wwPDB X-ray Structure Validation Summary Report (i)

Jun 25, 2024 – 09:03 PM EDT

PDB ID	:	6RP2
Title	:	Threonine to Cysteine (T225C) variant of E coli hydrogenase-1
Authors	:	Carr, S.B.; Armstrong, F.A.; Zhang, L.
Deposited on	:	2019-05-13
Resolution	:	1.35 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 (i) 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 (i)) were used in the production of this report:

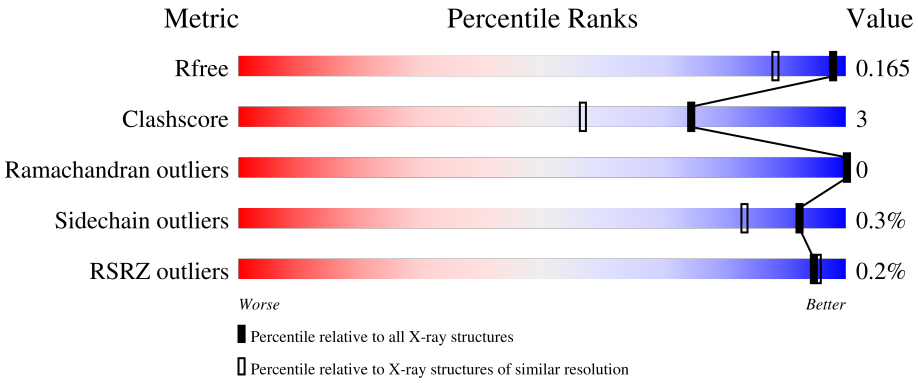
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.35 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	1509 (1.38-1.34)
Clashscore	141614	1551 (1.38-1.34)
Ramachandran outliers	138981	1530 (1.38-1.34)
Sidechain outliers	138945	1530 (1.38-1.34)
RSRZ outliers	127900	1487 (1.38-1.34)

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 <=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	S	324	% 74% 7% • 19%
1	T	324	75% 6% • 19%
2	L	582	93% 6%
2	M	582	92% 7%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
12	LI	L	605	-	-	-	X

2 Entry composition (i)

There are 13 unique types of molecules in this entry. The entry contains 15251 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 Hydrogenase-1 small chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	S	264	Total	C	N	O	S	0	14	0
			2103	1337	356	388	22			
1	T	264	Total	C	N	O	S	0	12	0
			2110	1340	365	382	23			

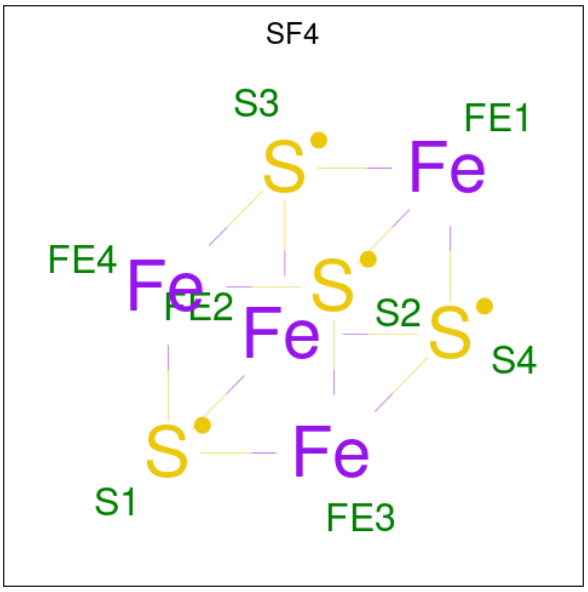
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	225	CYS	THR	conflict	UNP P69740
T	225	CYS	THR	conflict	UNP P69740

- Molecule 2 is a protein called Hydrogenase-1 large chain.

