



# Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 06:48 am BST

PDB ID : 3USE  
Title : Crystal Structure of E. coli hydrogenase-1 in its as-isolated form  
Authors : Volbeda, A.; Fontecilla-Camps, J.C.; Darnault, C.  
Deposited on : 2011-11-23  
Resolution : 1.67 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](mailto: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.

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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 : 2.11  
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) : 2.11

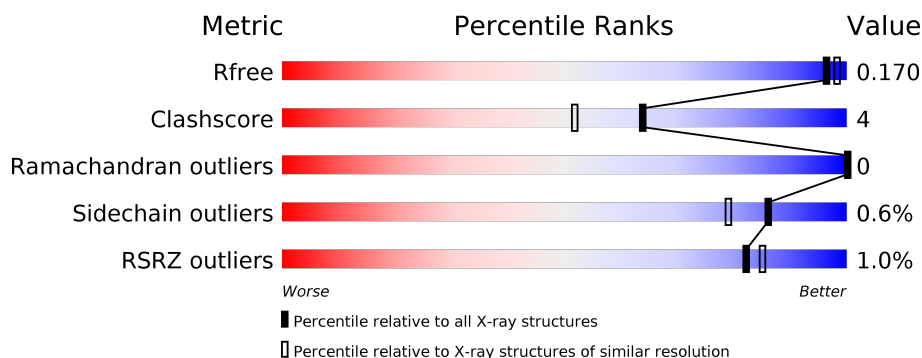
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.67 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	6780 (1.70-1.66)
Clashscore	141614	7310 (1.70-1.66)
Ramachandran outliers	138981	7173 (1.70-1.66)
Sidechain outliers	138945	7172 (1.70-1.66)
RSRZ outliers	127900	6661 (1.70-1.66)

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  $\geq 3$ , 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	S	335	<div> <div>%</div> <div> <div></div> <div>71%</div> <div>9%</div> <div>20%</div> </div> </div>
1	T	335	<div> <div>%</div> <div> <div></div> <div>73%</div> <div>7%</div> <div>20%</div> </div> </div>
2	L	582	<div> <div>%</div> <div> <div></div> <div>92%</div> <div>8%</div> </div> </div>
2	M	582	<div> <div>%</div> <div> <div></div> <div>93%</div> <div>7%</div> </div> </div>

## 2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 15199 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	268	Total	C	N	O	S	4	16	0
			2161	1376	370	394	21			
1	T	268	Total	C	N	O	S	0	17	0
			2172	1382	372	397	21			

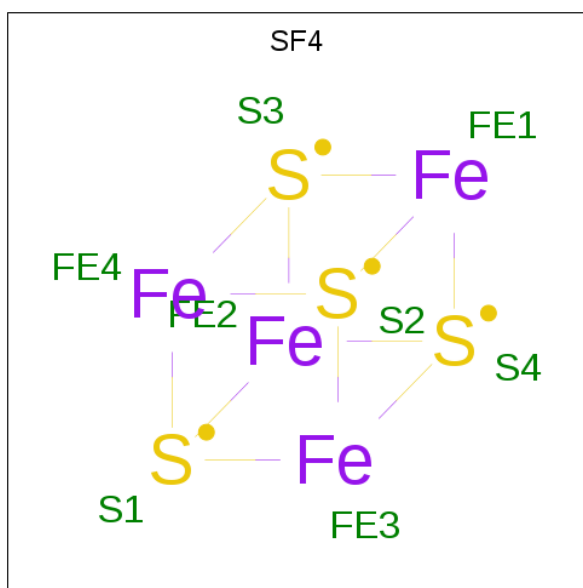
There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	328	ARG	-	EXPRESSION TAG	UNP P69739
S	329	SER	-	EXPRESSION TAG	UNP P69739
S	330	HIS	-	EXPRESSION TAG	UNP P69739
S	331	HIS	-	EXPRESSION TAG	UNP P69739
S	332	HIS	-	EXPRESSION TAG	UNP P69739
S	333	HIS	-	EXPRESSION TAG	UNP P69739
S	334	HIS	-	EXPRESSION TAG	UNP P69739
S	335	HIS	-	EXPRESSION TAG	UNP P69739
T	328	ARG	-	EXPRESSION TAG	UNP P69739
T	329	SER	-	EXPRESSION TAG	UNP P69739
T	330	HIS	-	EXPRESSION TAG	UNP P69739
T	331	HIS	-	EXPRESSION TAG	UNP P69739
T	332	HIS	-	EXPRESSION TAG	UNP P69739
T	333	HIS	-	EXPRESSION TAG	UNP P69739
T	334	HIS	-	EXPRESSION TAG	UNP P69739
T	335	HIS	-	EXPRESSION TAG	UNP P69739

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

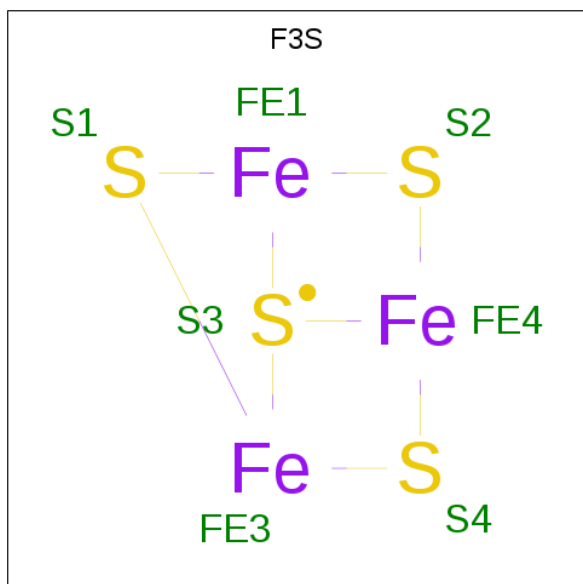
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	581	Total	C	N	O	S	0	40	0
			4788	3045	837	878	28			
2	M	581	Total	C	N	O	S	0	23	0
			4670	2974	810	858	28			

- Molecule 3 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula:  $\text{Fe}_4\text{S}_4$ ).



