



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 6, 2024 – 12:44 pm GMT

PDB ID : 5LRY
Title : E coli [NiFe] Hydrogenase Hyd-1 mutant E28D
Authors : Carr, S.B.; Phillips, S.E.V.; Evans, R.M.; Brooke, E.J.; Armstrong, F.A.
Deposited on : 2016-08-22
Resolution : 1.40 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 types of validation reports are described at

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

The following versions of software and data (see [references ⓘ](#)) 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

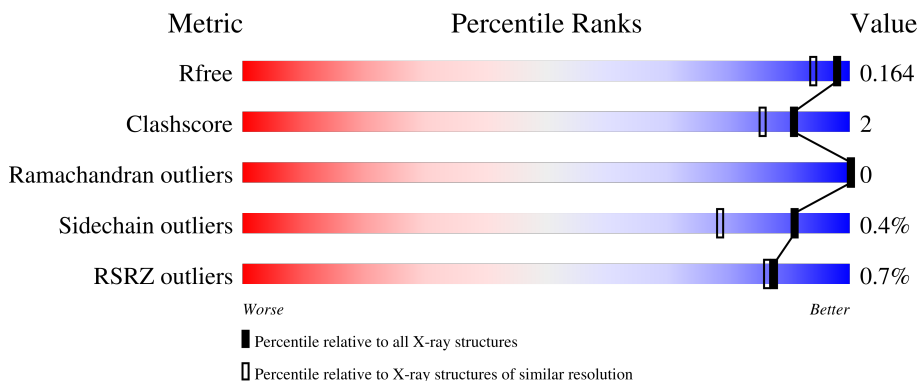
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


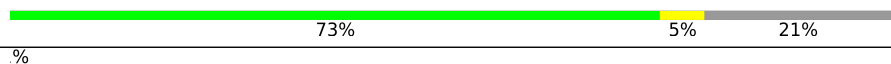
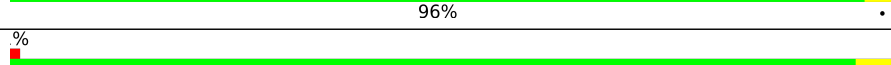

The reported resolution of this entry is 1.40 Å.

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	1714 (1.40-1.40)
Clashscore	141614	1812 (1.40-1.40)
Ramachandran outliers	138981	1763 (1.40-1.40)
Sidechain outliers	138945	1762 (1.40-1.40)
RSRZ outliers	127900	1674 (1.40-1.40)

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 $\leq 5\%$. 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	 74% 5% 21%
1	T	335	 73% 5% 21%
2	L	582	 96% 5%
2	M	582	 95% 5%

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 15125 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	263	2090	1327	358	385	20	0	10	0
1	T	263	2113	1340	366	386	21	0	12	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	328	ARG	-	expression tag	UNP P69740
S	329	SER	-	expression tag	UNP P69740
S	330	HIS	-	expression tag	UNP P69740
S	331	HIS	-	expression tag	UNP P69740
S	332	HIS	-	expression tag	UNP P69740
S	333	HIS	-	expression tag	UNP P69740
S	334	HIS	-	expression tag	UNP P69740
S	335	HIS	-	expression tag	UNP P69740
T	328	ARG	-	expression tag	UNP P69740
T	329	SER	-	expression tag	UNP P69740
T	330	HIS	-	expression tag	UNP P69740
T	331	HIS	-	expression tag	UNP P69740
T	332	HIS	-	expression tag	UNP P69740
T	333	HIS	-	expression tag	UNP P69740
T	334	HIS	-	expression tag	UNP P69740
T	335	HIS	-	expression tag	UNP P69740

