



Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 04:08 am BST

PDB ID : 3USC
Title : Crystal Structure of E. coli hydrogenase-1 in a ferricyanide-oxidized form
Authors : Volbeda, A.; Fontecilla-Camps, J.C.; Darnault, C.
Deposited on : 2011-11-23
Resolution : 2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The 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

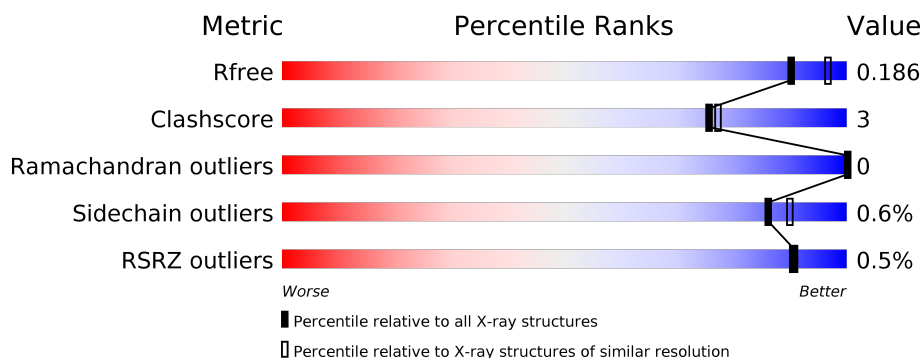
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	S	335	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> % <div style="width: 100%; height: 10px; background-color: green;"></div> 74% <div style="width: 10px; height: 10px; background-color: yellow;"></div> <div style="width: 10px; height: 10px; background-color: orange;"></div> <div style="width: 10px; height: 10px; background-color: red;"></div> 21% </div> </div>
1	T	335	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> % <div style="width: 100%; height: 10px; background-color: green;"></div> 71% <div style="width: 10px; height: 10px; background-color: yellow;"></div> <div style="width: 10px; height: 10px; background-color: orange;"></div> <div style="width: 10px; height: 10px; background-color: red;"></div> 21% </div> </div>
2	L	582	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> % <div style="width: 100%; height: 10px; background-color: green;"></div> 94% <div style="width: 10px; height: 10px; background-color: yellow;"></div> <div style="width: 10px; height: 10px; background-color: orange;"></div> <div style="width: 10px; height: 10px; background-color: red;"></div> 6% </div> </div>
2	M	582	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> % <div style="width: 100%; height: 10px; background-color: green;"></div> 95% <div style="width: 10px; height: 10px; background-color: yellow;"></div> <div style="width: 10px; height: 10px; background-color: orange;"></div> <div style="width: 10px; height: 10px; background-color: red;"></div> 5% </div> </div>

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 14932 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	265	Total	C	N	O	S	0	9	0
			2099	1333	360	385	21			
1	T	265	Total	C	N	O	S	0	10	0
			2107	1339	363	384	21			

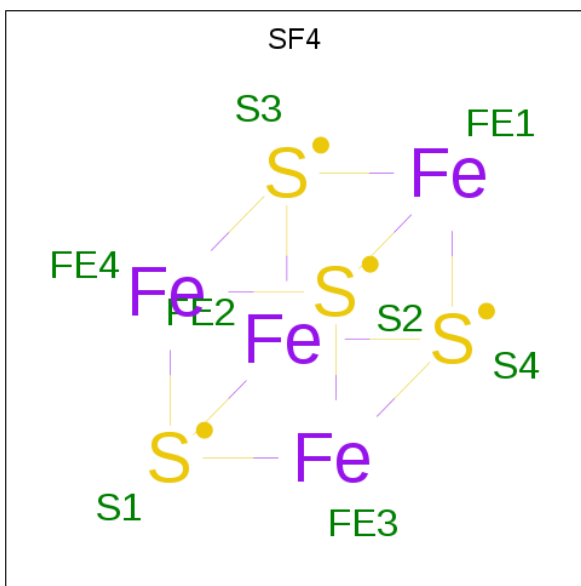
There are 16 discrepancies between the modelled and reference sequences:

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.

