



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 07:27 AM UTC

PDB ID : 3USE / pdb\_00003use  
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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
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

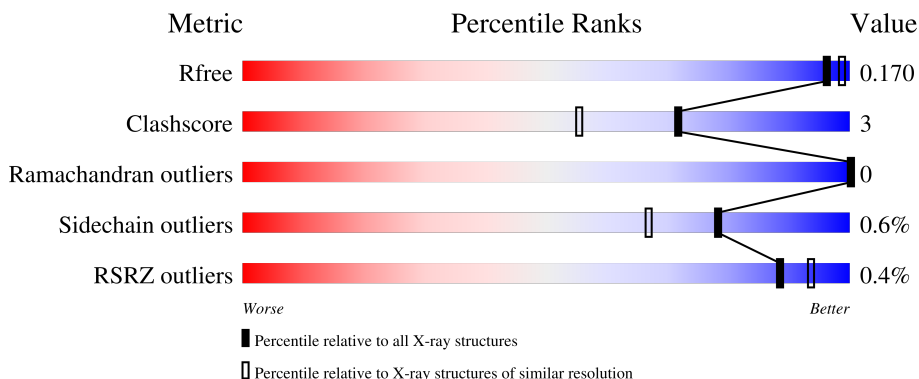
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.67 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))
$R_{free}$	180053	1054 (1.68-1.68)
Clashscore	190562	1078 (1.68-1.68)
Ramachandran outliers	187476	1068 (1.68-1.68)
Sidechain outliers	187428	1067 (1.68-1.68)
RSRZ outliers	180081	1055 (1.68-1.68)

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  $\geq 3$ , 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	 72% 8% 20%
1	T	335	 74% 6% 20%
2	L	582	 92% 7%
2	M	582	 93% 7%

## 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
			Total	C	N	O	S			
1	S	268	2161	1376	370	394	21	4	16	0
1	T	268	2172	1382	372	397	21	0	17	0

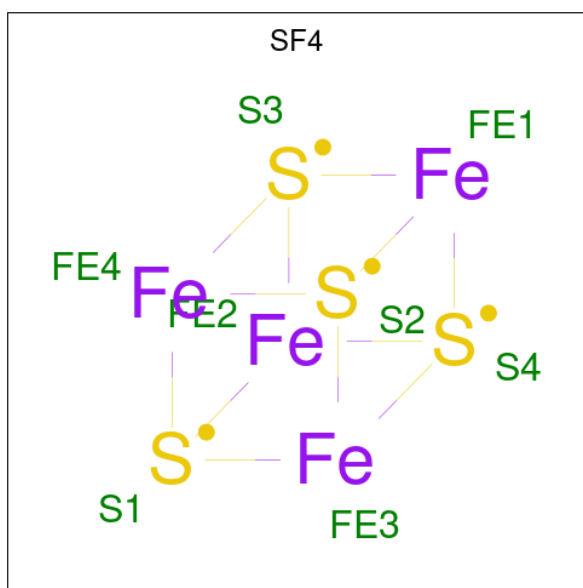
There are 16 discrepancies between the modelled and reference sequences:

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.

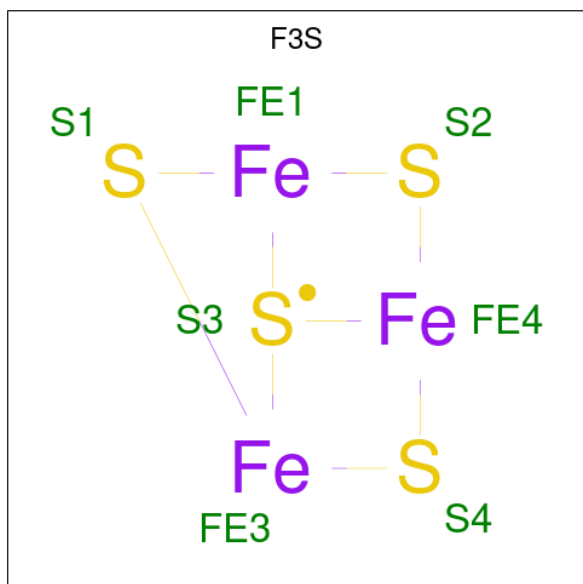
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	L	581	4788	3045	837	878	28	0	40	0
2	M	581	4670	2974	810	858	28	0	23	0

- Molecule 3 is IRON/SULFUR CLUSTER (CCD ID: 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 (CCD ID: F3S) (formula:  $\text{Fe}_3\text{S}_4$ ).