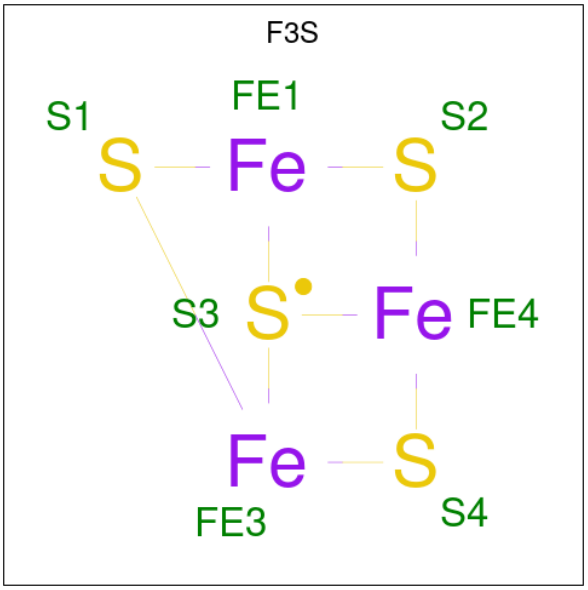
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	581	Total	C	N	O	S	0	25	0
			4693	2988	821	855	29			
2	M	581	Total	C	N	O	S	0	29	0
			4710	3005	811	863	31			

- Molecule 3 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



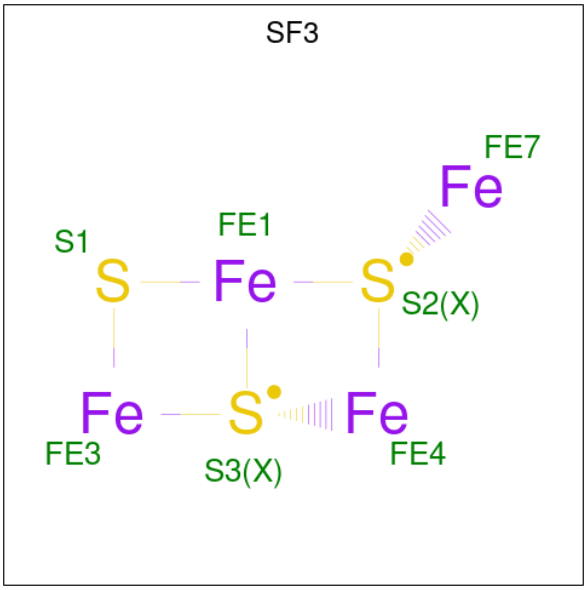
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	S	1	Total Fe S 8 4 4	0	0
3	T	1	Total Fe S 8 4 4	0	0

- Molecule 4 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe_3S_4).



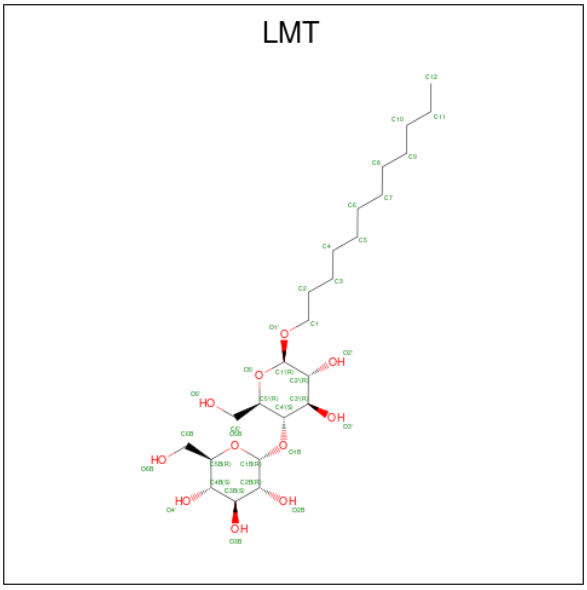
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	S	1	Total Fe S 7 3 4	0	0
4	T	1	Total Fe S 7 3 4	0	0

- Molecule 5 is FE4-S3 CLUSTER (three-letter code: SF3) (formula: Fe_4S_3).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	S	1	Total Fe S 8 5 3	0	1
5	T	1	Total Fe S 8 5 3	0	1

- Molecule 6 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).

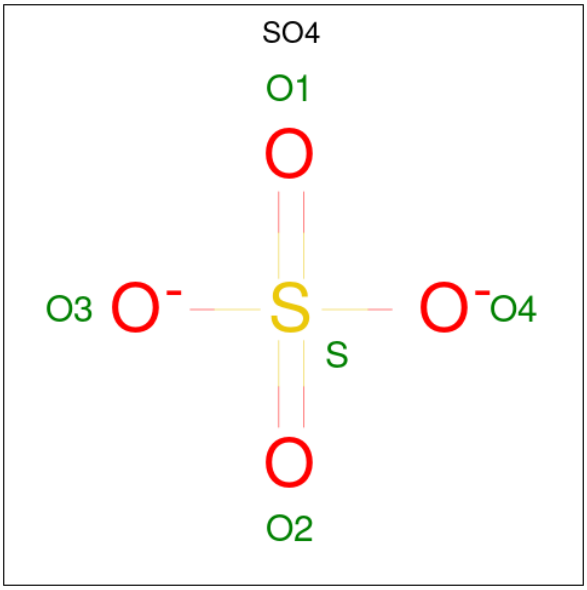


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	S	1	Total C O 24 18 6	0	0
6	T	1	Total C O 14 13 1	0	0