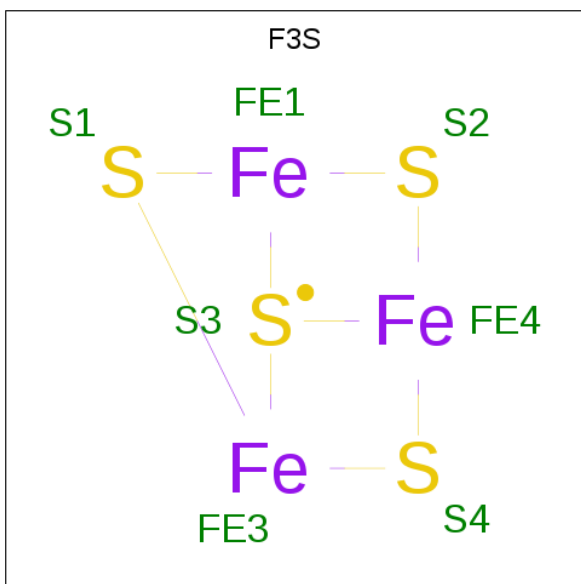
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	581	Total	C	N	O	S	0	30	0
			4724	3003	828	864	29			
2	M	581	Total	C	N	O	S	0	19	0
			4650	2958	808	856	28			

- 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	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: Fe_3S_4).



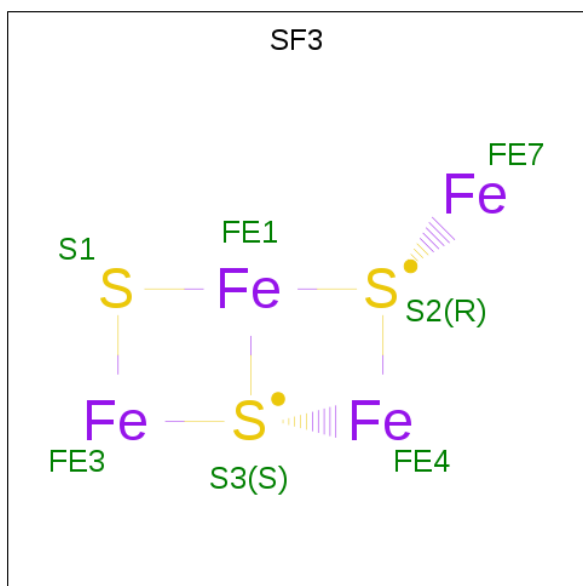
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	S	1	Total	Fe	S	0	0
			7	3	4		

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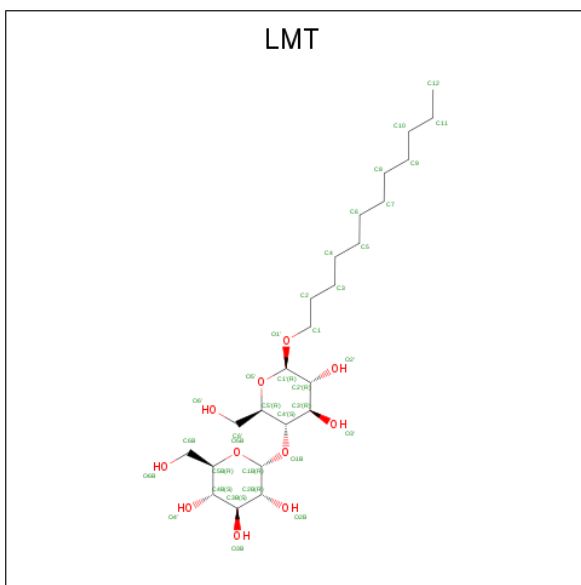
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	T	1	Total	Fe	S	0	0
			7	3	4		

- Molecule 5 is FE4-S3 CLUSTER (three-letter code: SF3) (formula: Fe₄S₃).



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

- Molecule 6 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: C₂₄H₄₆O₁₁).



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

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

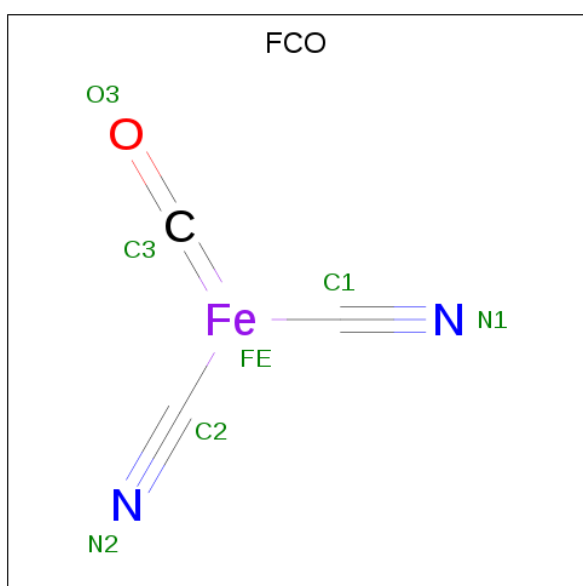
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	T	3	Total Cl 3 3	0	0
7	S	2	Total Cl 2 2	0	0

- Molecule 8 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- 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	0	0
			7	3	1	2	1		
9	M	1	Total	C	Fe	N	O	0	0
			7	3	1	2	1		

- Molecule 10 is NICKEL (III) ION (three-letter code: 3NI) (formula: Ni).

