5529 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.

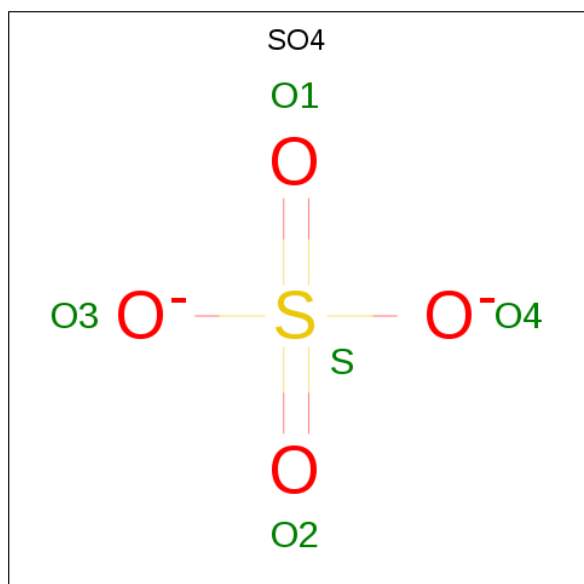
- Molecule 1 is a protein called Cysteine synthase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	339	Total	C	N	O	P	S	0	0	0
			2609	1655	441	497	1	15			
1	B	335	Total	C	N	O	P	S	0	0	0
			2572	1633	433	491	1	14			

There are 4 discrepancies between the modelled and reference sequences:

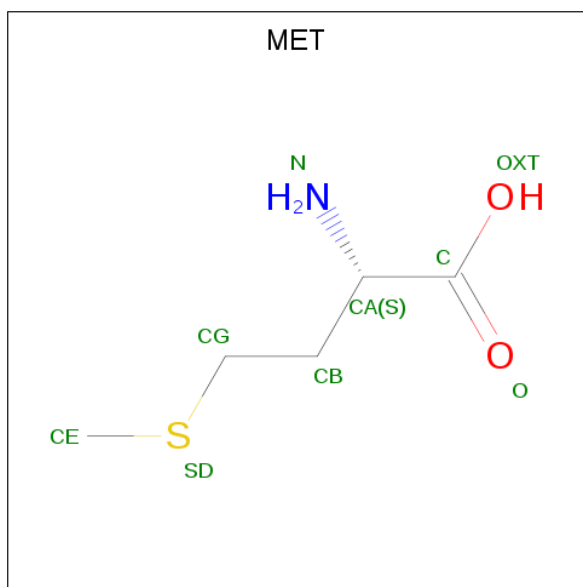
Chain	Residue	Modelled	Actual	Comment	Reference
A	338	HIS	-	EXPRESSION TAG	UNP O15570
A	339	HIS	-	EXPRESSION TAG	UNP O15570
B	338	HIS	-	EXPRESSION TAG	UNP O15570
B	339	HIS	-	EXPRESSION TAG	UNP O15570

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 3 is METHIONINE (three-letter code: MET) (formula: $C_5H_{11}NO_2S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C N O S 9 5 1 2 1	0	0

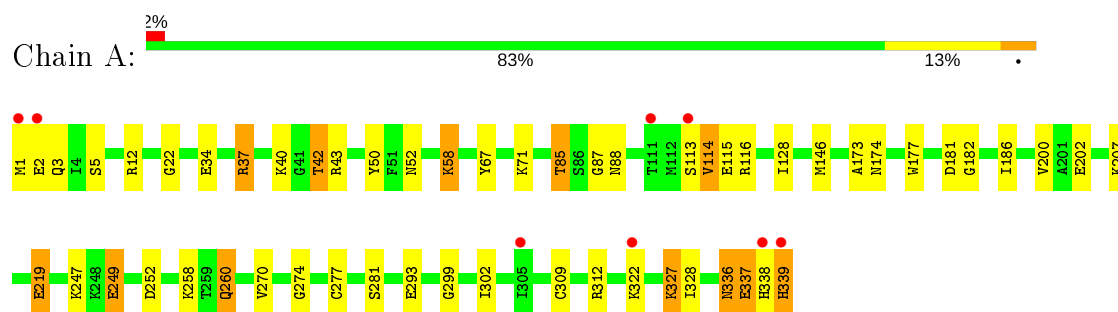
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	174	Total O 174 174	0	0
4	B	155	Total O 155 155	0	0

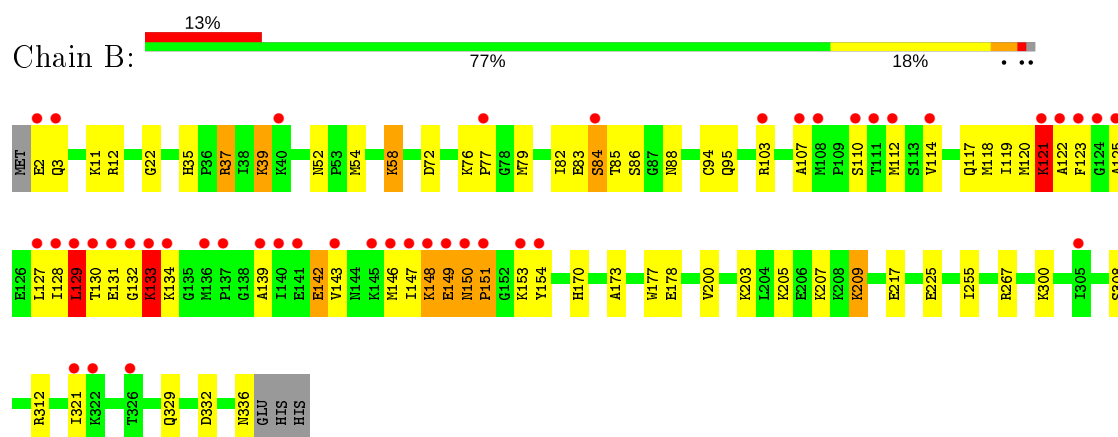
3 Residue-property plots [i](#)