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

- Molecule 4 is FE3-S4 CLUSTER (three-letter code: F3S) (formula:  $\text{Fe}_3\text{S}_4$ ).



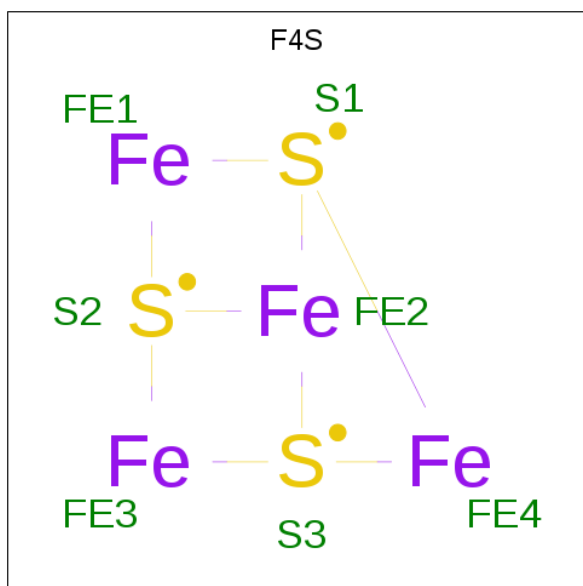
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	S	1	Total	Fe	S	0	0
			7	3	4		

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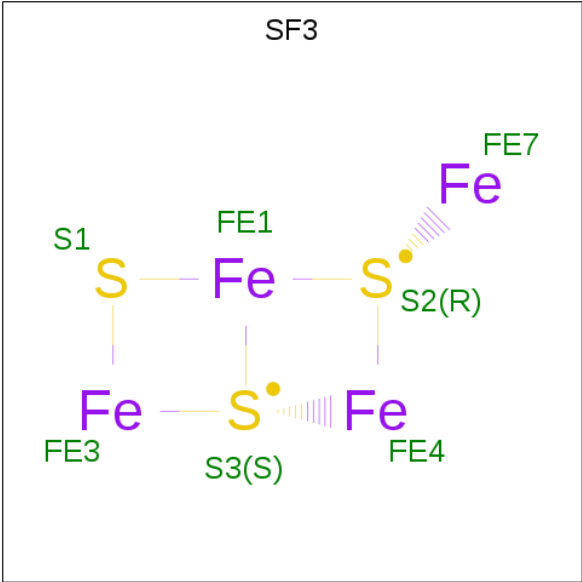
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	T	1	Total	Fe	S	0	0
			7	3	4		

- Molecule 5 is FE4-S3 CLUSTER (three-letter code: F4S) (formula:  $\text{Fe}_4\text{S}_3$ ).



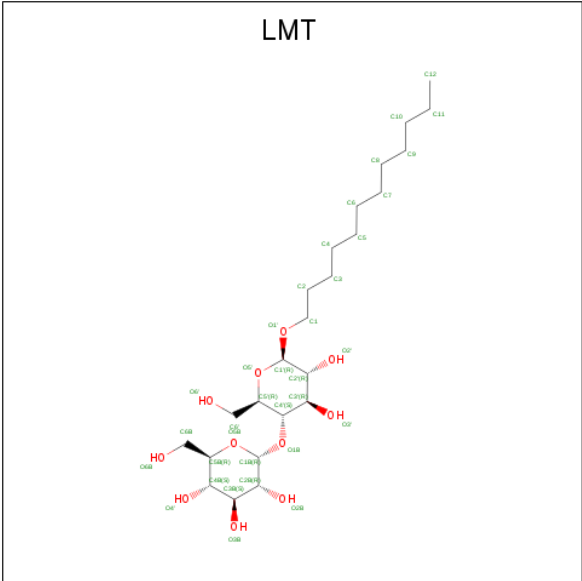
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	S	1	Total	Fe	S	0	1
			7	4	3		
5	T	1	Total	Fe	S	0	1
			7	4	3		

- Molecule 6 is FE4-S3 CLUSTER (three-letter code: SF3) (formula:  $\text{Fe}_4\text{S}_3$ ).



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

- Molecule 7 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: C<sub>24</sub>H<sub>46</sub>O<sub>11</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	S	1	Total	C	O	0	0
			14	13	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	T	1	Total	C	O	0	0
			14	13	1		

- Molecule 8 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 9 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

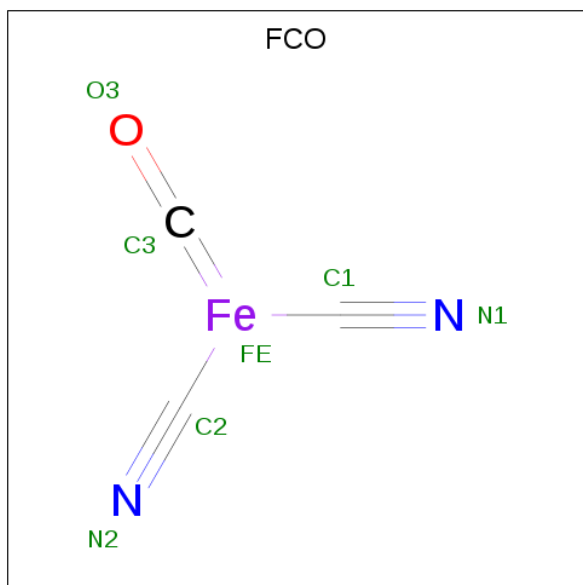
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	T	1	Total	Cl	0	0
			1	1		
9	S	1	Total	Cl	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	M	1	Total	Cl	0	0
			1	1		

- Molecule 10 is CARBONMONOXIDE-(DICYANO) IRON (three-letter code: FCO) (formula:  $C_3FeN_2O$ ).