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

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

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

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

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

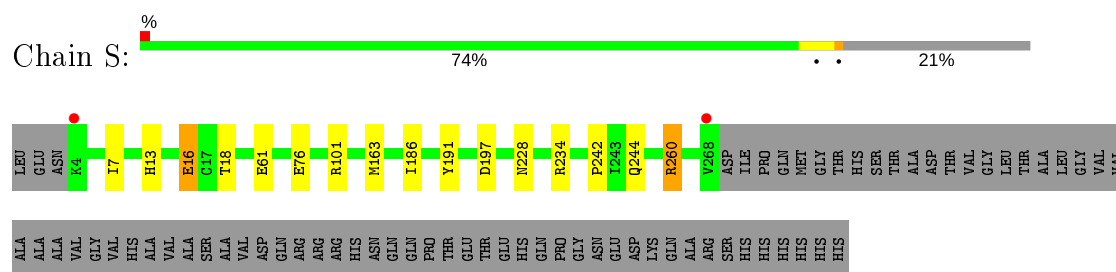
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	S	193	Total	O	0	1
			194	194		
13	L	410	Total	O	0	0
			410	410		
13	T	183	Total	O	0	1
			184	184		
13	M	446	Total	O	0	0
			446	446		

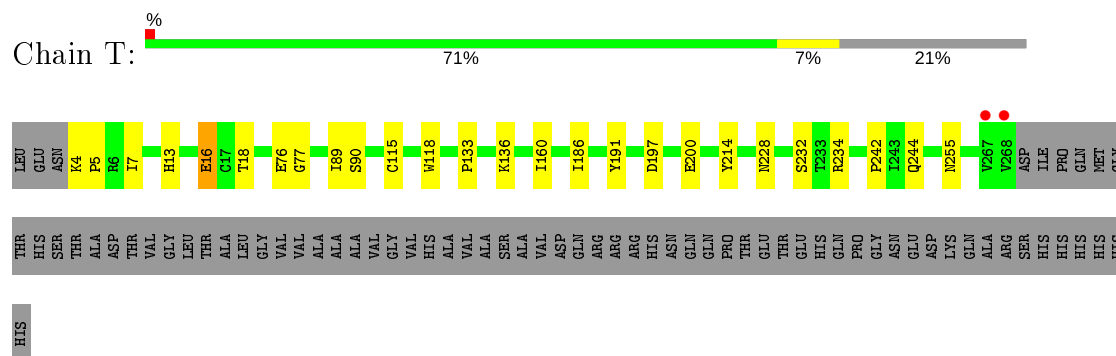
3 Residue-property plots [i](#)

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.

