Full wwPDB X-ray Structure Validation Report (i)

Jan 7, 2024 – 06:58 am GMT

PDB ID	:	6G7R
Title	:	Structure of fully reduced variant E28Q of E. coli hydrogenase-1 at pH 8
Authors	:	Carr, S.B.; Armstrong, F.A.; Evans, R.M.
Deposited on	:	2018-04-06
Resolution	:	1.20 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

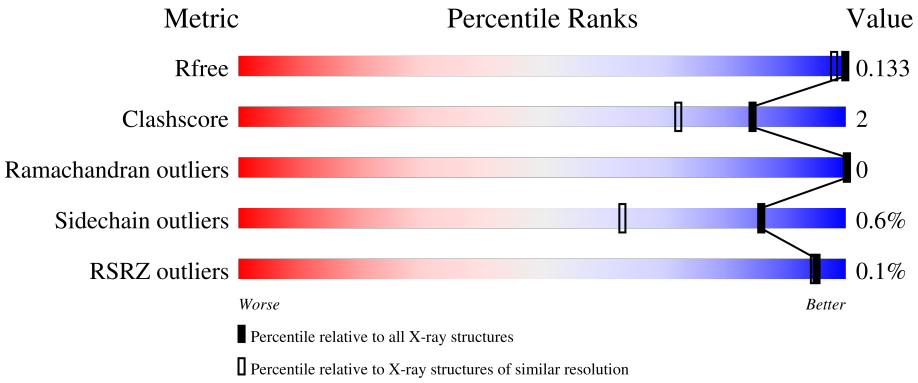
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.20 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	1223 (1.22-1.18)
Clashscore	141614	1286 (1.22-1.18)
Ramachandran outliers	138981	1240 (1.22-1.18)
Sidechain outliers	138945	1239 (1.22-1.18)
RSRZ outliers	127900	1200 (1.22-1.18)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	S	335	75% . 21%
1	T	335	74% . . 21%
2	L	582	95% 5%
2	M	582	96% .

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 28652 atoms, of which 13324 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	263	Total	C	H	N	O	S	148	7	0
			4110	1319	2034	359	378	20			
1	T	263	Total	C	H	N	O	S	157	10	0
			4173	1336	2070	367	379	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

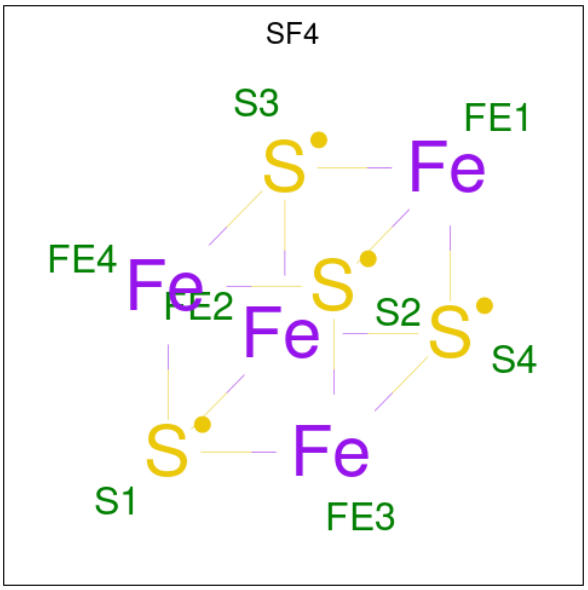
- Molecule 2 is a protein called Hydrogenase-1 large chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	L	581	Total	C	H	N	O	S	375	21	0
			9248	2961	4586	817	856	28			
2	M	581	Total	C	H	N	O	S	361	17	0
			9195	2948	4560	807	853	27			

There are 2 discrepancies between the modelled and reference sequences:

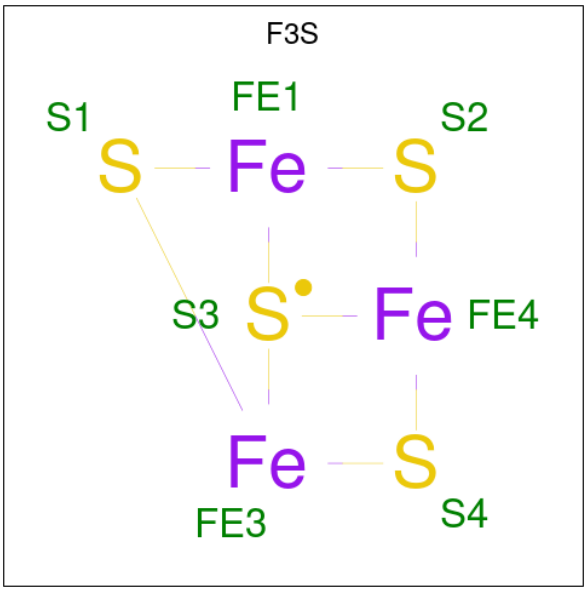
Chain	Residue	Modelled	Actual	Comment	Reference
L	28	GLN	GLU	conflict	UNP P0ACD8
M	28	GLN	GLU	conflict	UNP P0ACD8