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

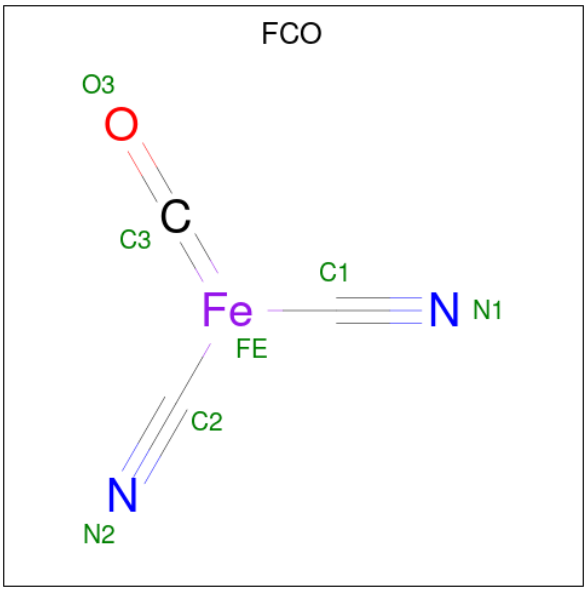
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	S	1	Total Cl 1 1	0	0
7	T	1	Total Cl 1 1	0	0

- Molecule 8 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	L	1	Total O S 5 4 1	0	0
8	M	1	Total O S 5 4 1	0	0

- Molecule 9 is CARBONMONOXIDE-(DICYANO) IRON (three-letter code: FCO) (formula: C_3FeN_2O).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	L	1	Total C Fe N O 7 3 1 2 1	0	0
9	M	1	Total C Fe N O 7 3 1 2 1	0	0

- Molecule 10 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	L	1	Total Ni 1 1	0	0
10	M	1	Total Ni 1 1	0	0

- Molecule 11 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	L	1	Total Mg 1 1	0	0
11	M	1	Total Mg 1 1	0	0

- Molecule 12 is LITHIUM ION (three-letter code: LI) (formula: Li).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	L	1	Total Li 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	M	1	Total Li 1 1	0	0

- Molecule 13 is water.

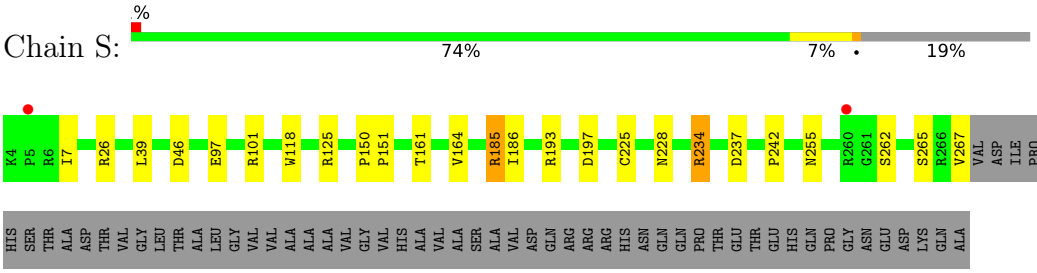
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	S	231	Total O 231 231	0	0
13	L	521	Total O 521 521	0	0
13	T	217	Total O 217 217	0	0
13	M	550	Total O 550 550	0	0

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.