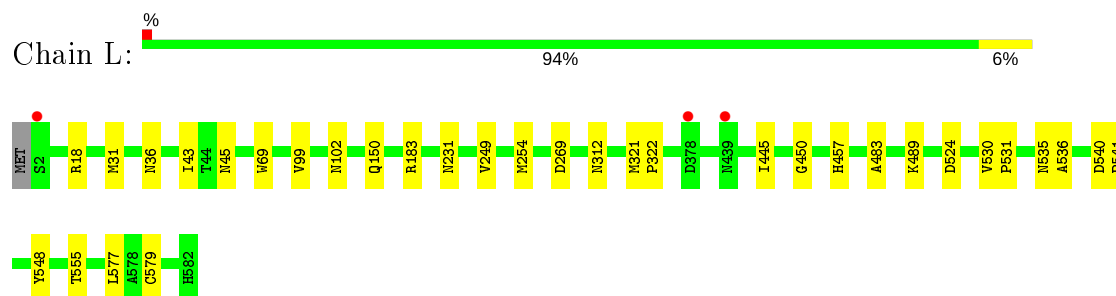
- Molecule 1: Hydrogenase-1 small chain



- Molecule 1: Hydrogenase-1 small chain

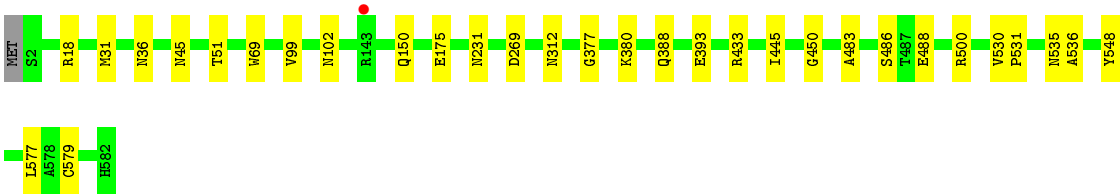


- Molecule 2: Hydrogenase-1 large chain



- 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, α , β , γ	94.17Å 98.16Å 183.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.00 29.72 – 2.00	Depositor EDS
% Data completeness (in resolution range)	87.6 (25.00-2.00) 87.6 (29.72-2.00)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.64 (at 2.00Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.141 , 0.177 0.151 , 0.186	Depositor DCC
R_{free} test set	5079 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	10.2	Xtriage
Anisotropy	0.641	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 42.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.026 for k,h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	14932	wwPDB-VP
Average B, all atoms (Å ²)	11.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.19% 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: MG, CL, SF4, LMT, SF3, 3NI, F3S, SO4, 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	0.63	0/2178	0.65	1/2955 (0.0%)
1	T	0.63	0/2189	0.64	0/2969
2	L	0.61	0/4925	0.61	0/6693
2	M	0.63	0/4826	0.62	0/6561
All	All	0.62	0/14118	0.62	1/19178 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S	260	ARG	NE-CZ-NH2	-5.42	117.59	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	2099	0	2050	17	0
1	T	2107	0	2068	18	0
2	L	4724	0	4670	31	0
2	M	4650	0	4578	28	0
3	S	8	0	0	0	0
3	T	8	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	14	0	25	5	0
6	T	14	0	25	2	0
7	S	2	0	0	0	0
7	T	3	0	0	0	0
8	M	5	0	0	0	0
8	S	5	0	0	0	0
8	T	10	0	0	0	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
13	L	410	0	0	8	0
13	M	446	0	0	6	0
13	S	194	0	0	2	0
13	T	184	0	0	1	0
All	All	14932	0	13416	85	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 (85) 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:L:457[A]:HIS:CD2	13:L:1030:HOH:O	1.81	1.30
2:M:269[A]:ASP:OD1	13:M:1130:HOH:O	1.54	1.21
1:S:61[B]:GLU:OE2	1:S:101[B]:ARG:NH1	1.78	1.15
2:M:175[B]:GLU:HG3	13:M:1138:HOH:O	0.93	1.09
2:L:150:GLN:HE22	2:M:150:GLN:HE22	1.15	0.89
1:T:7:ILE:HD13	6:T:404:LMT:H41	1.55	0.86
2:M:175[B]:GLU:CG	13:M:1138:HOH:O	1.63	0.85
2:L:457[A]:HIS:HD2	13:L:1030:HOH:O	1.33	0.82
2:L:269[A]:ASP:OD1	13:L:1103:HOH:O	2.00	0.80
1:S:234[B]:ARG:NH2	13:S:552:HOH:O	1.70	0.79
1:S:7:ILE:HD13	6:S:404:LMT:H42	1.66	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:486[A]:SER:OG	2:M:488[A]:GLU:OE1	2.05	0.72
2:L:18:ARG:HH11	2:L:36:ASN:HD21	1.36	0.71
2:M:18:ARG:HH11	2:M:36:ASN:HD21	1.38	0.69
1:S:234[A]:ARG:NH1	1:T:234[A]:ARG:HD3	2.09	0.68
2:L:99:VAL:H	2:L:312:ASN:HD21	1.41	0.68
2:M:36:ASN:HD22	2:M:45:ASN:HD22	1.41	0.66
1:S:234[A]:ARG:HD3	1:T:234[A]:ARG:NH1	2.12	0.65
2:L:150:GLN:NE2	2:M:150:GLN:HE22	1.91	0.65
2:M:99:VAL:H	2:M:312:ASN:HD21	1.45	0.64
2:L:36:ASN:HD22	2:L:45:ASN:HD22	1.48	0.62
2:M:530:VAL:CG1	2:M:531:PRO:HD2	2.30	0.62
1:T:186:ILE:HD11	1:T:228:ASN:HB3	1.81	0.62
1:S:7:ILE:HD13	6:S:404:LMT:C4	2.30	0.61
2:L:254[B]:MET:HA	2:L:254[B]:MET:HE2	1.85	0.59