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



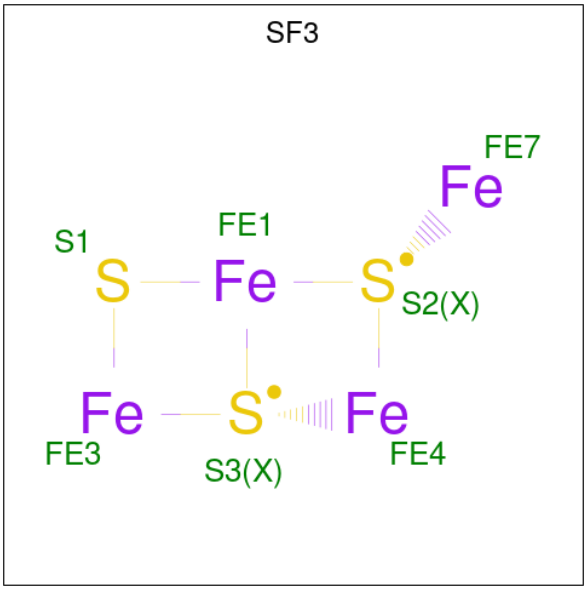
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	S	1	Total	Fe	S	0	0
			8	4	4		
3	T	1	Total	Fe	S	0	0
			8	4	4		

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



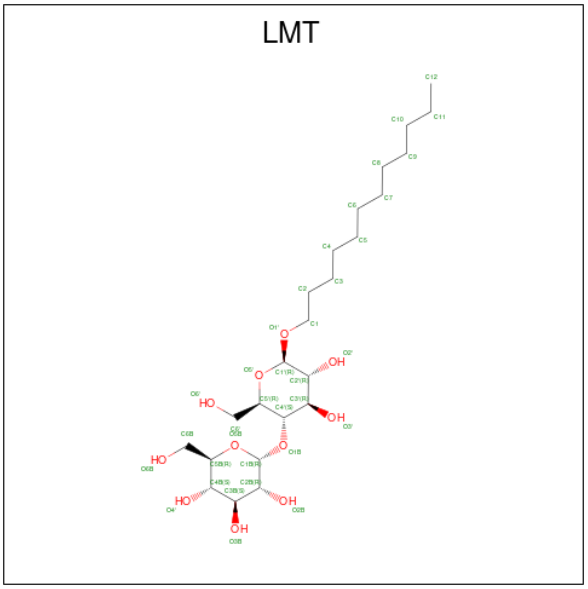
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	S	1	Total Fe S 7 3 4	0	0
4	T	1	Total Fe S 7 3 4	0	0

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



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

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

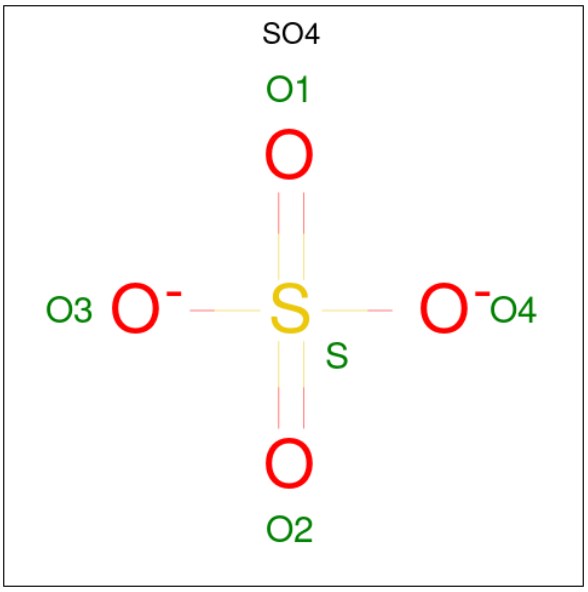


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	S	1	Total C H O 81 24 46 11	6	0
6	T	1	Total C H O 40 13 26 1	1	0

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

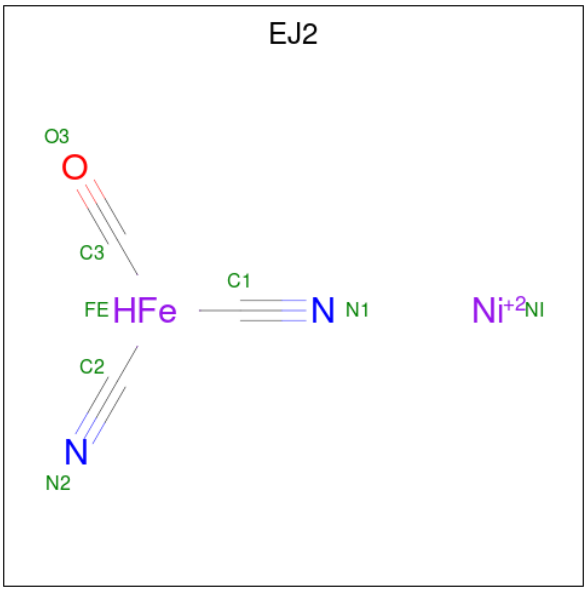
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	S	2	Total Cl 2 2	0	0
7	T	2	Total Cl 2 2	0	0

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



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

- Molecule 9 is NI-FE REDUCED ACTIVE CENTER (three-letter code: EJ2) (formula: C_3HFeN_2NiO).