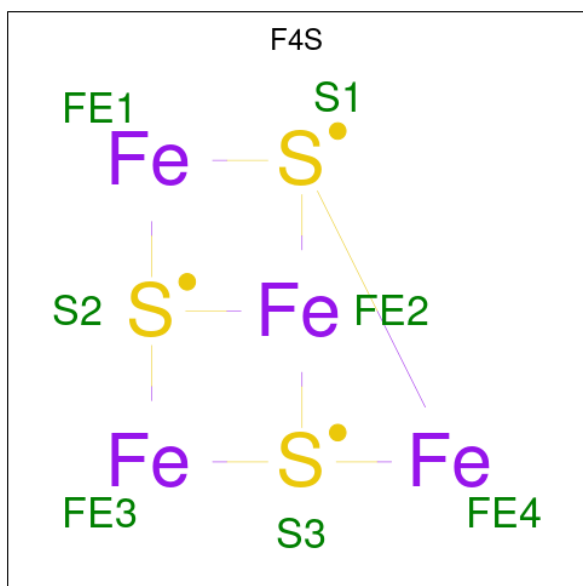
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	S	1	Total	Fe	S	0	0
			7	3	4		

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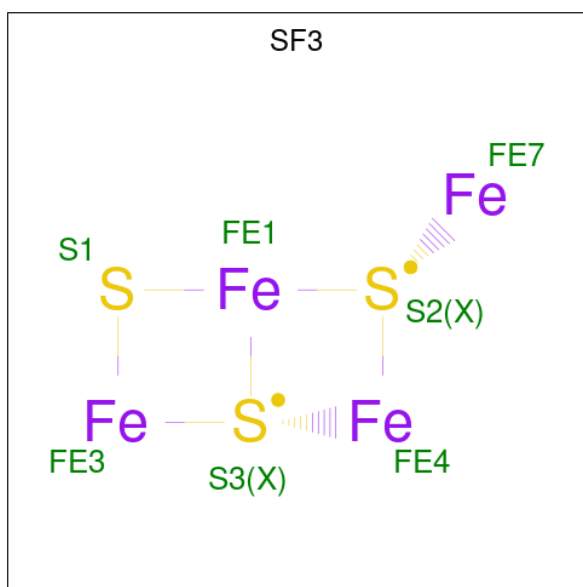
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
4	T	1	7	3	4	0	0

- Molecule 5 is FE4-S3 CLUSTER (CCD ID: F4S) (formula: Fe<sub>4</sub>S<sub>3</sub>).



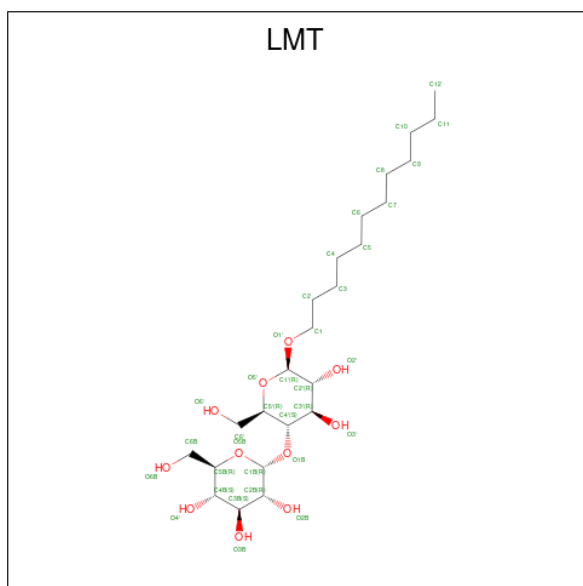
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
5	S	1	7	4	3	0	1
5	T	1	7	4	3	0	1

- Molecule 6 is FE4-S3 CLUSTER (CCD ID: SF3) (formula: Fe<sub>4</sub>S<sub>3</sub>).