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

- Molecule 11 is NICKEL (III) ION (three-letter code: 3NI) (formula: Ni).

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

- Molecule 12 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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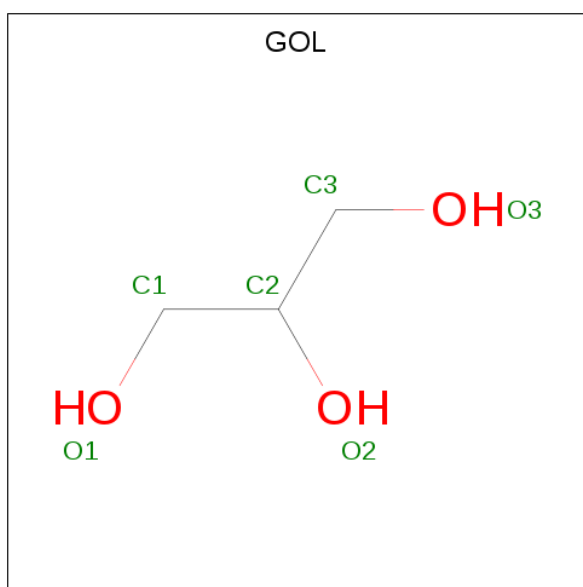
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	M	1	Total	Mg	0	0
			1	1		

- Molecule 13 is LITHIUM ION (three-letter code: LI) (formula: Li).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	L	1	Total	Li	0	0
			1	1		
13	M	1	Total	Li	0	0
			1	1		

- Molecule 14 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
14	L	1	Total	C	O	0	0
			6	3	3		
14	L	1	Total	C	O	0	0
			6	3	3		

- Molecule 15 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	S	202	Total	O	0	0
			202	202		
15	L	409	Total	O	0	0
			409	409		

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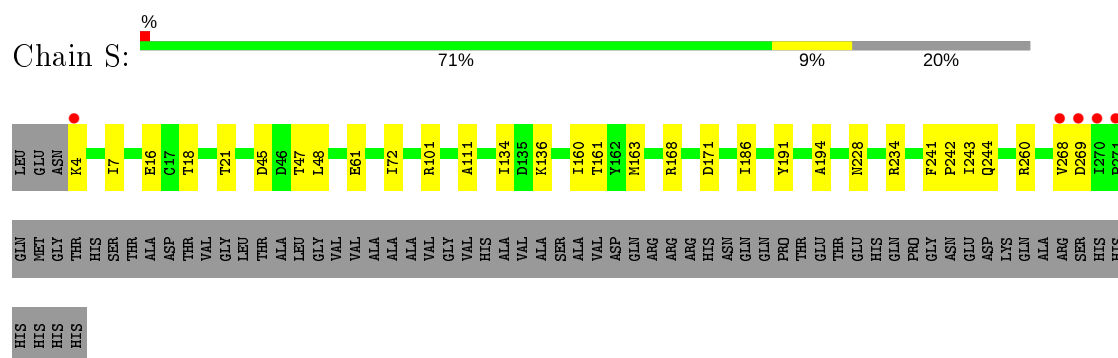
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	T	187	Total 187	O 187	0	0
15	M	459	Total 459	O 459	0	0

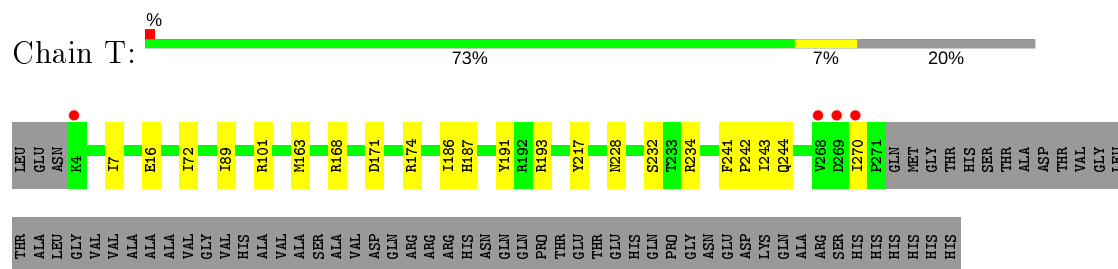
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

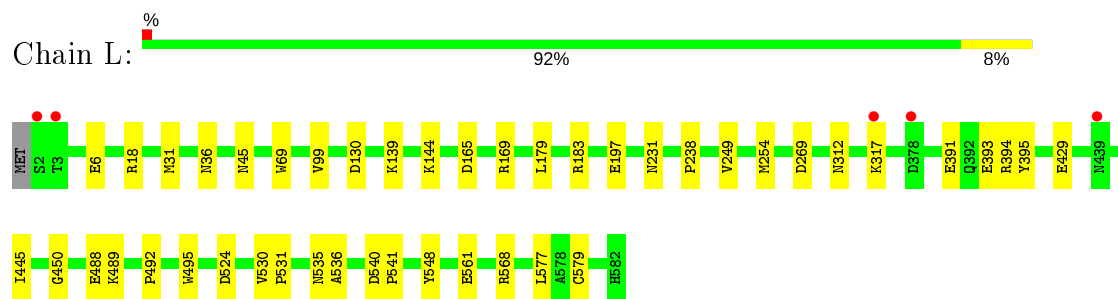
#### • Molecule 1: Hydrogenase-1 small chain