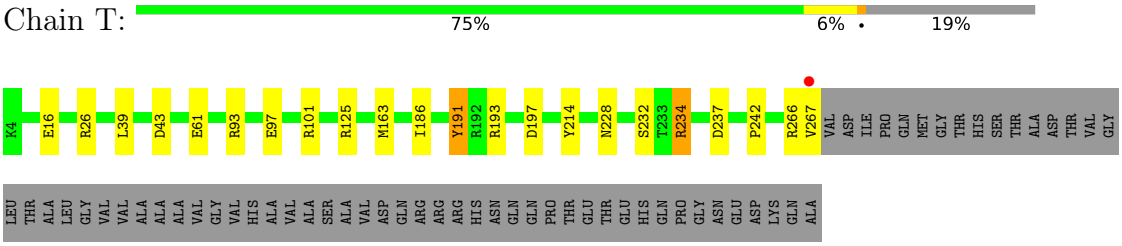
• Molecule 1: Hydrogenase-1 small chain

Chain S:



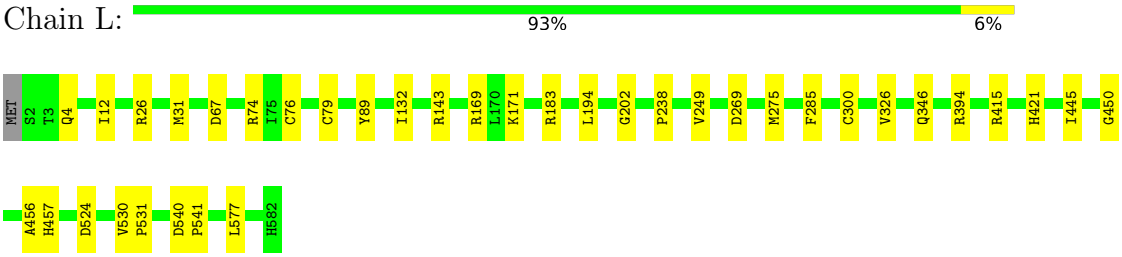
• Molecule 1: Hydrogenase-1 small chain

Chain T:



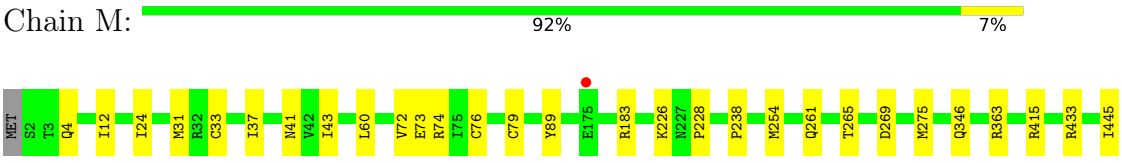
• Molecule 2: Hydrogenase-1 large chain

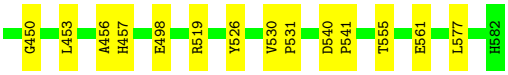
Chain L:



• Molecule 2: Hydrogenase-1 large chain

Chain M:




G450
L453
A456
H457
E498
R519
Y526
V530
P531
D540
P541
T555
E561
L577
H582

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	93.72Å 97.52Å 183.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	86.07 – 1.35 86.07 – 1.35	Depositor EDS
% Data completeness (in resolution range)	99.5 (86.07-1.35) 99.5 (86.07-1.35)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.32 (at 1.35Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.141 , 0.159 0.149 , 0.165	Depositor DCC
R_{free} test set	18097 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	13.3	Xtriage
Anisotropy	0.004	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 44.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	15251	wwPDB-VP
Average B, all atoms (Å^2)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.12% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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, CSO, LMT, MG, F3S, CL, FCO, LI, SF3, SF4, NI

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	S	0.76	1/2194 (0.0%)	0.97	9/2980 (0.3%)
1	T	0.75	1/2189 (0.0%)	0.98	12/2971 (0.4%)
2	L	0.73	0/4880	0.89	7/6632 (0.1%)
2	M	0.73	2/4907 (0.0%)	0.90	7/6671 (0.1%)
All	All	0.74	4/14170 (0.0%)	0.92	35/19254 (0.2%)

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	S	0	1
1	T	0	1
All	All	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	T	16	GLU	CD-OE2	-5.86	1.19	1.25
1	S	97	GLU	CD-OE1	-5.80	1.19	1.25
2	M	561	GLU	CD-OE1	5.30	1.31	1.25
2	M	73	GLU	CD-OE1	5.03	1.31	1.25

The worst 5 of 35 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	M	89	TYR	CB-CG-CD1	10.55	127.33	121.00
1	S	234	ARG	NE-CZ-NH1	-9.00	115.80	120.30
2	L	89	TYR	CB-CG-CD1	8.37	126.02	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	M	89	TYR	CB-CG-CD2	-8.26	116.04	121.00
1	T	193	ARG	NE-CZ-NH2	-7.93	116.34	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	S	26	ARG	Sidechain
1	T	26	ARG	Sidechain