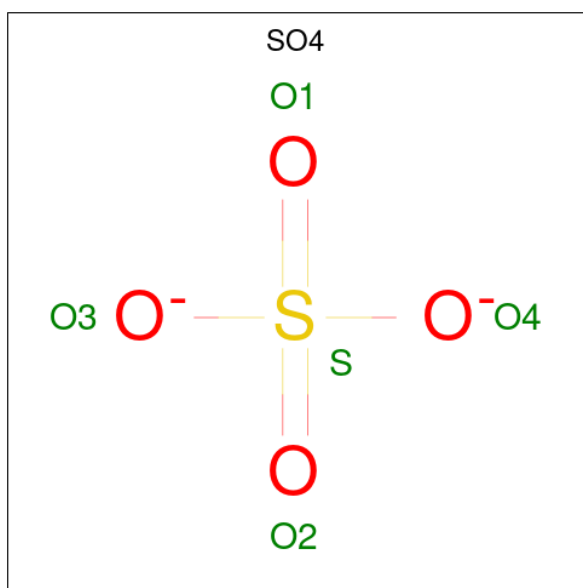
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	S	1	Total Fe S 7 4 3	0	1
6	T	1	Total Fe S 7 4 3	0	1

- Molecule 7 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula:  $C_{24}H_{46}O_{11}$ ).



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

- Molecule 8 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).

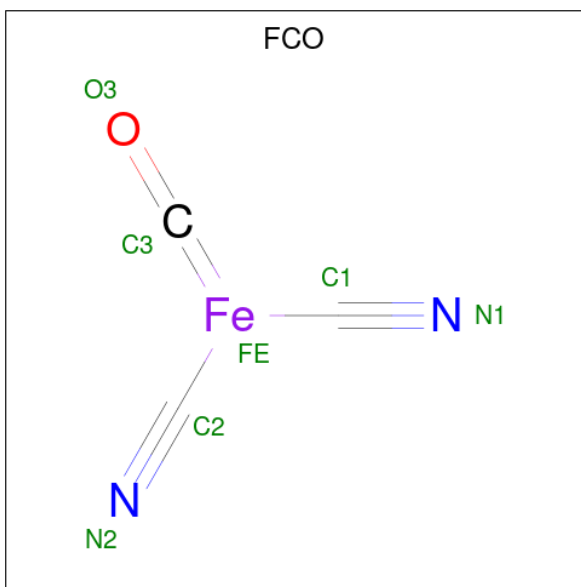


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	S	1	Total O S 5 4 1	0	0
8	S	1	Total O S 5 4 1	0	0
8	T	1	Total O S 5 4 1	0	0
8	T	1	Total O S 5 4 1	0	0
8	T	1	Total O S 5 4 1	0	0
8	M	1	Total O S 5 4 1	0	0

- Molecule 9 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 10 is CARBONMONOXIDE-(DICYANO) IRON (CCD ID: FCO) (formula: C<sub>3</sub>FeN<sub>2</sub>O).



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

- Molecule 11 is NICKEL (III) ION (CCD ID: 3NI) (formula: Ni).

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

- Molecule 12 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 13 is LITHIUM ION (CCD ID: LI) (formula: Li).

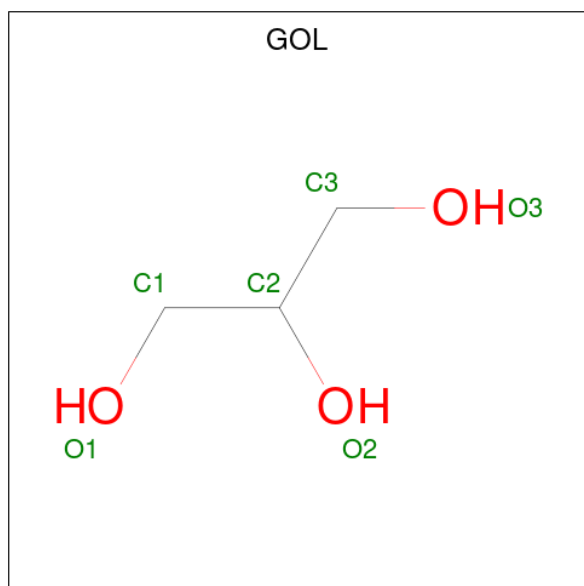
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Li		
13	L	1	1	1	0	0