#### • Molecule 1: Hydrogenase-1 small chain

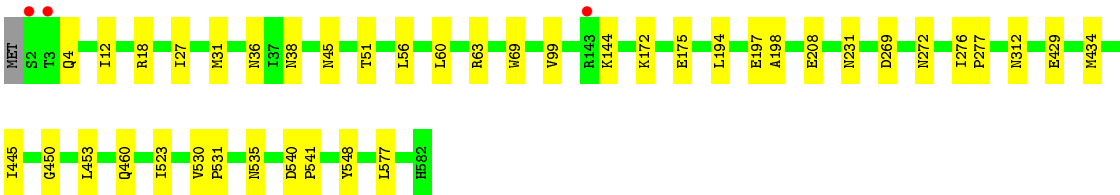


#### • Molecule 2: Hydrogenase-1 large chain



#### • Molecule 2: Hydrogenase-1 large chain





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	93.93Å 97.79Å 183.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.82 – 1.67 29.63 – 1.67	Depositor EDS
% Data completeness (in resolution range)	99.8 (29.82-1.67) 99.8 (29.63-1.67)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.45 (at 1.67Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.120 , 0.168 0.121 , 0.170	Depositor DCC
$R_{free}$ test set	9644 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	9.8	Xtriage
Anisotropy	0.294	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 44.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.016 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	15199	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.54% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: GOL, F4S, CL, SF4, LMT, MG, SF3, F3S, SO4, 3NI, LI, FCO

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	0.59	0/2262	0.70	4/3069 (0.1%)
1	T	0.57	0/2273	0.66	2/3084 (0.1%)
2	L	0.52	0/5013	0.59	0/6810
2	M	0.54	0/4858	0.59	0/6603
All	All	0.55	0/14406	0.62	6/19566 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	T	168	ARG	NE-CZ-NH1	8.80	124.70	120.30
1	T	168	ARG	NE-CZ-NH2	-8.25	116.17	120.30
1	S	168[A]	ARG	NE-CZ-NH1	6.69	123.65	120.30
1	S	168[B]	ARG	NE-CZ-NH1	6.69	123.65	120.30
1	S	168[A]	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	S	168[B]	ARG	NE-CZ-NH2	-5.64	117.48	120.30

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	S	2161	0	2138	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	T	2172	0	2144	16	0
2	L	4788	0	4750	38	0
2	M	4670	0	4615	33	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	7	0	0	0	0
5	T	7	0	0	0	0
6	S	7	0	0	0	0
6	T	7	0	0	0	0
7	S	14	0	25	7	0
7	T	14	0	25	4	0
8	M	5	0	0	0	0
8	S	10	0	0	0	0
8	T	15	0	0	1	0
9	M	1	0	0	1	0
9	S	1	0	0	0	0
9	T	1	0	0	0	0
10	L	7	0	0	0	0
10	M	7	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
12	M	1	0	0	0	0
13	L	1	0	0	0	0
13	M	1	0	0	0	0
14	L	12	0	16	1	0
15	L	409	0	0	11	0
15	M	459	0	0	12	0
15	S	202	0	0	8	0
15	T	187	0	0	3	0
All	All	15199	0	13713	115	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 4.