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

- Molecule 10 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 11 is water.

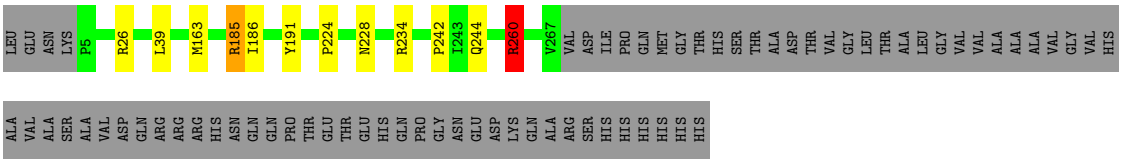
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	S	241	Total O 241 241	0	0
11	L	590	Total O 590 590	0	0
11	T	287	Total O 287 287	0	0
11	M	614	Total O 614 614	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

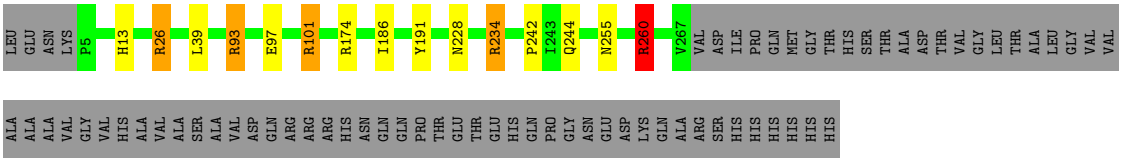
• Molecule 1: Hydrogenase-1 small chain

Chain S:



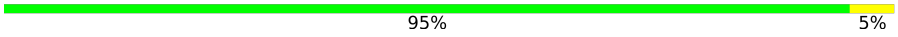
• Molecule 1: Hydrogenase-1 small chain

Chain T:



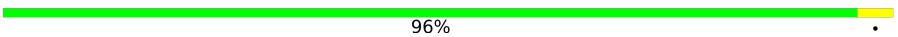
• Molecule 2: Hydrogenase-1 large chain

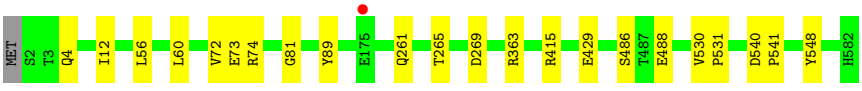
Chain L:



• Molecule 2: Hydrogenase-1 large chain

Chain M:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	94.07Å 97.81Å 183.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	67.89 – 1.20 67.80 – 1.20	Depositor EDS
% Data completeness (in resolution range)	96.5 (67.89-1.20) 96.5 (67.80-1.20)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.90 (at 1.20Å)	Xtriage
Refinement program	REFMAC 5.8.0222	Depositor
R, R_{free}	0.111 , 0.133 0.111 , 0.133	Depositor DCC
R_{free} test set	25633 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	10.2	Xtriage
Anisotropy	0.637	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 46.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o,F_c correlation	0.99	EDS
Total number of atoms	28652	wwPDB-VP
Average B, all atoms (Å^2)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.82% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SF3, F3S, MG, EJ2, SO4, SF4, CL, LMT

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	0.54	0/2143	0.91	6/2908 (0.2%)
1	T	0.53	0/2176	0.82	4/2951 (0.1%)
2	L	0.50	1/4844 (0.0%)	0.76	6/6586 (0.1%)
2	M	0.50	0/4802	0.76	5/6533 (0.1%)
All	All	0.51	1/13965 (0.0%)	0.79	21/18978 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	S	0	2
1	T	0	3
2	L	0	2
2	M	0	1
All	All	0	8

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	561	GLU	CD-OE1	5.37	1.31	1.25