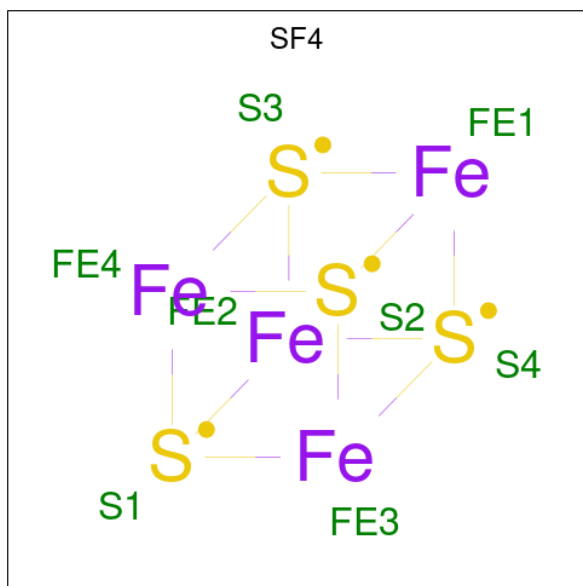
- Molecule 2 is a protein called Hydrogenase-1 large chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	L	581	4684	2975	814	865	30	0	25	0
2	M	581	4702	2992	814	866	30	0	28	0

There are 2 discrepancies between the modelled and reference sequences:

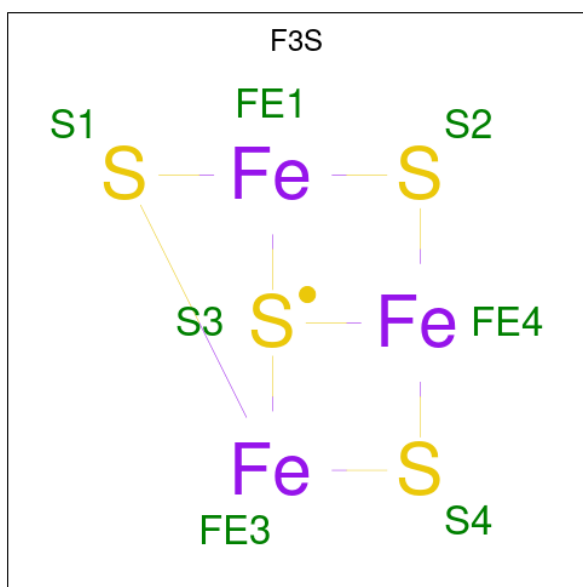
Chain	Residue	Modelled	Actual	Comment	Reference
L	28	ASP	GLU	conflict	UNP P0ACD8
M	28	ASP	GLU	conflict	UNP P0ACD8

- Molecule 3 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



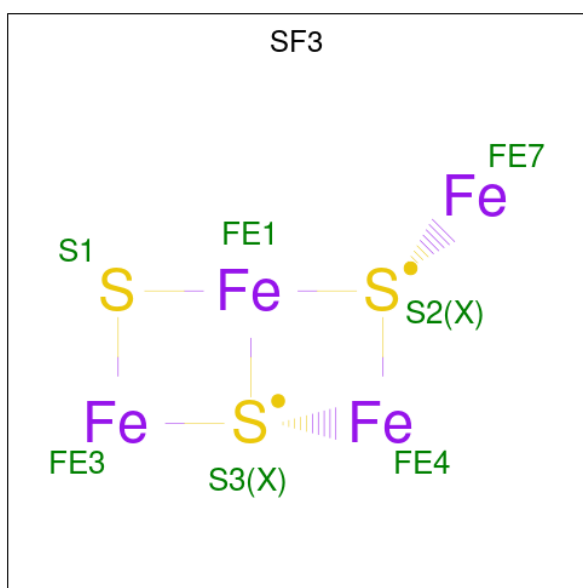
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	S	1	Total	Fe	S	0	0
			8	4	4		
3	T	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 4 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe₃S₄).