All (115) 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:M:175[B]:GLU:HG3	15:M:1139:HOH:O	1.06	1.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:269[A]:ASP:OD1	15:M:1133:HOH:O	1.68	1.08
1:S:61[B]:GLU:OE2	1:S:101[B]:ARG:NH1	1.87	1.06
1:S:161[A]:THR:HG23	15:S:682:HOH:O	1.58	1.03
2:L:488[B]:GLU:OE2	15:L:858:HOH:O	1.80	1.00
2:L:488[B]:GLU:OE2	15:L:842:HOH:O	1.83	0.95
9:M:606:CL:CL	15:M:1153:HOH:O	2.22	0.95
1:S:7:ILE:HD13	7:S:405:LMT:H42	1.45	0.95
2:L:269[A]:ASP:OD1	15:L:1089:HOH:O	1.83	0.94
2:L:6[A]:GLU:HG2	15:L:1087:HOH:O	1.67	0.94
2:L:139[B]:LYS:NZ	15:L:1099:HOH:O	2.02	0.91
1:S:21:THR:HG21	1:S:47[A]:THR:HG21	1.54	0.90
1:S:171[A]:ASP:OD1	15:S:700:HOH:O	1.90	0.89
2:M:175[B]:GLU:CG	15:M:1139:HOH:O	1.80	0.80
2:L:99:VAL:H	2:L:312:ASN:HD21	1.29	0.80
2:L:254[B]:MET:HA	2:L:254[B]:MET:HE2	1.65	0.79
2:M:99:VAL:H	2:M:312:ASN:HD21	1.31	0.77
2:L:18:ARG:HH11	2:L:36:ASN:HD21	1.32	0.76
2:L:269[B]:ASP:OD1	15:L:1076:HOH:O	2.04	0.75
1:S:234[A]:ARG:CZ	15:T:559:HOH:O	2.34	0.75
2:M:208[A]:GLU:OE1	15:M:862:HOH:O	2.04	0.75
1:T:7:ILE:HD13	7:T:405:LMT:H41	1.69	0.73
2:L:179:LEU:HD22	14:L:606:GOL:H12	1.71	0.72
1:T:171[B]:ASP:OD1	15:T:612:HOH:O	2.09	0.70
1:S:163:MET:HB3	7:S:405:LMT:H52	1.74	0.69
2:M:18:ARG:HH11	2:M:36:ASN:HD21	1.39	0.68
2:M:36:ASN:HD22	2:M:45:ASN:HD22	1.43	0.65
2:L:429[B]:GLU:OE1	15:L:1084:HOH:O	2.13	0.64
2:M:197[B]:GLU:OE2	15:M:975:HOH:O	0.62	0.61
1:S:61[B]:GLU:HG2	15:S:623:HOH:O	2.01	0.61
2:M:269[B]:ASP:OD1	15:M:1127:HOH:O	2.16	0.60
1:S:260[A]:ARG:NH2	15:S:696:HOH:O	0.75	0.60
15:S:555:HOH:O	1:T:234[A]:ARG:CZ	2.50	0.59
1:S:260[A]:ARG:HH21	1:S:260[A]:ARG:HG3	1.69	0.58
2:L:165:ASP:O	2:L:169[A]:ARG:HG2	2.04	0.58
2:L:99:VAL:H	2:L:312:ASN:ND2	2.02	0.57
2:M:269[A]:ASP:CG	15:M:1133:HOH:O	2.30	0.57
2:M:36:ASN:ND2	2:M:45:ASN:HD22	2.02	0.57
1:T:186:ILE:HD11	1:T:228:ASN:HB3	1.88	0.56
2:M:99:VAL:H	2:M:312:ASN:ND2	2.02	0.56
2:M:172:LYS:O	2:M:175[A]:GLU:HG2	2.05	0.56
1:S:234[A]:ARG:CZ	1:S:244:GLN:HE22	2.21	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:36:ASN:HD22	2:L:45:ASN:HD22	1.56	0.53
2:L:530:VAL:CG1	2:L:531:PRO:HD2	2.38	0.53
1:T:234[A]:ARG:CZ	1:T:244:GLN:HE22	2.21	0.53
2:M:530:VAL:CG1	2:M:531:PRO:HD2	2.40	0.52
2:L:269[A]:ASP:CG	15:L:1089:HOH:O	2.40	0.52
2:L:445:ILE:O	2:L:450:GLY:HA3	2.09	0.52
2:M:31:MET:HB2	2:M:577:LEU:HG	1.91	0.51
2:M:208[B]:GLU:OE1	15:M:1065:HOH:O	2.18	0.50
1:S:268:VAL:HG23	1:S:269:ASP:H	1.76	0.50
1:S:7:ILE:HG21	7:S:405:LMT:H62	1.93	0.50
2:L:183[B]:ARG:NH2	15:L:909:HOH:O	0.65	0.50
1:S:7:ILE:HD13	7:S:405:LMT:C4	2.29	0.50
1:T:187:HIS:CE1	1:T:193:ARG:HD3	2.47	0.49
2:M:535:ASN:HB3	2:M:548:TYR:CE1	2.48	0.49
1:S:161[A]:THR:CG2	15:S:682:HOH:O	2.36	0.48
1:S:194:ALA:HB2	1:T:193:ARG:HG3	1.93	0.48
2:L:535:ASN:HB3	2:L:548:TYR:CE1	2.48	0.48
2:M:429[B]:GLU:HG3	15:M:940:HOH:O	2.13	0.48
2:M:63:ARG:HB2	2:M:523[B]:ILE:HD12	1.96	0.48
2:M:69:TRP:HH2	2:M:231:ASN:HD22	1.62	0.48
2:L:254[B]:MET:CA	2:L:254[B]:MET:HE2	2.36	0.47
2:M:434[B]:MET:SD	2:M:453:LEU:HB3	2.54	0.47
2:M:144[B]:LYS:HG2	15:M:923:HOH:O	2.14	0.47
1:S:260[A]:ARG:HG3	1:S:260[A]:ARG:NH2	2.29	0.47
1:S:186:ILE:HD11	1:S:228:ASN:HB3	1.97	0.47
1:S:45:ASP:OD1	1:S:47[A]:THR:HG22	2.15	0.47
1:T:163:MET:HB3	7:T:405:LMT:H51	1.95	0.47
2:L:540:ASP:HB2	2:L:541:PRO:CD	2.45	0.46
1:S:260[A]:ARG:CG	1:S:260[A]:ARG:NH2	2.79	0.45
1:S:72:ILE:HG13	7:S:405:LMT:H71	1.97	0.45
2:L:393[B]:GLU:HB2	2:L:394[B]:ARG:H	1.67	0.45
2:L:530:VAL:HG12	2:L:531:PRO:HD2	1.98	0.45
1:S:163:MET:HE3	7:S:405:LMT:H72	1.98	0.45
2:L:536:ALA:HB2	2:L:548:TYR:CE2	2.52	0.44
1:S:47[A]:THR:HG23	1:S:48:LEU:HG	1.99	0.44
1:S:18:THR:HG22	1:S:18:THR:O	2.18	0.44
1:T:72:ILE:HG13	7:T:405:LMT:H71	2.00	0.44
2:L:31:MET:HB2	2:L:577:LEU:HG	2.00	0.43
1:S:234[A]:ARG:NH2	15:T:559:HOH:O	2.51	0.43
1:T:174[B]:ARG:HG3	8:T:408:SO4:O1	2.18	0.43
2:L:561[A]:GLU:CD	2:L:561[A]:GLU:H	2.21	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:194:LEU:HB3	2:M:198:ALA:HB3	2.00	0.42
2:M:530:VAL:HG12	2:M:531:PRO:HD2	2.01	0.42
2:M:56:LEU:O	2:M:60:LEU:HD23	2.19	0.42
1:S:111:ALA:HB2	1:S:134[B]:ILE:HD11	2.00	0.42
2:L:254[B]:MET:HE3	2:L:254[B]:MET:HB2	1.87	0.42
2:L:269[A]:ASP:OD2	15:L:1090:HOH:O	2.22	0.42
2:L:69:TRP:HH2	2:L:231:ASN:HD22	1.68	0.42
1:T:217:TYR:CE1	1:T:270:ILE:HD11	2.54	0.42
2:M:276:ILE:HB	2:M:277:PRO:HD3	2.02	0.41
2:L:144:LYS:HB3	2:L:197[A]:GLU:HG2	2.02	0.41
2:M:4:GLN:HA	2:M:12:ILE:O	2.20	0.41
2:M:445:ILE:O	2:M:450:GLY:HA3	2.20	0.41
1:T:89:ILE:HB	2:M:51:THR:HB	2.02	0.41
1:S:136[A]:LYS:HE3	15:S:600:HOH:O	2.20	0.41
2:L:249:VAL:HB	1:T:232[B]:SER:OG	2.21	0.41
2:L:130:ASP:HB3	2:L:568:ARG:HG2	2.03	0.41
2:L:391:GLU:HA	2:L:395:TYR:CD2	2.56	0.41
2:L:530:VAL:HG11	2:L:579:CYS:HB3	2.02	0.41
1:S:241:PHE:CE2	1:S:243:ILE:HB	2.56	0.41
1:S:234[A]:ARG:NH1	1:T:234[A]:ARG:HD3	2.35	0.41
2:M:540:ASP:HB2	2:M:541:PRO:CD	2.50	0.41
2:L:492:PRO:HA	2:L:495:TRP:CD2	2.56	0.40
2:L:489[A]:LYS:HE2	15:L:1088:HOH:O	2.22	0.40
2:M:38:ASN:HB2	15:M:1098:HOH:O	2.21	0.40
2:M:272:ASN:OD1	2:M:460:GLN:HG3	2.21	0.40
1:S:160:ILE:HG12	7:S:405:LMT:H92	2.02	0.40
15:S:534:HOH:O	2:L:238:PRO:HG2	2.21	0.40
2:M:27:ILE:HD12	2:M:577:LEU:HD23	2.02	0.40
1:S:268:VAL:HG23	1:S:269:ASP:N	2.36	0.40
1:T:241:PHE:CE2	1:T:243:ILE:HB	2.57	0.40
1:T:7:ILE:HG21	7:T:405:LMT:H62	2.03	0.40