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	S	2103	0	2057	17	0
1	T	2110	0	2069	16	0
2	L	4693	0	4649	25	0
2	M	4710	0	4666	32	0
3	S	8	0	0	0	0
3	T	8	0	0	0	0
4	S	7	0	0	0	0
4	T	7	0	0	0	0
5	S	8	0	0	0	0
5	T	8	0	0	0	0
6	S	24	0	35	1	0
6	T	14	0	25	1	0
7	S	1	0	0	0	0
7	T	1	0	0	0	0
8	L	5	0	0	0	0
8	M	5	0	0	1	0
9	L	7	0	0	0	0
9	M	7	0	0	0	0
10	L	1	0	0	0	0
10	M	1	0	0	0	0
11	L	1	0	0	0	0
11	M	1	0	0	0	0
12	L	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	M	1	0	0	0	0
13	L	521	0	0	10	0
13	M	550	0	0	11	0
13	S	231	0	0	7	0
13	T	217	0	0	5	0
All	All	15251	0	13501	86	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 3.

The worst 5 of 86 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:T:39[B]:LEU:HD11	13:T:699:HOH:O	1.19	1.28
1:T:93[B]:ARG:CZ	1:T:97:GLU:OE1	1.86	1.22
2:M:269[B]:ASP:OD1	13:M:701:HOH:O	1.54	1.20
2:L:346[B]:GLN:OE1	13:L:702:HOH:O	1.57	1.18
2:M:457[A]:HIS:CD2	13:M:1007:HOH:O	1.95	1.15

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	S	276/324 (85%)	263 (95%)	13 (5%)	0	100	100
1	T	274/324 (85%)	264 (96%)	10 (4%)	0	100	100
2	L	604/582 (104%)	586 (97%)	18 (3%)	0	100	100
2	M	609/582 (105%)	593 (97%)	16 (3%)	0	100	100
All	All	1763/1812 (97%)	1706 (97%)	57 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	S	230/263 (88%)	229 (100%)	1 (0%)	91 81
1	T	228/263 (87%)	226 (99%)	2 (1%)	78 53
2	L	505/480 (105%)	504 (100%)	1 (0%)	93 84
2	M	510/480 (106%)	510 (100%)	0	100 100
All	All	1473/1486 (99%)	1469 (100%)	4 (0%)	92 83

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

Mol	Chain	Res	Type
1	S	242	PRO
2	L	524	ASP
1	T	191	TYR
1	T	242	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
2	M	439	ASN
2	M	467	GLN
2	L	421	HIS
2	M	61	GLN
2	M	261	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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	$\#\|Z\| > 2$
2	CSO	M	79	10,2,9	3,6,7	0.72	0	0,6,8	-	-
2	CSO	L	79	10,2,9	3,6,7	0.71	0	0,6,8	-	-

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	CSO	M	79	10,2,9	-	0/1/5/7	-
2	CSO	L	79	10,2,9	-	0/1/5/7	-

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.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	M	79	CSO	2	0
2	L	79	CSO	2	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 22 ligands modelled in this entry, 8 are monoatomic - leaving 14 for Mogul analysis.

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	$\#\|Z\| > 2$
8	SO4	L	601	-	4,4,4	0.31	0	6,6,6	0.31	0
5	SF3	T	403[B]	1	0,8,8	-	-	-		
4	F3S	T	402	1	0,9,9	-	-	-		
5	SF3	S	403[B]	1	0,8,8	-	-	-		
8	SO4	M	604	-	4,4,4	0.38	0	6,6,6	0.26	0
5	SF3	T	403[A]	1	0,8,8	-	-	-		
9	FCO	M	601	13,2	0,6,6	-	-	-		
4	F3S	S	402	1	0,9,9	-	-	-		
5	SF3	S	403[A]	1	0,8,8	-	-	-		
6	LMT	T	404	-	13,13,36	0.27	0	12,12,47	0.60	0
3	SF4	T	401	1	0,12,12	-	-	-		
6	LMT	S	404	-	24,24,36	0.68	0	29,29,47	1.46	6 (20%)
3	SF4	S	401	1	0,12,12	-	-	-		
9	FCO	L	602	13,2	0,6,6	-	-	-		