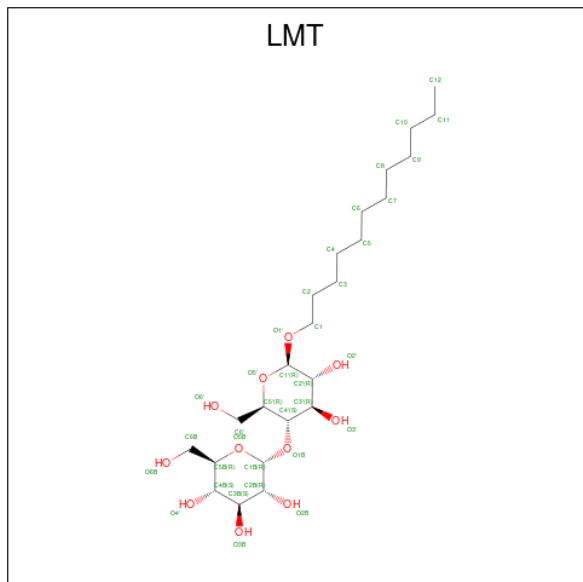
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	S	1	Total Fe S 7 3 4	0	0
4	T	1	Total Fe S 7 3 4	0	0

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



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-MALTOSE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



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

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

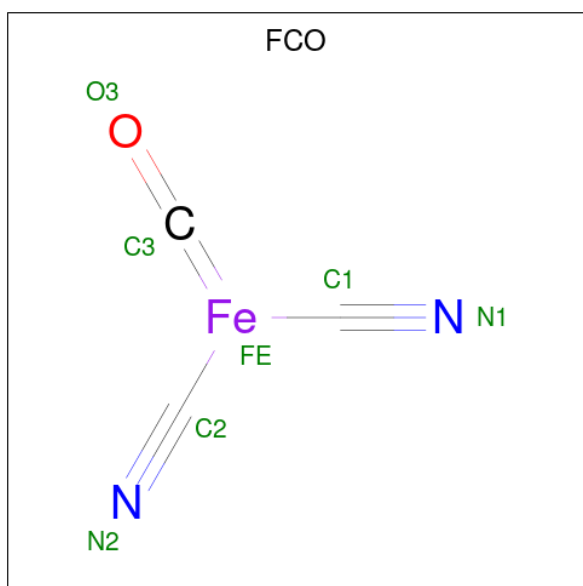
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	S	1	Total	Cl	0	0
			1	1		
7	T	1	Total	Cl	0	0
			1	1		

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	S	1	Total	O	S	0	0
			5	4	1		
8	L	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: C₃FeN₂O).



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 (II) ION (three-letter code: NI) (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	M	1	Total	Li	0	0
			1	1		

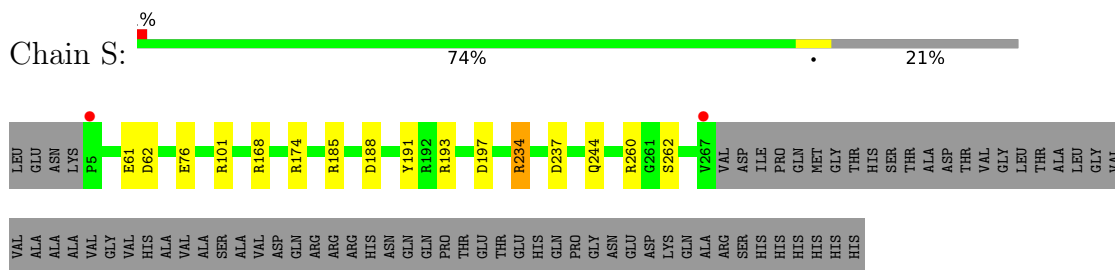
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	S	226	Total	O	0	0
			226	226		
13	L	481	Total	O	0	0
			481	481		
13	T	200	Total	O	0	0
			200	200		
13	M	521	Total	O	0	0
			521	521		

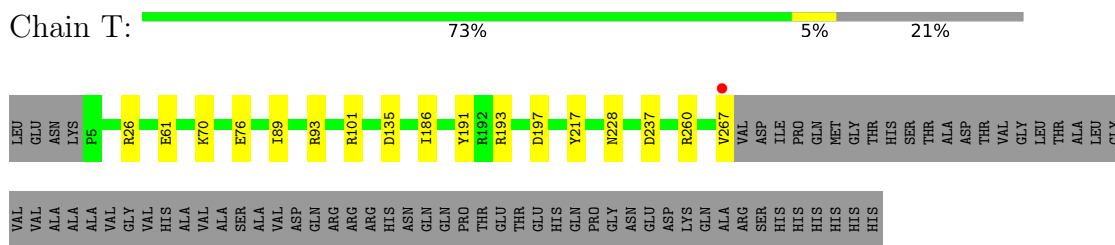
3 Residue-property plots [i](#)

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.