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	282/335 (84%)	267 (95%)	15 (5%)	0	100	100
1	T	283/335 (84%)	271 (96%)	12 (4%)	0	100	100
2	L	619/582 (106%)	600 (97%)	19 (3%)	0	100	100
2	M	602/582 (103%)	586 (97%)	16 (3%)	0	100	100
All	All	1786/1834 (97%)	1724 (96%)	62 (4%)	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	237/274 (86%)	233 (98%)	4 (2%)	60	43
1	T	238/274 (87%)	234 (98%)	4 (2%)	60	43
2	L	519/481 (108%)	518 (100%)	1 (0%)	93	89
2	M	503/481 (105%)	503 (100%)	0	100	100
All	All	1497/1510 (99%)	1488 (99%)	9 (1%)	86	79

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	S	4	LYS
1	S	16	GLU
1	S	191	TYR
1	S	242	PRO
2	L	524	ASP
1	T	16	GLU
1	T	101	ARG
1	T	191	TYR
1	T	242	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	S	244	GLN
2	L	36	ASN
2	L	108	ASN
2	L	231	ASN
2	L	258	ASN
2	L	312	ASN
2	L	328	ASN
2	L	332	ASN
2	L	479	ASN
2	L	544	GLN
1	T	244	GLN
2	M	36	ASN
2	M	108	ASN
2	M	231	ASN
2	M	258	ASN
2	M	312	ASN
2	M	328	ASN
2	M	544	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 29 ligands modelled in this entry, 9 are monoatomic - leaving 20 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
10	FCO	L	601	2,15	0,6,6	0.00	-	-		
8	SO4	T	407	-	4,4,4	0.14	0	6,6,6	0.15	0
3	SF4	T	401	1	0,12,12	0.00	-	-		
4	F3S	S	402	1	0,9,9	0.00	-	-		
14	GOL	L	605	-	5,5,5	0.51	0	5,5,5	0.52	0
8	SO4	T	406	-	4,4,4	0.11	0	6,6,6	0.15	0
8	SO4	S	407	-	4,4,4	0.16	0	6,6,6	0.21	0
5	F4S	S	403[A]	1	0,9,9	0.00	-	-		
10	FCO	M	601	2,15	0,6,6	0.00	-	-		
7	LMT	S	405	-	13,13,36	0.13	0	12,12,47	1.01	1 (8%)
8	SO4	S	406	-	4,4,4	0.16	0	6,6,6	0.28	0
8	SO4	M	604	-	4,4,4	0.12	0	6,6,6	0.26	0
6	SF3	T	404[B]	1	0,8,8	0.00	-	-		
7	LMT	T	405	-	13,13,36	0.12	0	12,12,47	0.69	0
8	SO4	T	408	-	4,4,4	0.21	0	6,6,6	0.53	0
14	GOL	L	606	-	5,5,5	0.33	0	5,5,5	0.42	0
4	F3S	T	402	1	0,9,9	0.00	-	-		
5	F4S	T	403[A]	1	0,9,9	0.00	-	-		
6	SF3	S	404[B]	1	0,8,8	0.00	-	-		
3	SF4	S	401	1	0,12,12	0.00	-	-		