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

- Molecule 14 is GLYCEROL (CCD ID: 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		
15	T	187	Total	O	0	0
			187	187		
15	M	459	Total	O	0	0
			459	459		





## 4 Data and refinement statistics i

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 29.82 – 1.67	Depositor EDS
% Data completeness (in resolution range)	99.8 (29.82-1.67) 99.7 (29.82-1.67)	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)	Xtrriage
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	Xtrriage
Anisotropy	0.294	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 40.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.016 for k,h,-l	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	15199	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	13.0	wwPDB-VP

Xtrriage'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, F3S, FCO, CL, SF4, LMT, MG, LI, F4S, SO4, 3NI, SF3

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	0.68	0/2262	0.77	0/3069
1	T	0.69	0/2273	0.77	0/3084
2	L	0.61	0/5013	0.73	2/6810 (0.0%)
2	M	0.62	0/4858	0.74	0/6603
All	All	0.64	0/14406	0.74	2/19566 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	379[A]	VAL	N-CA-C	5.32	120.40	109.34
2	L	379[B]	VAL	N-CA-C	5.32	120.40	109.34

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	25	0
1	T	2172	0	2144	15	0
2	L	4788	0	4750	29	0
2	M	4670	0	4615	25	0
3	S	8	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	6	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	0	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	1	0
15	M	459	0	0	3	0
15	S	202	0	0	3	0
15	T	187	0	0	0	0
All	All	15199	0	13713	90	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.

All (90) 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:S:61[B]:GLU:OE2	1:S:101[B]:ARG:NH1	1.87	1.06
1:S:7:ILE:HD13	7:S:405:LMT:H42	1.45	0.95
1:S:21:THR:HG21	1:S:47[A]:THR:HG21	1.54	0.90
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
1:S:61[B]:GLU:HG2	15:S:623:HOH:O	2.01	0.61
1:T:159:ILE:HG22	1:T:163:MET:HE2	1.83	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: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
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: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
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
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: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:561[A]:GLU:H	2:L:561[A]:GLU:CD	2.21	0.47
2:L:254[B]:MET:HE2	2:L:254[B]:MET:CA	2.36	0.47
2:L:486:SER:OG	2:L:488[B]:GLU:OE1	2.22	0.47
2:M:434[B]:MET:SD	2:M:453:LEU:HB3	2.54	0.47
1:S:260[A]:ARG:HG3	1:S:260[A]:ARG:NH2	2.29	0.47
2:M:144[B]:LYS:HG2	15:M:923:HOH:O	2.14	0.47
1:S:45:ASP:OD1	1:S:47[A]:THR:HG22	2.15	0.47
1:S:186:ILE:HD11	1:S:228:ASN:HB3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:NH2	1:S:260[A]:ARG:CG	2.79	0.45
1:S:72:ILE:HG13	7:S:405:LMT:H71	1.97	0.45
1:S:159:ILE:HG22	1:S:163:MET:HE2	1.98	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
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:T:174[B]:ARG:HG3	8:T:408:SO4:O1	2.18	0.43
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
1:S:111:ALA:HB2	1:S:134[B]:ILE:HD11	2.00	0.42
2:M:56:LEU:O	2:M:60:LEU:HD23	2.19	0.42
2:L:254[B]:MET:HE3	2:L:254[B]:MET:HB2	1.87	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
1:S:234[A]:ARG:NH1	1:T:234[A]:ARG:HD3	2.35	0.41
1:S:241:PHE:CE2	1:S:243:ILE:HB	2.56	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
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
1:S:160:ILE:HG12	7:S:405:LMT:H92	2.02	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:268:VAL:HG23	1:S:269:ASP:N	2.36	0.40
15:S:534:HOH:O	2:L:238:PRO:HG2	2.21	0.40
1:T:7:ILE:HG21	7:T:405:LMT:H62	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:241:PHE:CE2	1:T:243:ILE:HB	2.57	0.40
2:M:27:ILE:HD12	2:M:577:LEU:HD23	2.02	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 [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	S	237/274 (86%)	233 (98%)	4 (2%)	53	29
1	T	238/274 (87%)	236 (99%)	2 (1%)	73	59
2	L	519/481 (108%)	514 (99%)	5 (1%)	68	52