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	S	185[A]	ARG	NE-CZ-NH1	10.48	125.54	120.30
1	S	185[B]	ARG	NE-CZ-NH1	10.48	125.54	120.30
1	S	185[A]	ARG	NE-CZ-NH2	-10.30	115.15	120.30
1	S	185[B]	ARG	NE-CZ-NH2	-10.30	115.15	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	L	89	TYR	CB-CG-CD1	8.40	126.04	121.00
2	L	89	TYR	CB-CG-CD2	-7.91	116.26	121.00
2	L	363	ARG	NE-CZ-NH1	-7.90	116.35	120.30
2	M	363	ARG	NE-CZ-NH2	7.73	124.17	120.30
2	M	89	TYR	CB-CG-CD1	7.68	125.61	121.00
2	L	363	ARG	NE-CZ-NH2	6.93	123.76	120.30
2	M	89	TYR	CB-CG-CD2	-6.65	117.01	121.00
1	T	234[A]	ARG	NE-CZ-NH2	-6.64	116.98	120.30
1	T	234[B]	ARG	NE-CZ-NH2	-6.64	116.98	120.30
1	S	260	ARG	NE-CZ-NH2	-6.32	117.14	120.30
2	M	548	TYR	CB-CG-CD1	6.14	124.68	121.00
1	T	26	ARG	NE-CZ-NH2	-5.77	117.41	120.30
2	L	548	TYR	CB-CG-CD1	5.31	124.19	121.00
2	M	415	ARG	NE-CZ-NH2	-5.28	117.66	120.30
2	L	356	TYR	CB-CG-CD2	-5.11	117.93	121.00
1	T	260	ARG	NE-CZ-NH2	-5.05	117.78	120.30
1	S	260	ARG	CG-CD-NE	-5.01	101.29	111.80

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	L	169	ARG	Sidechain
2	L	74	ARG	Sidechain
2	M	74	ARG	Sidechain
1	S	26	ARG	Sidechain
1	S	260	ARG	Sidechain
1	T	26	ARG	Sidechain
1	T	260	ARG	Sidechain
1	T	93[A]	ARG	Sidechain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	S	2076	2034	2027	15	0
1	T	2103	2070	2065	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	L	4662	4586	4590	21	0
2	M	4635	4560	4558	11	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	35	46	46	1	0
6	T	14	26	25	0	0
7	S	2	0	0	0	0
7	T	2	0	0	0	0
8	L	5	0	0	0	0
9	L	8	1	0	0	0
9	M	8	1	0	0	0
10	L	1	0	0	0	0
10	M	1	0	0	0	0
11	L	590	0	0	13	0
11	M	614	0	0	3	0
11	S	241	0	0	0	0
11	T	287	0	0	2	0
All	All	15328	13324	13311	63	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 2.