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	SF4	T	401	1	-	-	0/6/5/5
4	F3S	S	402	1	-	-	0/3/3/3
14	GOL	L	605	-	-	3/4/4/4	-
6	SF3	T	404[B]	1	-	-	0/2/2/2
5	F4S	S	403[A]	1	-	-	0/3/3/3
7	LMT	S	405	-	-	4/11/11/61	-
6	SF3	S	404[B]	1	-	-	0/2/2/2
14	GOL	L	606	-	-	0/4/4/4	-
7	LMT	T	405	-	-	5/11/11/61	-
4	F3S	T	402	1	-	-	0/3/3/3
5	F4S	T	403[A]	1	-	-	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SF4	S	401	1	-	-	0/6/5/5

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
7	S	405	LMT	C7-C6-C5	-2.46	101.94	114.42

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	S	405	LMT	O1'-C1-C2-C3
7	T	405	LMT	C2-C1-O1'-C1'
7	T	405	LMT	O1'-C1-C2-C3
7	T	405	LMT	C2-C3-C4-C5
14	L	605	GOL	O1-C1-C2-C3
14	L	605	GOL	C1-C2-C3-O3
7	T	405	LMT	C4-C5-C6-C7
7	S	405	LMT	C2-C1-O1'-C1'
14	L	605	GOL	O1-C1-C2-O2
7	S	405	LMT	C7-C8-C9-C10
7	T	405	LMT	C1-C2-C3-C4
7	S	405	LMT	C2-C3-C4-C5

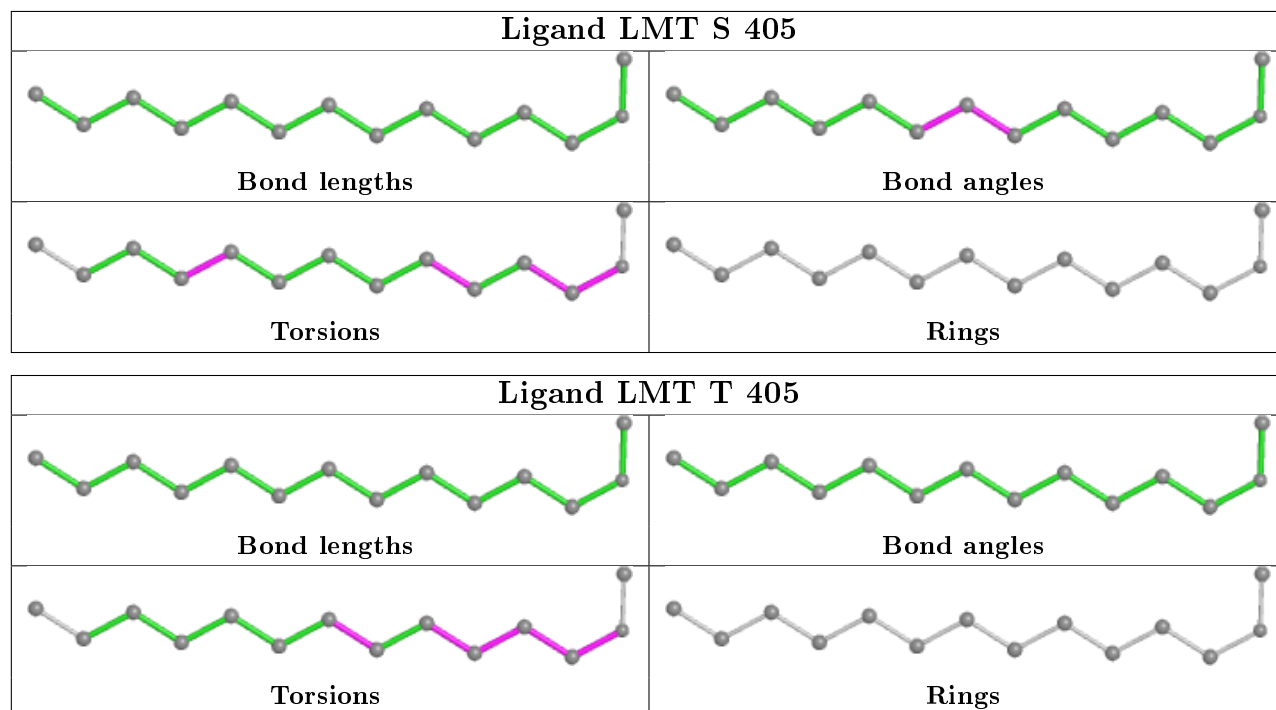
There are no ring outliers.

4 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	S	405	LMT	7	0
7	T	405	LMT	4	0
8	T	408	SO4	1	0
14	L	606	GOL	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 than 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 [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	S	268/335 (80%)	-0.51	5 (1%)	66	70	6, 10, 19, 44	6 (2%)
1	T	268/335 (80%)	-0.52	4 (1%)	73	77	6, 11, 21, 54	6 (2%)
2	L	581/582 (99%)	-0.52	5 (0%)	84	87	6, 11, 22, 34	3 (0%)
2	M	581/582 (99%)	-0.59	3 (0%)	91	92	6, 11, 20, 34	1 (0%)
All	All	1698/1834 (92%)	-0.55	17 (1%)	82	85	6, 11, 21, 54	16 (0%)

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	S	268	VAL	8.3
1	T	268	VAL	6.7
2	L	2	SER	4.2
1	S	4	LYS	4.2
1	S	271	PRO	4.2
2	M	2	SER	3.8
1	S	269	ASP	3.4
1	T	269	ASP	3.4
1	S	270	ILE	3.3
2	L	3[A]	THR	3.0
2	L	439[A]	ASN	2.6
1	T	270	ILE	2.5
1	T	4	LYS	2.4
2	M	3	THR	2.4
2	L	378	ASP	2.3
2	M	143	ARG	2.1
2	L	317[A]	LYS	2.0

### 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 ⓘ

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. The B-factors column lists the minimum, median, 95<sup>th</sup> 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.