2:M:269[A]:ASP:CG	13:M:1130:HOH:O	2.22	0.59
1:S:18:THR:HA	1:S:76[A]:GLU:OE1	2.02	0.59
2:M:36:ASN:ND2	2:M:45:ASN:HD22	2.00	0.58
2:L:457[A]:HIS:NE2	13:L:1030:HOH:O	2.14	0.57
2:M:530:VAL:HG12	2:M:531:PRO:HD2	1.87	0.56
1:S:163:MET:HB3	6:S:404:LMT:H52	1.88	0.55
1:S:197:ASP:OD2	1:T:197:ASP:OD2	2.23	0.55
1:S:186:ILE:HD11	1:S:228:ASN:HB3	1.91	0.52
2:L:183[B]:ARG:NH2	13:L:912:HOH:O	0.67	0.51
1:S:234[A]:ARG:CZ	1:S:244:GLN:HE22	2.23	0.51
2:L:530:VAL:CG1	2:L:531:PRO:HD2	2.41	0.51
1:T:4:LYS:HG3	1:T:5:PRO:HD2	1.90	0.51
1:T:234[A]:ARG:CZ	1:T:244:GLN:HE22	2.25	0.50
2:M:380[A]:LYS:HB2	2:M:388:GLN:HB2	1.94	0.50
1:S:13:HIS:HD2	1:S:16[B]:GLU:OE2	1.96	0.49
2:L:150:GLN:HE22	2:M:150:GLN:NE2	1.97	0.49
1:S:18:THR:HG22	1:S:18:THR:O	2.13	0.49
2:L:269[A]:ASP:CG	13:L:1103:HOH:O	2.49	0.48
2:L:99:VAL:H	2:L:312:ASN:ND2	2.09	0.48
2:M:31:MET:HB2	2:M:577:LEU:HG	1.95	0.48
2:L:445:ILE:O	2:L:450:GLY:HA3	2.13	0.48
2:L:530:VAL:HG11	2:L:579:CYS:HB3	1.94	0.47
2:L:31:MET:HB2	2:L:577:LEU:HG	1.95	0.47
1:S:163:MET:HE3	6:S:404:LMT:H71	1.96	0.47
1:T:18:THR:HA	1:T:76[A]:GLU:OE1	2.16	0.46
2:L:535:ASN:HB3	2:L:548:TYR:CE1	2.51	0.46
1:S:61[B]:GLU:HG2	13:S:623:HOH:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:115:CYS:HB2	13:T:522:HOH:O	2.15	0.46
2:M:433[B]:ARG:NH2	13:M:1063:HOH:O	2.49	0.46
1:S:7:ILE:HG21	6:S:404:LMT:H61	1.99	0.45
2:L:536:ALA:HB2	2:L:548:TYR:CE2	2.50	0.45
2:L:36:ASN:ND2	2:L:45:ASN:HD22	2.13	0.45
2:M:99:VAL:H	2:M:312:ASN:ND2	2.12	0.45
2:L:69:TRP:HH2	2:L:231:ASN:HD22	1.65	0.45
2:M:69:TRP:HH2	2:M:231:ASN:HD22	1.65	0.45
2:L:269[B]:ASP:OD1	13:L:1086:HOH:O	2.21	0.45
2:L:254[B]:MET:CA	2:L:254[B]:MET:HE2	2.46	0.45
2:L:540:ASP:HB2	2:L:541:PRO:CD	2.47	0.44
2:M:535:ASN:HB3	2:M:548:TYR:CE1	2.53	0.44
1:T:160:ILE:HG12	6:T:404:LMT:H92	2.00	0.44
2:M:500[B]:ARG:NH2	13:M:1015:HOH:O	2.52	0.43
1:S:234[A]:ARG:NH1	1:T:234[A]:ARG:CD	2.79	0.43
2:M:377:GLY:HA3	2:M:393[A]:GLU:OE1	2.18	0.43
1:T:89:ILE:HB	2:M:51:THR:HB	2.00	0.42
1:T:133:PRO:HG2	1:T:136:LYS:HG2	2.01	0.42
1:T:118:TRP:CD2	1:T:255:ASN:HB2	2.55	0.42
1:T:13:HIS:HD2	1:T:16[B]:GLU:OE1	2.02	0.42
2:L:489[A]:LYS:HE2	13:L:1099:HOH:O	2.19	0.42
2:L:43:ILE:HD12	2:L:555:THR:HB	2.01	0.42
1:T:77:GLY:HA2	1:T:115:CYS:HB3	2.01	0.42
1:T:200:GLU:HB3	1:T:214:TYR:CD2	2.55	0.42
2:M:530:VAL:HG13	2:M:531:PRO:HD2	2.00	0.41
2:M:445:ILE:O	2:M:450:GLY:HA3	2.21	0.41
2:M:530:VAL:HG11	2:M:579:CYS:HB3	2.02	0.41
2:L:249:VAL:HB	1:T:232[B]:SER:OG	2.21	0.41
2:M:536:ALA:HB2	2:M:548:TYR:CE2	2.56	0.41
2:L:102:ASN:HB2	2:L:483:ALA:O	2.21	0.41
2:L:530:VAL:HG12	2:L:531:PRO:HD2	2.02	0.40
2:L:321:MET:HA	2:L:322:PRO:HD3	1.94	0.40
2:M:102:ASN:HB2	2:M:483:ALA:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	272/335 (81%)	259 (95%)	13 (5%)	0	100	100
1	T	273/335 (82%)	260 (95%)	13 (5%)	0	100	100
2	L	609/582 (105%)	590 (97%)	19 (3%)	0	100	100
2	M	598/582 (103%)	583 (98%)	15 (2%)	0	100	100
All	All	1752/1834 (96%)	1692 (97%)	60 (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	227/274 (83%)	222 (98%)	5 (2%)	52	55
1	T	228/274 (83%)	222 (97%)	6 (3%)	46	48
2	L	509/481 (106%)	508 (100%)	1 (0%)	93	95
2	M	499/481 (104%)	499 (100%)	0	100	100
All	All	1463/1510 (97%)	1451 (99%)	12 (1%)	86	86