All (63) 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:28:GLN:CD	11:L:703:HOH:O	1.73	1.24
1:T:93[B]:ARG:CZ	1:T:97:GLU:OE1	1.98	1.12
2:L:28:GLN:CG	11:L:703:HOH:O	1.91	1.10
1:T:101:ARG:HH11	1:T:101:ARG:HG3	1.25	1.00
2:L:28:GLN:NE2	11:L:703:HOH:O	1.91	0.99
1:S:234[A]:ARG:NH1	1:T:234[A]:ARG:NH2	2.12	0.96
2:L:183[B]:ARG:NH1	11:L:704:HOH:O	1.99	0.93
2:L:165[B]:ASP:OD1	11:L:702:HOH:O	1.86	0.92
2:L:28:GLN:HG3	11:L:703:HOH:O	1.59	0.82
1:T:93[B]:ARG:NE	1:T:97:GLU:OE1	2.14	0.80
1:S:234[A]:ARG:CZ	1:T:234[A]:ARG:CZ	2.59	0.80
2:L:269[B]:ASP:OD1	11:L:705:HOH:O	2.02	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:254[B]:MET:HA	2:L:254[B]:MET:HE2	1.70	0.73
1:T:101:ARG:HH11	1:T:101:ARG:CG	1.99	0.73
1:S:234[A]:ARG:CZ	1:T:234[A]:ARG:NH2	2.52	0.73
1:S:234[A]:ARG:HH11	1:T:234[A]:ARG:NH2	1.87	0.73
1:S:234[A]:ARG:NH1	1:T:234[A]:ARG:HH21	1.86	0.72
2:M:429[B]:GLU:HG3	11:M:735:HOH:O	1.92	0.69
11:L:1247:HOH:O	1:T:39[A]:LEU:HD11	1.94	0.67
1:T:234[B]:ARG:CZ	1:T:244:GLN:HE22	2.08	0.67
2:M:269[B]:ASP:OD1	11:M:701:HOH:O	2.13	0.65
1:S:234[A]:ARG:NH1	1:T:234[A]:ARG:CZ	2.59	0.65
2:L:562:GLN:OE1	11:L:706:HOH:O	2.14	0.64
1:T:13:HIS:HD2	11:T:578:HOH:O	1.81	0.63
1:T:39[A]:LEU:HG	11:T:741:HOH:O	2.01	0.60
1:S:260:ARG:HG3	1:S:260:ARG:NH1	2.19	0.58
2:L:135:LEU:HD22	2:L:187:TRP:CD1	2.38	0.58
1:T:260:ARG:NH1	1:T:260:ARG:HG3	2.18	0.57
2:M:60[B]:LEU:HD11	2:M:72:VAL:CG1	2.36	0.56
1:S:234[A]:ARG:HH11	1:T:234[A]:ARG:HH21	1.47	0.56
1:S:234[B]:ARG:NH2	1:T:234[B]:ARG:HD3	2.21	0.55
1:S:39[A]:LEU:HD11	11:M:1266:HOH:O	2.07	0.55
2:L:393:GLU:OE1	11:L:707:HOH:O	2.18	0.54
1:T:101:ARG:CG	1:T:101:ARG:NH1	2.67	0.54
2:L:183[B]:ARG:CZ	11:L:704:HOH:O	2.46	0.53
1:T:260:ARG:HG3	1:T:260:ARG:HH11	1.73	0.52
1:T:255:ASN:O	1:T:260:ARG:NH2	2.36	0.52
1:S:234[B]:ARG:NH1	1:S:244:GLN:HE22	2.07	0.52
2:L:144:LYS:HB3	2:L:197[A]:GLU:HG2	1.92	0.52
2:L:519[B]:ARG:HG2	2:L:520:ASP:OD2	2.10	0.51
1:T:101:ARG:HG3	1:T:101:ARG:NH1	2.07	0.51
1:S:185[A]:ARG:HD2	1:S:224:PRO:O	2.13	0.48
2:L:169:ARG:NH2	11:L:715:HOH:O	2.46	0.48
2:L:530:VAL:CG1	2:L:531:PRO:HD2	2.44	0.48
2:M:486[A]:SER:OG	2:M:488[A]:GLU:OE1	2.31	0.47
2:M:530:VAL:CG1	2:M:531:PRO:HD2	2.46	0.45
2:L:4:GLN:HA	2:L:12:ILE:O	2.16	0.44
2:L:445:ILE:O	2:L:450:GLY:HA3	2.18	0.43
1:T:93[B]:ARG:NH2	1:T:97:GLU:OE1	2.45	0.43
2:L:530:VAL:HG11	2:L:579:CYS:HB3	1.99	0.43
1:S:234[A]:ARG:NE	1:T:234[A]:ARG:NH2	2.66	0.42
2:L:169:ARG:NH1	11:L:716:HOH:O	2.46	0.42
2:M:261:GLN:HE21	2:M:265[B]:THR:HG23	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:260:ARG:NH1	1:T:260:ARG:CG	2.78	0.42
2:M:56:LEU:O	2:M:60[A]:LEU:HD23	2.20	0.42
1:S:186:ILE:HD11	1:S:228:ASN:HB3	2.03	0.41
2:M:4:GLN:HA	2:M:12:ILE:O	2.20	0.41
2:M:540:ASP:HB2	2:M:541:PRO:CD	2.50	0.41
2:M:60[B]:LEU:HD11	2:M:72:VAL:HG13	2.03	0.41
2:L:530:VAL:HG13	2:L:531:PRO:HD2	2.03	0.41
1:S:163:MET:HB3	6:S:404:LMT:H52	2.03	0.41
2:M:73[B]:GLU:OE2	2:M:81:GLY:N	2.54	0.41
1:T:186:ILE:HD11	1:T:228:ASN:HB3	2.04	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	268/335 (80%)	256 (96%)	12 (4%)	0	100	100
1	T	271/335 (81%)	259 (96%)	12 (4%)	0	100	100
2	L	600/582 (103%)	585 (98%)	15 (2%)	0	100	100
2	M	596/582 (102%)	582 (98%)	14 (2%)	0	100	100
All	All	1735/1834 (95%)	1682 (97%)	53 (3%)	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	223/274 (81%)	220 (99%)	3 (1%)	69 33
1	T	226/274 (82%)	221 (98%)	5 (2%)	52 14
2	L	501/481 (104%)	499 (100%)	2 (0%)	91 76
2	M	497/481 (103%)	497 (100%)	0	100 100
All	All	1447/1510 (96%)	1437 (99%)	10 (1%)	86 59

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	S	191	TYR
1	S	242	PRO
1	S	260	ARG
2	L	169	ARG
2	L	524	ASP
1	T	101	ARG
1	T	174[A]	ARG
1	T	174[B]	ARG
1	T	191	TYR
1	T	242	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	T	13	HIS
1	T	244	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 17 ligands modelled in this entry, 6 are monoatomic - leaving 11 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	$\#\|Z\| > 2$
5	SF3	T	403	1	0,8,8	-	-	-		
8	SO4	L	601	-	4,4,4	0.11	0	6,6,6	0.32	0
3	SF4	T	401	1	0,12,12	-	-	-		
4	F3S	S	402	1	0,9,9	-	-	-		
6	LMT	S	404	-	36,36,36	0.68	0	47,47,47	1.26	5 (10%)
9	EJ2	M	601	2	1,6,6	2.48	1 (100%)	-		
4	F3S	T	402	1	0,9,9	-	-	-		
3	SF4	S	401	1	0,12,12	-	-	-		
6	LMT	T	404	-	13,13,36	0.40	0	12,12,47	0.45	0
5	SF3	S	403	1	0,8,8	-	-	-		
9	EJ2	L	602	2	1,6,6	3.13	1 (100%)	-		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	SF3	T	403	1	-	-	0/2/2/2
3	SF4	T	401	1	-	-	0/6/5/5
4	F3S	S	402	1	-	-	0/3/3/3
6	LMT	S	404	-	-	2/21/61/61	0/2/2/2
4	F3S	T	402	1	-	-	0/3/3/3
3	SF4	S	401	1	-	-	0/6/5/5
6	LMT	T	404	-	-	2/11/11/61	-
5	SF3	S	403	1	-	-	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	L	602	EJ2	O3-C3	-3.13	1.12	1.16
9	M	601	EJ2	O3-C3	-2.48	1.12	1.16