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	M	503/481 (105%)	503 (100%)	0	100	100
All	All	1497/1510 (99%)	1486 (99%)	11 (1%)	78	62

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	S	4	LYS
1	S	7	ILE
1	S	16	GLU
1	S	242	PRO
2	L	6[A]	GLU
2	L	6[B]	GLU
2	L	524	ASP
2	L	561[A]	GLU
2	L	561[B]	GLU
1	T	16	GLU
1	T	242	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	S	68	ASN
1	S	244	GLN
2	L	36	ASN
2	L	108	ASN
2	L	150	GLN
2	L	231	ASN
2	L	258	ASN
2	L	312	ASN
2	L	332	ASN
2	L	479	ASN
2	M	4	GLN
2	M	36	ASN
2	M	108	ASN
2	M	150	GLN
2	M	231	ASN
2	M	258	ASN
2	M	312	ASN
2	M	460	GLN
2	M	479	ASN

### 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 oligosaccharides 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	$\# Z  > 2$
8	SO4	T	406	-	4,4,4	0.21	0	6,6,6	0.15	0
8	SO4	S	406	-	4,4,4	0.26	0	6,6,6	0.27	0
7	LMT	T	405	-	13,13,36	0.11	0	12,12,47	0.69	0
6	SF3	S	404[B]	1	0,8,8	-	-	-		
3	SF4	T	401	1	0,12,12	-	-	-		
7	LMT	S	405	-	13,13,36	0.13	0	12,12,47	1.02	1 (8%)
8	SO4	S	407	-	4,4,4	0.25	0	6,6,6	0.18	0
4	F3S	S	402	1	0,9,9	-	-	-		
8	SO4	M	604	-	4,4,4	0.22	0	6,6,6	0.24	0
3	SF4	S	401	1	0,12,12	-	-	-		
14	GOL	L	605	-	5,5,5	0.52	0	5,5,5	0.57	0
14	GOL	L	606	-	5,5,5	0.33	0	5,5,5	0.47	0
10	FCO	L	601	15,2	0,6,6	-	-	-		
5	F4S	T	403[A]	1	0,9,9	-	-	-		
4	F3S	T	402	1	0,9,9	-	-	-		
8	SO4	T	407	-	4,4,4	0.22	0	6,6,6	0.19	0
8	SO4	T	408	-	4,4,4	0.13	0	6,6,6	0.54	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	SF3	T	404[B]	1	0,8,8	-	-	-	-	-
5	F4S	S	403[A]	1	0,9,9	-	-	-	-	-
10	FCO	M	601	15,2	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
7	LMT	S	405	-	-	4/11/11/61	-
14	GOL	L	606	-	-	0/4/4/4	-
6	SF3	T	404[B]	1	-	-	0/2/2/2
5	F4S	S	403[A]	1	-	-	0/4/3/3
5	F4S	T	403[A]	1	-	-	0/4/3/3
4	F3S	T	402	1	-	-	0/3/3/3
3	SF4	S	401	1	-	-	0/6/5/5
7	LMT	T	405	-	-	5/11/11/61	-
4	F3S	S	402	1	-	-	0/3/3/3
6	SF3	S	404[B]	1	-	-	0/2/2/2
14	GOL	L	605	-	-	4/4/4/4	-
3	SF4	T	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(°)	Ideal(°)
7	S	405	LMT	C7-C6-C5	-2.46	101.94	114.37

There are no chirality outliers.

All (13) 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'
14	L	605	GOL	O1-C1-C2-C3
14	L	605	GOL	C1-C2-C3-O3
7	T	405	LMT	O1'-C1-C2-C3
7	T	405	LMT	C2-C3-C4-C5
7	S	405	LMT	C2-C1-O1'-C1'