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	S	16[A]	GLU
1	S	16[B]	GLU

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Mol	Chain	Res	Type
1	S	191	TYR
1	S	242	PRO
1	S	260	ARG
2	L	524	ASP
1	T	16[A]	GLU
1	T	16[B]	GLU
1	T	90[A]	SER
1	T	90[B]	SER
1	T	191	TYR
1	T	242	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	S	13	HIS
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	328	ASN
2	L	332	ASN
2	L	544	GLN
2	M	36	ASN
2	M	108	ASN
2	M	231	ASN
2	M	258	ASN
2	M	312	ASN
2	M	479	ASN
2	M	544	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 26 ligands modelled in this entry, 10 are monoatomic - leaving 16 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
3	SF4	S	401	1	0,12,12	0.00	-	-		
8	SO4	T	409	-	4,4,4	0.13	0	6,6,6	0.27	0
4	F3S	S	402	1	0,9,9	0.00	-	-		
6	LMT	S	404	-	13,13,36	0.30	0	12,12,47	0.44	0
5	SF3	T	403[B]	1	0,8,8	0.00	-	-		
9	FCO	M	601	13,2	0,6,6	0.00	-	-		
5	SF3	T	403[C]	1	0,8,8	0.00	-	-		
8	SO4	T	408	-	4,4,4	0.11	0	6,6,6	0.19	0
6	LMT	T	404	-	13,13,36	0.29	0	12,12,47	0.47	0
5	SF3	S	403[C]	1	0,8,8	0.00	-	-		
4	F3S	T	402	1	0,9,9	0.00	-	-		
3	SF4	T	401	1	0,12,12	0.00	-	-		
8	SO4	M	604	-	4,4,4	0.18	0	6,6,6	0.16	0
9	FCO	L	601	13,2	0,6,6	0.00	-	-		
8	SO4	S	407	-	4,4,4	0.24	0	6,6,6	0.30	0
5	SF3	S	403[B]	1	0,8,8	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	S	401	1	-	-	0/6/5/5
4	F3S	S	402	1	-	-	0/3/3/3
6	LMT	S	404	-	-	4/11/11/61	-
5	SF3	T	403[B]	1	-	-	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SF4	T	401	1	-	-	0/6/5/5
5	SF3	T	403[C]	1	-	-	0/2/2/2
6	LMT	T	404	-	-	7/11/11/61	-
5	SF3	S	403[C]	1	-	-	0/2/2/2
4	F3S	T	402	1	-	-	0/3/3/3
5	SF3	S	403[B]	1	-	-	0/2/2/2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	T	404	LMT	O1'-C1-C2-C3
6	T	404	LMT	C2-C3-C4-C5
6	S	404	LMT	O1'-C1-C2-C3
6	S	404	LMT	C5-C6-C7-C8
6	S	404	LMT	C1-C2-C3-C4
6	T	404	LMT	C4-C5-C6-C7
6	S	404	LMT	C2-C1-O1'-C1'
6	T	404	LMT	C1-C2-C3-C4
6	T	404	LMT	C9-C10-C11-C12
6	T	404	LMT	C2-C1-O1'-C1'
6	T	404	LMT	C7-C8-C9-C10