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	S	404	LMT	C6-C5-C4	3.26	130.97	114.42
6	S	404	LMT	O6B-C6B-C5B	-3.04	100.87	111.29
6	S	404	LMT	O5B-C5B-C4B	3.01	115.16	109.69
6	S	404	LMT	C8-C7-C6	2.56	127.43	114.42
6	S	404	LMT	C6'-C5'-C4'	2.41	120.35	113.33

There are no chirality outliers.

All (4) torsion outliers are listed below:

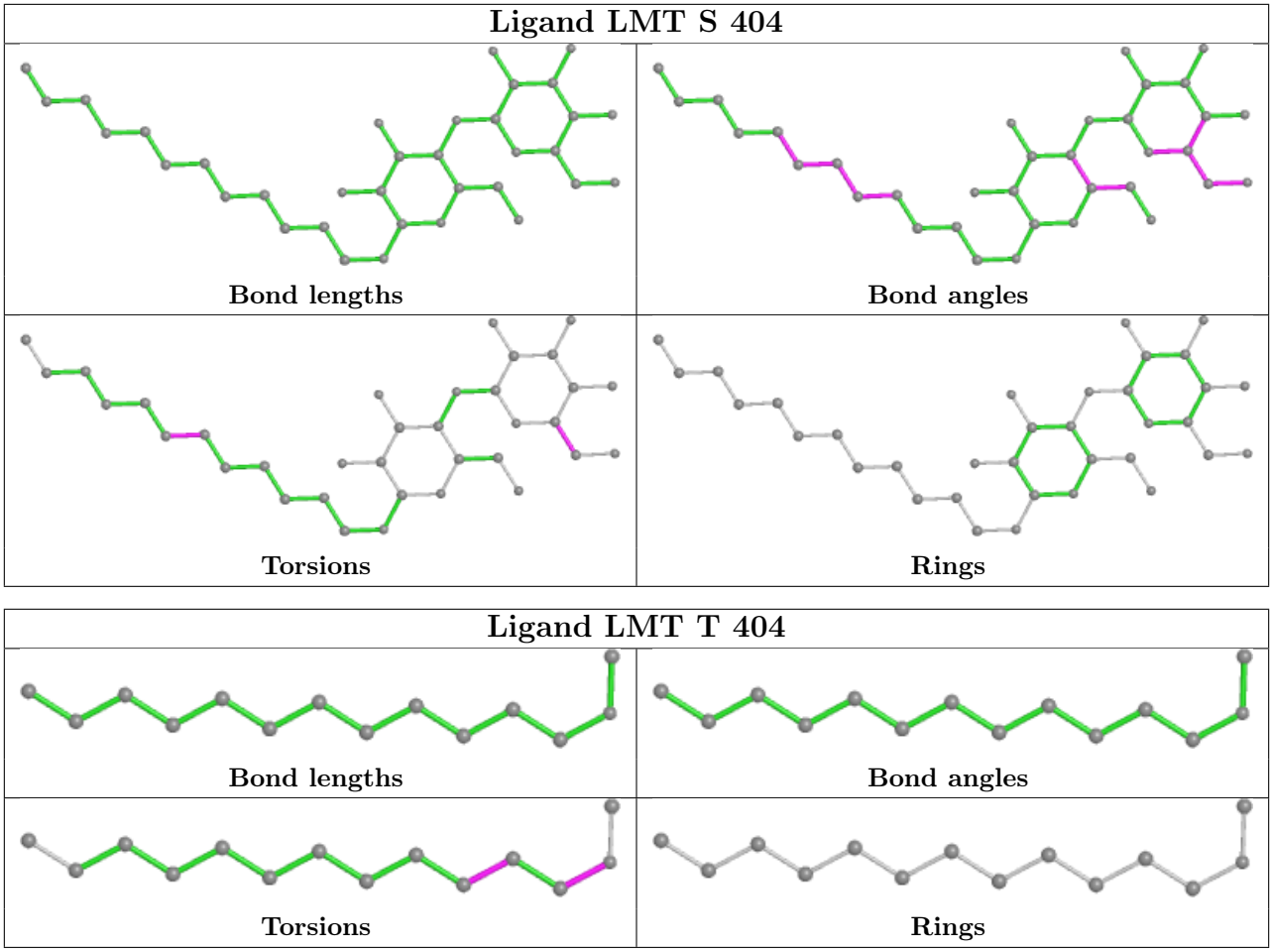
Mol	Chain	Res	Type	Atoms
6	T	404	LMT	C2-C1-O1'-C1'
6	T	404	LMT	C1-C2-C3-C4
6	S	404	LMT	C5-C6-C7-C8
6	S	404	LMT	C4B-C5B-C6B-O6B