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: Cysteine synthase



• Molecule 1: Cysteine synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α , β , γ	80.42Å 80.42Å 112.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.43 – 2.00 28.43 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.5 (28.43-2.00) 97.6 (28.43-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.15 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.178 , 0.225 0.185 , 0.227	Depositor DCC
R_{free} test set	2334 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	23.0	Xtriage
Anisotropy	0.120	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 49.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.024 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5529	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.54% 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: LLP, 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	1.03	1/2628 (0.0%)	1.00	7/3539 (0.2%)
1	B	1.09	1/2589 (0.0%)	1.04	10/3487 (0.3%)
All	All	1.06	2/5217 (0.0%)	1.02	17/7026 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	337	GLU	CD-OE2	-7.46	1.17	1.25
1	B	308	SER	C-N	5.04	1.45	1.34

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	37	ARG	NE-CZ-NH2	-8.48	116.06	120.30
1	B	12	ARG	NE-CZ-NH1	7.69	124.14	120.30
1	A	12	ARG	NE-CZ-NH1	7.54	124.07	120.30
1	B	72	ASP	CB-CG-OD1	-7.40	111.64	118.30
1	B	72	ASP	CB-CG-OD2	7.28	124.85	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	2609	0	2664	36	0
1	B	2572	0	2632	103	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
3	B	9	0	8	1	0
4	A	174	0	0	1	0
4	B	155	0	0	3	0
All	All	5529	0	5304	138	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 13.

The worst 5 of 138 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:258:LYS:HB3	1:A:260:GLN:NE2	1.51	1.24
1:B:110:SER:HA	1:B:129:LEU:CD1	1.69	1.22
1:B:121:LYS:HE2	1:B:122:ALA:HB2	1.24	1.11
1:A:258:LYS:HB3	1:A:260:GLN:HE21	1.01	1.06
1:B:110:SER:HA	1:B:129:LEU:HD12	1.37	1.02

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	336/339 (99%)	329 (98%)	7 (2%)	0	100	100
1	B	332/339 (98%)	310 (93%)	16 (5%)	6 (2%)	8	3
All	All	668/678 (98%)	639 (96%)	23 (3%)	6 (1%)	17	11

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	121	LYS
1	B	149	GLU
1	B	133	LYS
1	B	148	LYS
1	B	150	ASN

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	278/278 (100%)	261 (94%)	17 (6%)	18	14
1	B	274/278 (99%)	259 (94%)	15 (6%)	21	17
All	All	552/556 (99%)	520 (94%)	32 (6%)	20	15

5 of 32 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	322	LYS
1	B	2	GLU
1	B	209	LYS
1	A	339	HIS
1	B	3	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	144	ASN
1	A	260	GLN
1	B	52	ASN
1	A	88	ASN
1	B	3	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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$
1	LLP	B	58	1	23,24,25	2.44	7 (30%)	25,32,34	1.82	9 (36%)
1	LLP	A	58	1	23,24,25	2.67	5 (21%)	25,32,34	1.55	5 (20%)

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
1	LLP	B	58	1	-	1/16/17/19	0/1/1/1
1	LLP	A	58	1	-	0/16/17/19	0/1/1/1

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	58	LLP	C3-C2	8.30	1.49	1.40
1	B	58	LLP	C3-C2	7.60	1.48	1.40
1	A	58	LLP	C4-C3	5.44	1.49	1.40
1	A	58	LLP	C4'-NZ	4.86	1.43	1.27
1	B	58	LLP	C4-C3	4.50	1.47	1.40

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	58	LLP	C4-C3-C2	-3.87	117.80	120.19
1	B	58	LLP	C6-N1-C2	3.68	125.99	119.17
1	A	58	LLP	C6-N1-C2	2.82	124.39	119.17
1	B	58	LLP	C4-C3-C2	-2.75	118.48	120.19
1	B	58	LLP	OP4-C5'-C5	2.74	114.57	109.35

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	58	LLP	CG-CD-CE-NZ

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	58	LLP	2	0
1	A	58	LLP	2	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	$\# Z > 2$
3	MET	B	401	-	4,8,8	1.44	1 (25%)	2,9,9	0.83	0
2	SO4	A	401	-	4,4,4	0.49	0	6,6,6	0.44	0
2	SO4	B	402	-	4,4,4	0.39	0	6,6,6	0.32	0

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
3	MET	B	401	-	-	0/4/8/8	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	401	MET	CA-N	2.75	1.53	1.47

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	401	MET	1	0

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	338/339 (99%)	-0.01	8 (2%) 59 57	12, 21, 42, 68	0
1	B	334/339 (98%)	0.47	44 (13%) 3 2	10, 22, 64, 111	0
All	All	672/678 (99%)	0.23	52 (7%) 13 12	10, 22, 55, 111	0

The worst 5 of 52 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	127	LEU	7.0
1	B	141	GLU	6.3
1	B	123	PHE	5.6
1	B	133	LYS	5.4
1	B	143	VAL	5.3

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	LLP	A	58	24/25	0.98	0.14	12,14,16,16	0
1	LLP	B	58	24/25	0.99	0.17	11,14,15,16	0

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(Å ²)	Q<0.9
2	SO4	B	402	5/5	0.93	0.18	63,65,72,73	0
3	MET	B	401	9/9	0.95	0.14	26,28,32,35	0
2	SO4	A	401	5/5	0.97	0.16	47,50,52,61	0

6.5 Other polymers [i](#)

There are no such residues in this entry.