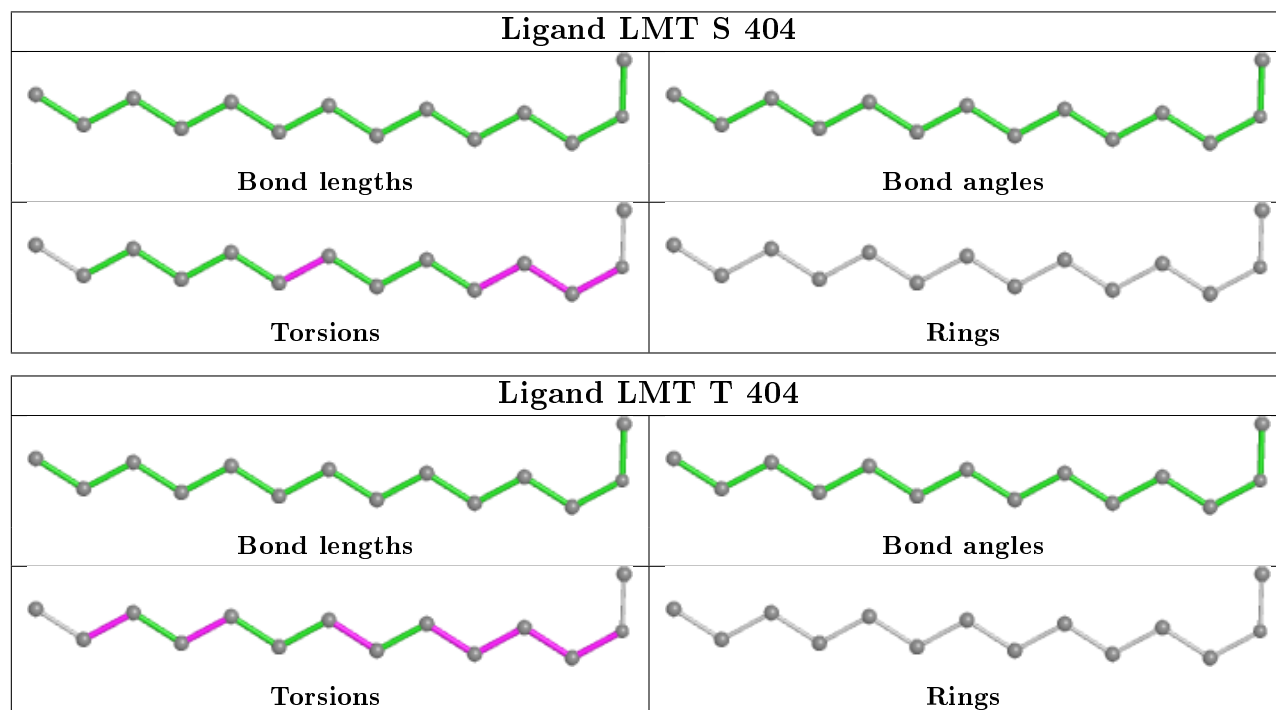
There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	S	404	LMT	5	0
6	T	404	LMT	2	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, 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	S	265/335 (79%)	-0.61	2 (0%) 86 85	4, 9, 18, 41	4 (1%)
1	T	265/335 (79%)	-0.57	2 (0%) 86 85	4, 9, 19, 41	5 (1%)
2	L	581/582 (99%)	-0.60	3 (0%) 91 90	4, 10, 21, 34	4 (0%)
2	M	581/582 (99%)	-0.65	1 (0%) 95 94	4, 10, 20, 33	0
All	All	1692/1834 (92%)	-0.61	8 (0%) 91 90	4, 9, 20, 41	13 (0%)

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	T	268	VAL	5.9
1	S	268	VAL	5.4
1	T	267	VAL	3.9
2	L	2	SER	3.0
1	S	4	LYS	2.9
2	M	143	ARG	2.4
2	L	378	ASP	2.3
2	L	439[A]	ASN	2.3

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 carbohydrates in this entry.