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	S	404	LMT	1	0

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



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	S	263/335 (78%)	-0.72	0	100	100	7, 11, 18, 28	0
1	T	263/335 (78%)	-0.71	0	100	100	7, 11, 20, 29	0
2	L	581/582 (99%)	-0.80	0	100	100	7, 12, 26, 49	0
2	M	581/582 (99%)	-0.80	1 (0%)	95	94	7, 12, 22, 35	0
All	All	1688/1834 (92%)	-0.77	1 (0%)	95	95	7, 12, 23, 49	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	M	175	GLU	3.1

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

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

6.3 Carbohydrates

There are no monosaccharides 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^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	LMT	S	404	35/35	0.82	0.22	22,26,37,49	6

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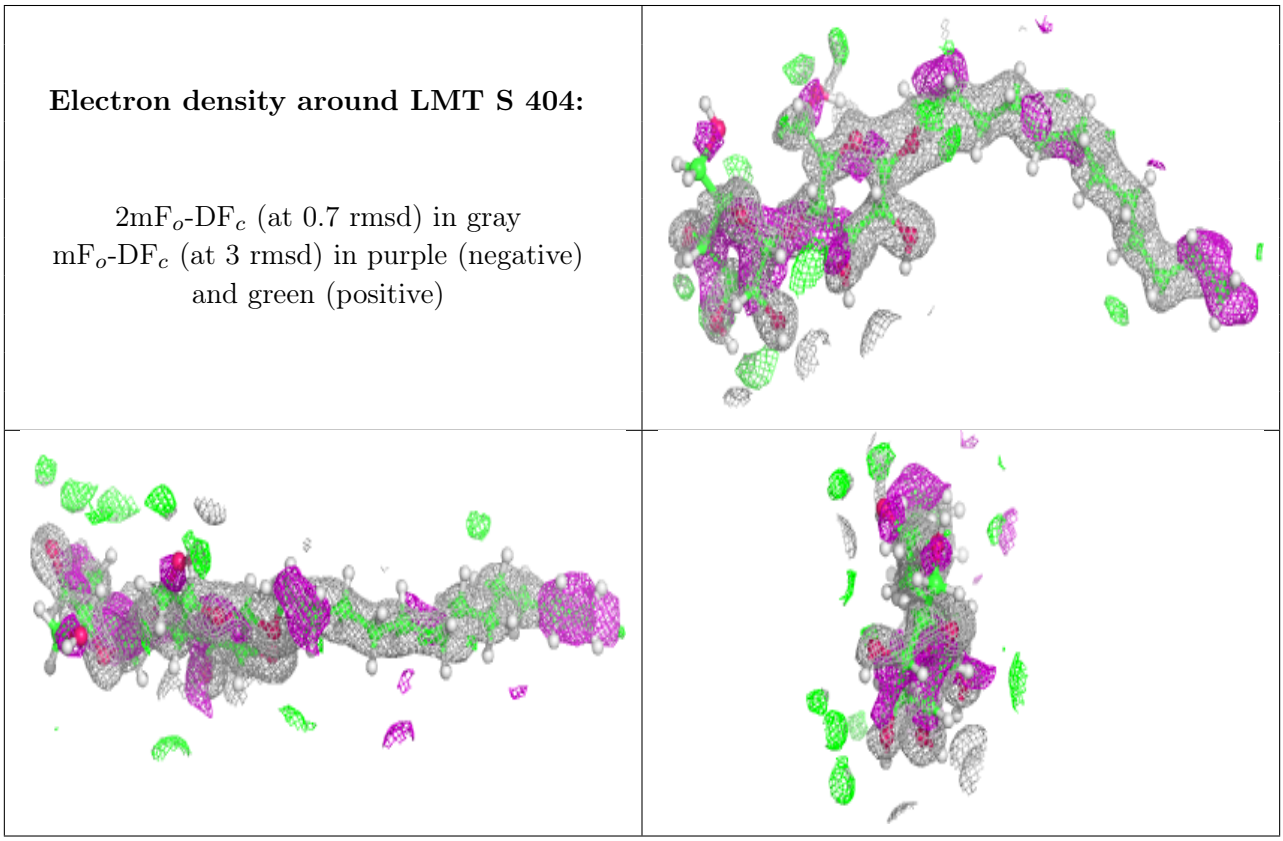
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	LMT	T	404	14/35	0.90	0.12	0,18,29,35	40
8	SO4	L	601	5/5	0.98	0.08	14,14,18,19	5
7	CL	T	406	1/1	0.99	0.12	30,30,30,30	0
5	SF3	S	403	7/7	1.00	0.07	7,7,7,8	0
5	SF3	T	403	7/7	1.00	0.06	8,8,8,8	0
3	SF4	S	401	8/8	1.00	0.07	7,7,8,8	0
3	SF4	T	401	8/8	1.00	0.07	7,7,7,8	0
7	CL	S	405	1/1	1.00	0.04	13,13,13,13	0
7	CL	S	406	1/1	1.00	0.12	27,27,27,27	0
7	CL	T	405	1/1	1.00	0.04	15,15,15,15	0
4	F3S	S	402	7/7	1.00	0.07	7,8,8,8	0
4	F3S	T	402	7/7	1.00	0.07	8,8,8,8	0
9	EJ2	L	602	8/8	1.00	0.06	8,9,10,11	0
9	EJ2	M	601	8/8	1.00	0.07	8,8,9,11	0
10	MG	L	603	1/1	1.00	0.12	6,6,6,6	0
10	MG	M	602	1/1	1.00	0.12	6,6,6,6	0