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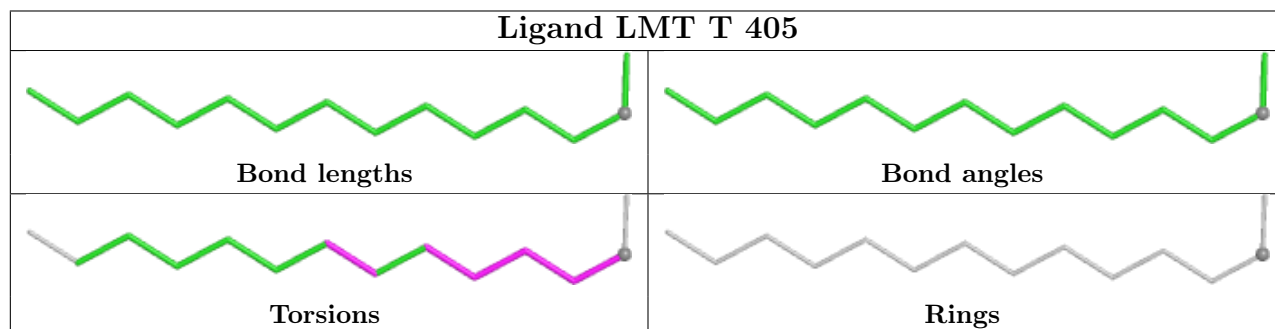
Mol	Chain	Res	Type	Atoms
7	T	405	LMT	C4-C5-C6-C7
14	L	605	GOL	O1-C1-C2-O2
7	S	405	LMT	C7-C8-C9-C10
7	T	405	LMT	C1-C2-C3-C4
7	S	405	LMT	C2-C3-C4-C5
14	L	605	GOL	O2-C2-C3-O3

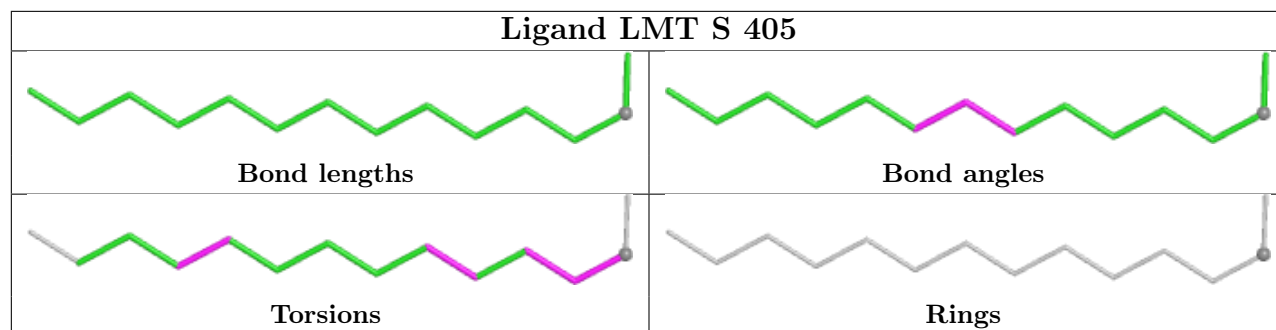
There are no ring outliers.

4 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	T	405	LMT	4	0
7	S	405	LMT	6	0
14	L	606	GOL	1	0
8	T	408	SO4	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%)	-0.90	3 (1%) 78 85	4, 10, 18, 37	21 (7%)
1	T	268/335 (80%)	-0.86	4 (1%) 72 80	5, 10, 20, 45	23 (8%)
2	L	581/582 (99%)	-0.91	0 100 100	5, 11, 20, 34	43 (7%)
2	M	581/582 (99%)	-0.97	0 100 100	5, 10, 20, 34	24 (4%)
All	All	1698/1834 (92%)	-0.92	7 (0%) 88 93	4, 10, 20, 45	111 (6%)

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	T	270	ILE	6.3
1	S	270	ILE	5.1
1	S	268	VAL	5.1
1	T	268	VAL	4.2
1	T	271	PRO	4.2
1	S	271	PRO	3.7
1	T	4	LYS	2.5