6.4 Ligands ⓘ

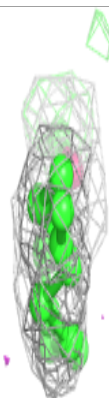
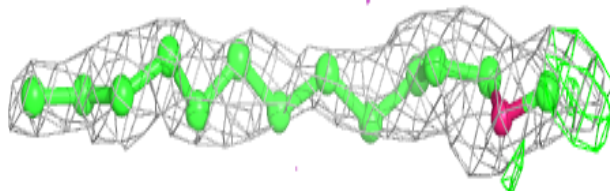
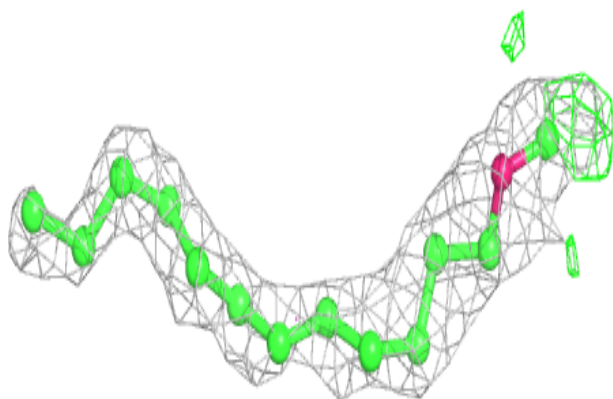
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	SO4	T	408	5/5	0.80	0.22	23,24,31,31	5
8	SO4	M	604	5/5	0.83	0.26	40,41,42,45	5
6	LMT	S	404	14/35	0.86	0.20	28,31,40,40	0
12	LI	L	604	1/1	0.86	0.27	9,9,9,9	0
6	LMT	T	404	14/35	0.86	0.20	30,33,43,43	0
7	CL	T	407	1/1	0.87	0.08	34,34,34,34	1
8	SO4	T	409	5/5	0.92	0.22	35,36,39,40	5
8	SO4	S	407	5/5	0.93	0.19	19,21,23,25	5
7	CL	T	406	1/1	0.98	0.14	14,14,14,14	1
7	CL	S	406	1/1	0.99	0.14	9,9,9,9	1
10	3NI	L	602	1/1	0.99	0.02	11,11,11,11	0
7	CL	T	405	1/1	0.99	0.04	14,14,14,14	0
7	CL	S	405	1/1	0.99	0.05	13,13,13,13	0
9	FCO	M	601	7/7	1.00	0.06	6,6,7,8	0
5	SF3	S	403[C]	7/7	1.00	0.03	7,7,9,13	1
4	F3S	T	402	7/7	1.00	0.04	5,6,7,7	0
11	MG	L	603	1/1	1.00	0.04	6,6,6,6	0
9	FCO	L	601	7/7	1.00	0.06	6,6,7,7	0
5	SF3	S	403[B]	7/7	1.00	0.03	7,7,9,11	1
11	MG	M	603	1/1	1.00	0.08	4,4,4,4	0
4	F3S	S	402	7/7	1.00	0.04	6,6,6,7	0
5	SF3	T	403[B]	7/7	1.00	0.03	8,9,10,11	1
5	SF3	T	403[C]	7/7	1.00	0.03	8,9,10,15	1
10	3NI	M	602	1/1	1.00	0.03	12,12,12,12	0
3	SF4	T	401	8/8	1.00	0.04	6,7,8,8	0
3	SF4	S	401	8/8	1.00	0.04	6,7,8,8	0

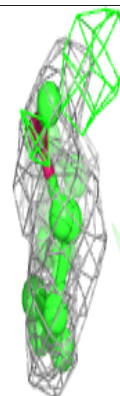
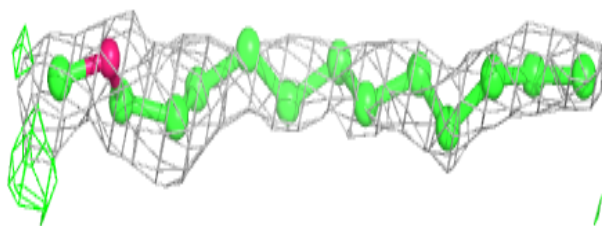
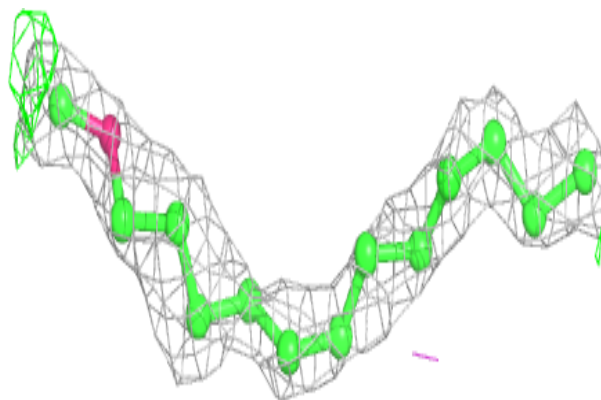
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around LMT 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 ⓘ

There are no such residues in this entry.