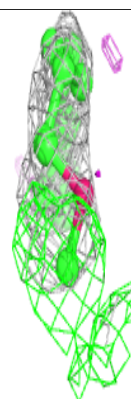
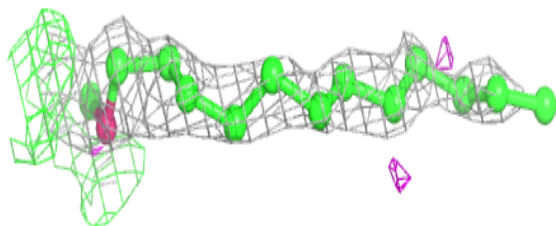
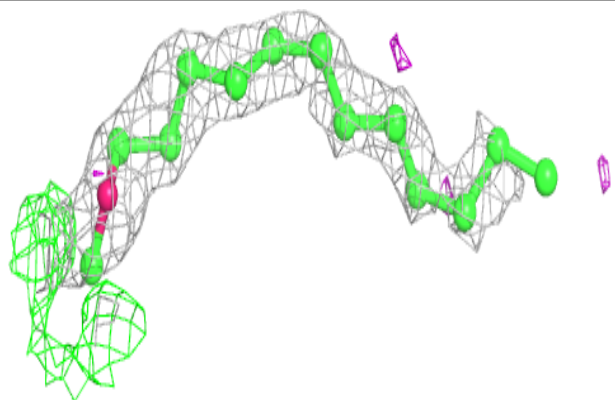
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
14	GOL	L	606	6/6	0.80	0.22	27,32,35,35	0
8	SO4	M	604	5/5	0.83	0.17	32,33,37,37	5
14	GOL	L	605	6/6	0.84	0.27	35,45,47,49	0
7	LMT	T	405	14/35	0.89	0.16	29,35,39,40	0
7	LMT	S	405	14/35	0.90	0.17	20,23,31,31	14
8	SO4	T	408	5/5	0.90	0.22	23,26,29,29	5
8	SO4	T	406	5/5	0.91	0.14	17,17,23,24	5
8	SO4	T	407	5/5	0.92	0.16	33,34,35,35	5
8	SO4	S	407	5/5	0.93	0.17	32,32,34,35	5
13	LI	L	604	1/1	0.97	0.32	12,12,12,12	0
9	CL	M	606	1/1	0.98	0.05	28,28,28,28	1
13	LI	M	605	1/1	0.98	0.12	11,11,11,11	0
8	SO4	S	406	5/5	0.99	0.11	16,17,18,18	5
3	SF4	S	401	8/8	1.00	0.04	7,7,8,8	0
12	MG	L	603	1/1	1.00	0.04	6,6,6,6	0
9	CL	S	408	1/1	1.00	0.05	13,13,13,13	0
11	3NI	M	602	1/1	1.00	0.03	11,11,11,11	0
3	SF4	T	401	8/8	1.00	0.05	7,7,8,8	0
5	F4S	S	403[A]	7/7	1.00	0.04	8,8,10,10	7
4	F3S	S	402	7/7	1.00	0.05	6,6,7,7	0
12	MG	M	603	1/1	1.00	0.06	6,6,6,6	0
10	FCO	M	601	7/7	1.00	0.05	7,7,8,8	0
6	SF3	T	404[B]	7/7	1.00	0.04	7,8,10,10	7
10	FCO	L	601	7/7	1.00	0.05	7,8,9,9	0
6	SF3	S	404[B]	7/7	1.00	0.04	8,8,10,10	7
11	3NI	L	602	1/1	1.00	0.02	11,11,11,11	0
5	F4S	T	403[A]	7/7	1.00	0.04	7,8,10,11	7
9	CL	T	409	1/1	1.00	0.03	13,13,13,13	0
4	F3S	T	402	7/7	1.00	0.05	6,7,7,8	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.

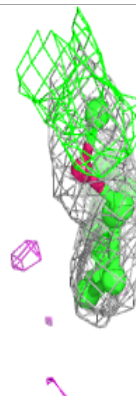
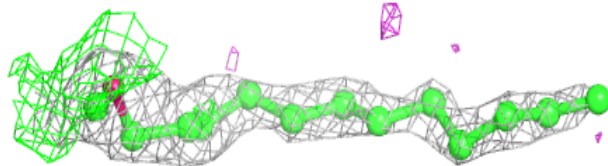
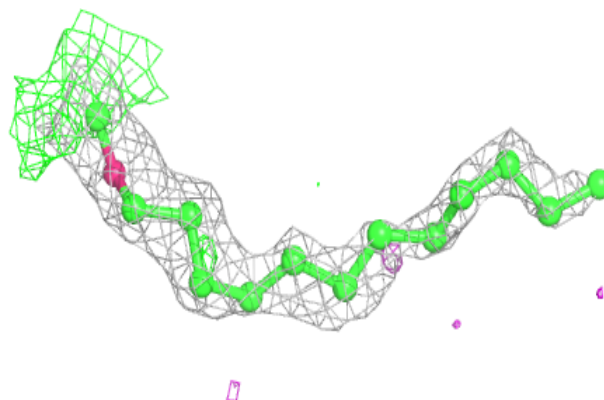
**Electron density around LMT T 405:**

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



**Electron density around LMT S 405:**

$2mF_o-DF_c$  (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.