### 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 [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands

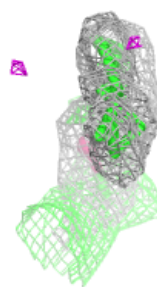
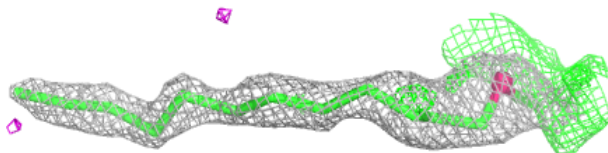
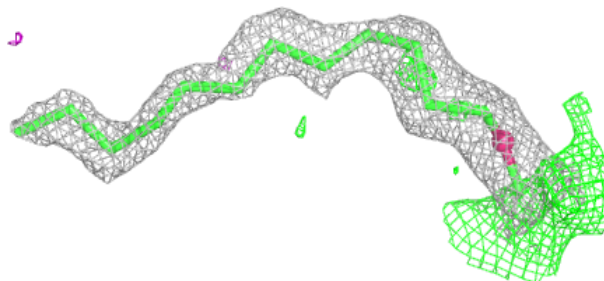
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
7	LMT	S	405	14/35	0.77	0.17	20,23,31,31	14
7	LMT	T	405	14/35	0.81	0.12	29,35,39,40	0
8	SO4	M	604	5/5	0.82	0.15	32,33,37,37	5
14	GOL	L	605	6/6	0.83	0.13	35,45,47,49	0
14	GOL	L	606	6/6	0.87	0.13	27,32,35,35	0
8	SO4	T	407	5/5	0.88	0.12	33,34,35,35	5
8	SO4	S	407	5/5	0.89	0.10	32,32,34,35	5
8	SO4	T	408	5/5	0.90	0.13	23,26,29,29	5
8	SO4	T	406	5/5	0.92	0.10	17,17,23,24	5
13	LI	M	605	1/1	0.97	0.03	11,11,11,11	0
9	CL	M	606	1/1	0.98	0.04	28,28,28,28	1
13	LI	L	604	1/1	0.99	0.35	12,12,12,12	0
8	SO4	S	406	5/5	0.99	0.04	16,17,18,18	5
5	F4S	T	403[A]	7/7	1.00	0.01	7,8,10,11	7
6	SF3	S	404[B]	7/7	1.00	0.01	8,8,10,10	7
6	SF3	T	404[B]	7/7	1.00	0.01	7,8,10,10	7
9	CL	S	408	1/1	1.00	0.01	13,13,13,13	0
9	CL	T	409	1/1	1.00	0.03	13,13,13,13	0
3	SF4	S	401	8/8	1.00	0.01	7,7,8,8	0
10	FCO	L	601	7/7	1.00	0.03	7,8,9,9	0
10	FCO	M	601	7/7	1.00	0.02	7,7,8,8	0
11	3NI	L	602	1/1	1.00	0.02	11,11,11,11	0
11	3NI	M	602	1/1	1.00	0.01	11,11,11,11	0
12	MG	L	603	1/1	1.00	0.01	6,6,6,6	0
12	MG	M	603	1/1	1.00	0.01	6,6,6,6	0
3	SF4	T	401	8/8	1.00	0.01	7,7,8,8	0
4	F3S	S	402	7/7	1.00	0.01	6,6,7,7	0
4	F3S	T	402	7/7	1.00	0.01	6,7,7,8	0
5	F4S	S	403[A]	7/7	1.00	0.01	8,8,10,10	7

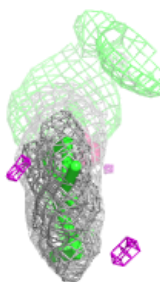
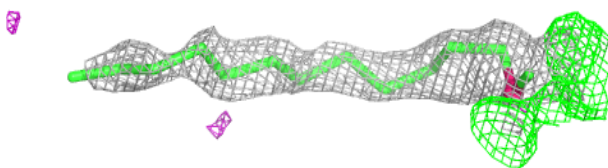
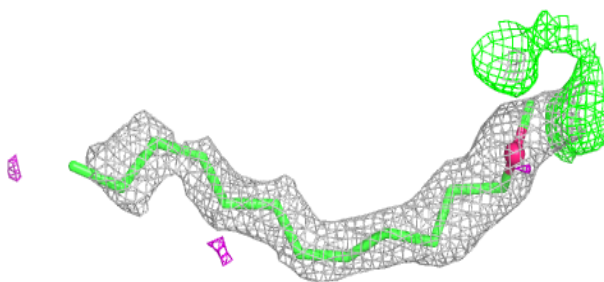
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around LMT S 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 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)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.