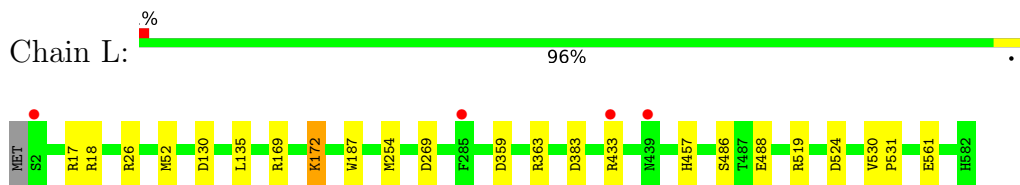
- Molecule 1: Hydrogenase-1 small chain



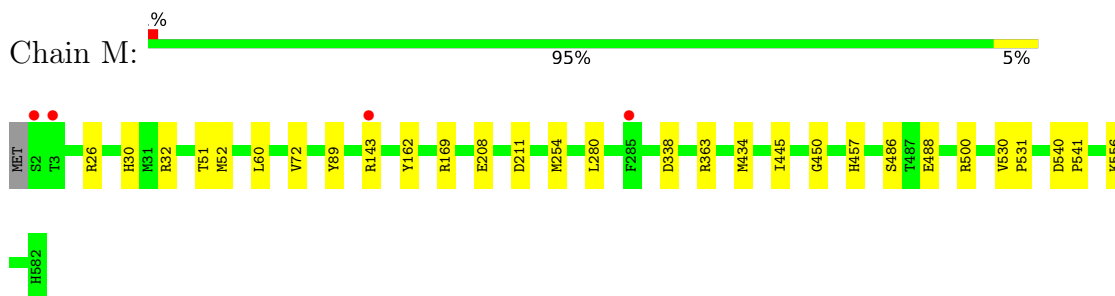
- Molecule 1: Hydrogenase-1 small chain



- Molecule 2: Hydrogenase-1 large chain



- Molecule 2: Hydrogenase-1 large chain



4 Data and refinement statistics i

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	94.76Å 98.75Å 185.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	92.79 – 1.40 55.01 – 1.40	Depositor EDS
% Data completeness (in resolution range)	99.2 (92.79-1.40) 99.2 (55.01-1.40)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.79 (at 1.40Å)	Xtrriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.146 , 0.163 0.147 , 0.164	Depositor DCC
R_{free} test set	16837 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	10.2	Xtrriage
Anisotropy	0.103	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 48.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.018 for k,h,-l	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	15125	wwPDB-VP
Average B, all atoms (Å ²)	13.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.04% 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: NI, SF4, LI, CL, F3S, MG, CSD, SF3, FCO, SO4, 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	0.89	2/2169 (0.1%)	1.01	16/2943 (0.5%)
1	T	0.87	1/2195 (0.0%)	0.99	12/2977 (0.4%)
2	L	0.85	1/4865 (0.0%)	0.85	14/6615 (0.2%)
2	M	0.84	0/4889	0.85	12/6647 (0.2%)
All	All	0.85	4/14118 (0.0%)	0.90	54/19182 (0.3%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S	260	ARG	CZ-NH1	6.24	1.41	1.33
1	S	262	SER	CB-OG	5.81	1.49	1.42
1	T	260	ARG	CZ-NH1	5.54	1.40	1.33
2	L	561	GLU	CD-OE1	5.24	1.31	1.25