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

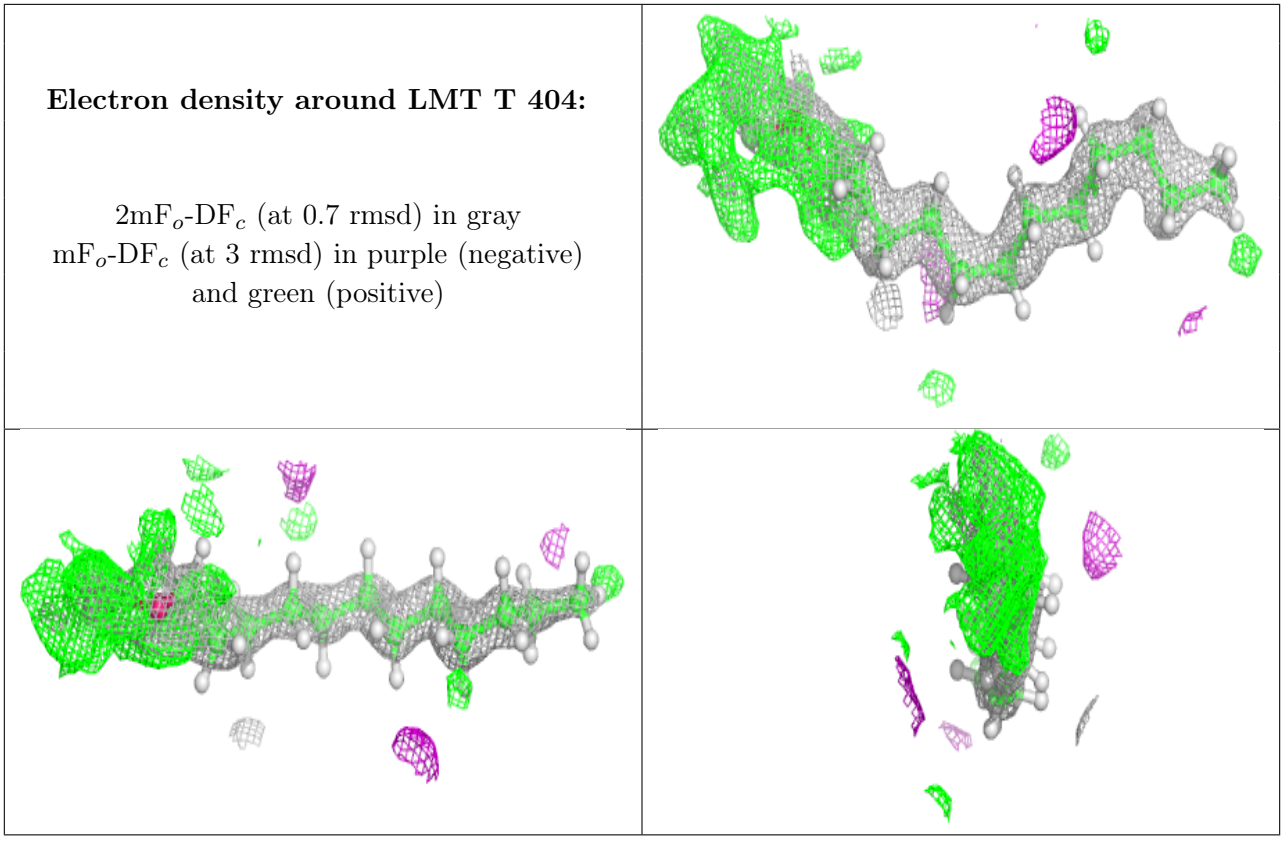
Electron density around LMT S 404:

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



Electron density around LMT T 404:

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



6.5 Other polymers (i)

There are no such residues in this entry.