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
5	SF3	T	403[B]	1	-	-	0/2/2/2
4	F3S	T	402	1	-	-	0/3/3/3
5	SF3	S	403[B]	1	-	-	0/2/2/2
5	SF3	T	403[A]	1	-	-	0/2/2/2
4	F3S	S	402	1	-	-	0/3/3/3
6	LMT	T	404	-	-	5/11/11/61	-
5	SF3	S	403[A]	1	-	-	0/2/2/2
3	SF4	T	401	1	-	-	0/6/5/5
6	LMT	S	404	-	-	4/15/35/61	0/1/1/2
3	SF4	S	401	1	-	-	0/6/5/5

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	S	404	LMT	C1-O1'-C1'	4.57	121.43	113.84
6	S	404	LMT	C3-C2-C1	2.58	124.94	113.49
6	S	404	LMT	O5'-C1'-C2'	-2.44	105.19	110.35
6	S	404	LMT	O5'-C5'-C6'	2.17	111.82	106.44
6	S	404	LMT	O3'-C3'-C2'	2.12	115.26	110.35

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

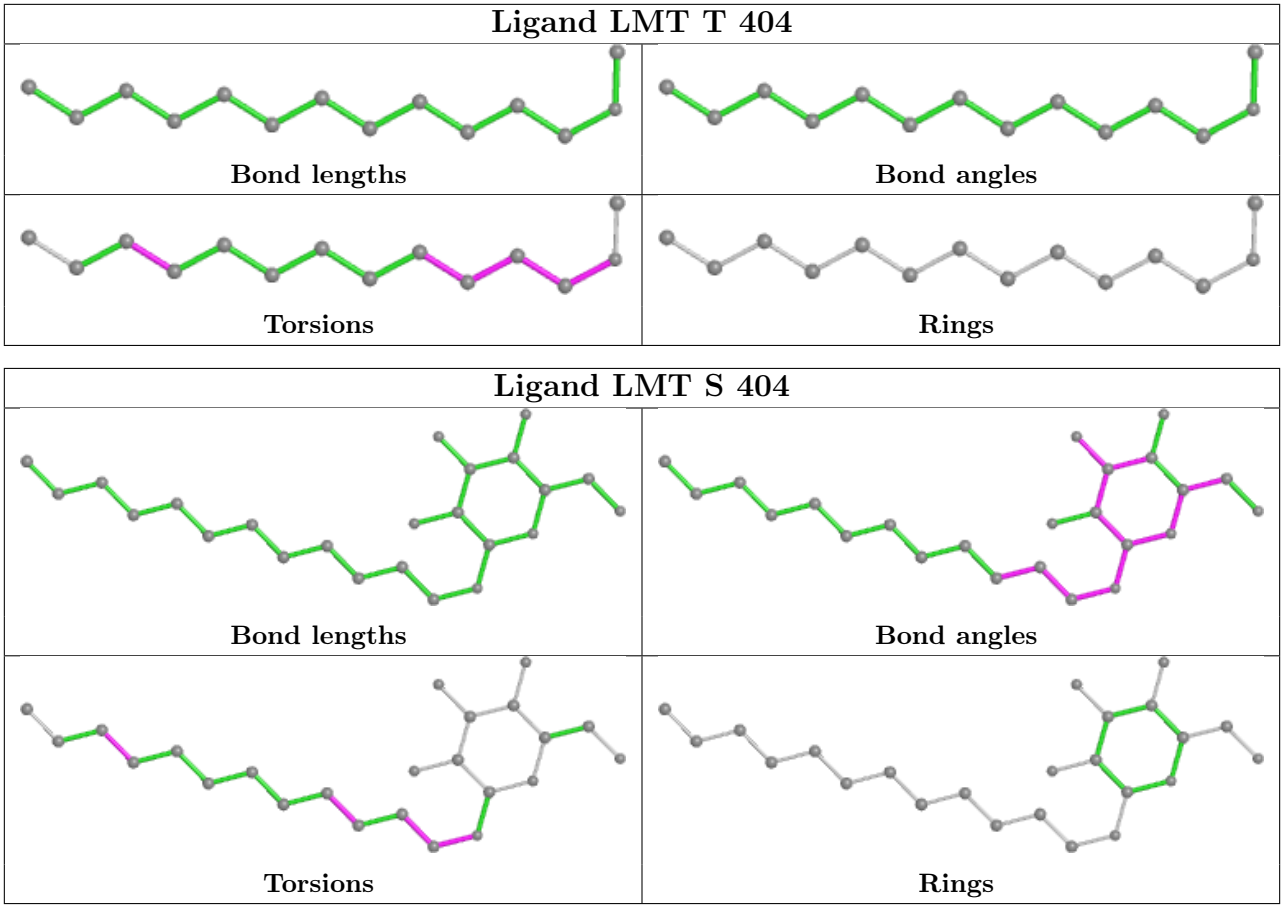
Mol	Chain	Res	Type	Atoms
6	S	404	LMT	C2-C1-O1'-C1'
6	T	404	LMT	O1'-C1-C2-C3
6	S	404	LMT	O1'-C1-C2-C3
6	T	404	LMT	C2-C3-C4-C5
6	T	404	LMT	C1-C2-C3-C4

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	M	604	SO4	1	0
6	T	404	LMT	1	0
6	S	404	LMT	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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, 95^{th} 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	S	264/324 (81%)	-0.08	2 (0%)	86	89	9, 12, 21, 40	0
1	T	264/324 (81%)	-0.04	1 (0%)	92	93	10, 13, 22, 37	1 (0%)
2	L	580/582 (99%)	-0.09	0	100	100	9, 13, 24, 42	2 (0%)
2	M	580/582 (99%)	-0.13	1 (0%)	95	95	9, 13, 22, 40	1 (0%)
All	All	1688/1812 (93%)	-0.10	4 (0%)	95	95	9, 13, 23, 42	4 (0%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	S	260	ARG	2.2
2	M	175	GLU	2.2
1	S	5	PRO	2.2
1	T	267	VAL	2.1

6.2 Non-standard residues in protein, DNA, RNA chains

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, 95^{th} 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	CSO	L	79	7/8	0.97	0.09	11,11,12,19	1
2	CSO	M	79	7/8	0.97	0.09	10,11,12,15	1

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands (i)

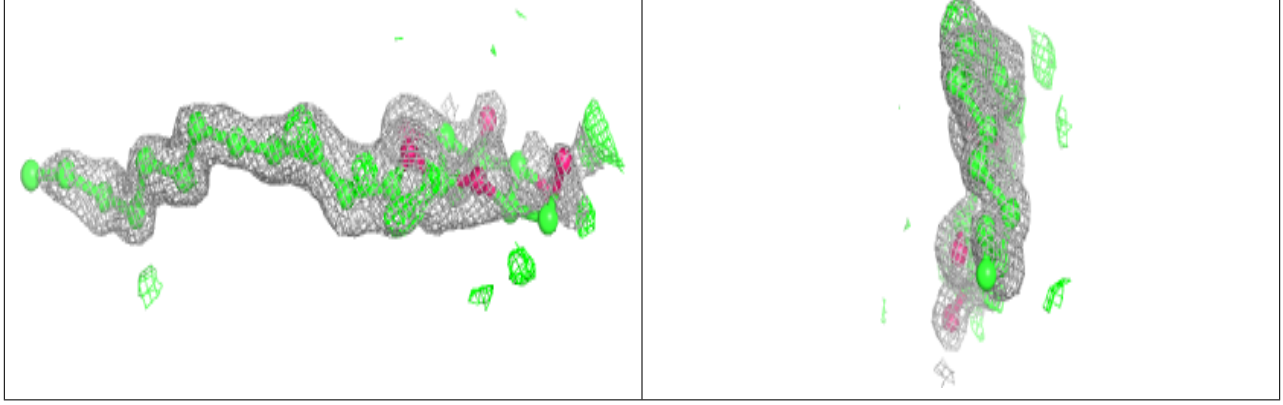
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
6	LMT	S	404	24/35	0.73	0.18	18,25,30,35	24
12	LI	L	605	1/1	0.74	0.49	17,17,17,17	0
6	LMT	T	404	14/35	0.76	0.26	17,19,26,27	14
8	SO4	M	604	5/5	0.89	0.12	27,28,30,30	5
8	SO4	L	601	5/5	0.94	0.17	20,23,24,25	0
12	LI	M	605	1/1	0.95	0.11	16,16,16,16	0
5	SF3	T	403[A]	7/7	0.99	0.07	9,11,11,12	1
5	SF3	T	403[B]	7/7	0.99	0.07	10,11,12,16	1
9	FCO	M	601	7/7	0.99	0.07	10,11,12,12	0
10	NI	L	603	1/1	0.99	0.06	16,16,16,16	0
10	NI	M	602	1/1	0.99	0.05	16,16,16,16	0
7	CL	S	405	1/1	0.99	0.07	15,15,15,15	0
7	CL	T	405	1/1	0.99	0.07	16,16,16,16	0
3	SF4	T	401	8/8	1.00	0.06	10,10,11,11	0
9	FCO	L	602	7/7	1.00	0.07	10,11,11,11	0
4	F3S	S	402	7/7	1.00	0.06	10,10,11,11	0
4	F3S	T	402	7/7	1.00	0.07	10,10,11,11	0
5	SF3	S	403[A]	7/7	1.00	0.07	8,10,11,11	1
11	MG	L	604	1/1	1.00	0.07	9,9,9,9	0
11	MG	M	603	1/1	1.00	0.08	9,9,9,9	0
5	SF3	S	403[B]	7/7	1.00	0.07	10,10,11,16	1
3	SF4	S	401	8/8	1.00	0.06	10,10,11,11	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

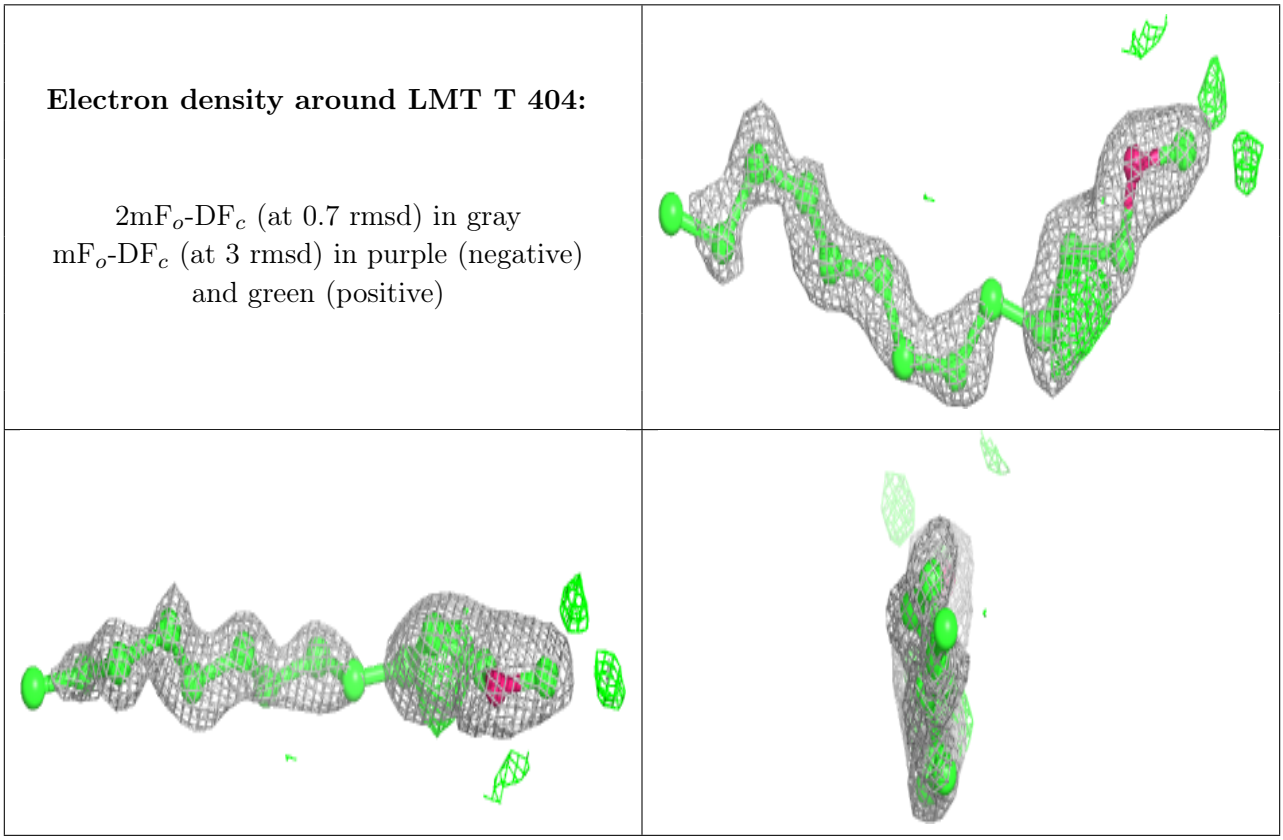
Electron density around LMT S 404:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around LMT T 404:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.