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	T	260	ARG	NE-CZ-NH2	-10.70	114.95	120.30
1	S	260	ARG	NE-CZ-NH2	-10.46	115.07	120.30
1	S	193	ARG	NE-CZ-NH2	-9.99	115.30	120.30
2	L	363	ARG	NE-CZ-NH1	9.88	125.24	120.30
2	M	363	ARG	NE-CZ-NH1	9.16	124.88	120.30
1	T	193	ARG	NE-CZ-NH2	-8.88	115.86	120.30
2	L	363	ARG	NE-CZ-NH2	-8.83	115.88	120.30
1	S	193	ARG	NE-CZ-NH1	8.69	124.64	120.30
1	S	185	ARG	NE-CZ-NH1	8.39	124.49	120.30
1	S	197[A]	ASP	CB-CG-OD1	8.38	125.84	118.30
1	S	197[B]	ASP	CB-CG-OD1	8.38	125.84	118.30
1	T	197[A]	ASP	CB-CG-OD1	8.36	125.82	118.30
1	T	197[B]	ASP	CB-CG-OD1	8.36	125.82	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	T	193	ARG	NE-CZ-NH1	7.70	124.15	120.30
2	L	26	ARG	NE-CZ-NH1	7.11	123.85	120.30
1	T	260	ARG	NE-CZ-NH1	6.72	123.66	120.30
1	S	260	ARG	NE-CZ-NH1	6.62	123.61	120.30
1	T	135	ASP	CB-CG-OD1	6.59	124.23	118.30
2	M	500[A]	ARG	NE-CZ-NH2	-6.44	117.08	120.30
2	M	500[B]	ARG	NE-CZ-NH2	-6.44	117.08	120.30
1	T	193	ARG	CG-CD-NE	-6.32	98.52	111.80
2	M	89	TYR	CB-CG-CD1	6.32	124.79	121.00
2	L	26	ARG	NE-CZ-NH2	-5.96	117.32	120.30
1	S	193	ARG	CG-CD-NE	-5.95	99.30	111.80
2	M	89	TYR	CB-CG-CD2	-5.93	117.44	121.00
2	M	211	ASP	CB-CG-OD1	5.91	123.62	118.30
1	S	168	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	S	237	ASP	CB-CG-OD2	-5.66	113.21	118.30
2	L	359	ASP	CB-CG-OD1	5.66	123.39	118.30
1	T	26	ARG	NE-CZ-NH2	-5.63	117.48	120.30
2	L	383	ASP	CB-CG-OD1	5.62	123.36	118.30
1	T	237	ASP	CB-CG-OD2	-5.58	113.28	118.30
2	M	143	ARG	NE-CZ-NH2	-5.52	117.54	120.30
2	M	338	ASP	CB-CG-OD1	5.48	123.24	118.30
2	M	169	ARG	NE-CZ-NH1	5.43	123.02	120.30
2	M	26	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	S	174	ARG	NE-CZ-NH1	5.30	122.95	120.30
2	L	17[A]	ARG	NE-CZ-NH2	-5.25	117.67	120.30
2	L	17[B]	ARG	NE-CZ-NH2	-5.25	117.67	120.30
2	M	32	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	S	62	ASP	CB-CG-OD1	5.22	123.00	118.30
2	L	269[A]	ASP	CB-CG-OD1	5.20	122.98	118.30
2	L	269[B]	ASP	CB-CG-OD1	5.20	122.98	118.30
2	L	18	ARG	NE-CZ-NH1	5.19	122.90	120.30
1	T	93[A]	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	T	93[B]	ARG	NE-CZ-NH1	5.18	122.89	120.30
2	M	169	ARG	NE-CZ-NH2	-5.15	117.73	120.30
1	S	188	ASP	CB-CG-OD1	5.10	122.89	118.30
2	L	130	ASP	CB-CG-OD1	5.09	122.88	118.30
2	L	519[A]	ARG	NE-CZ-NH1	-5.05	117.78	120.30
2	L	519[B]	ARG	NE-CZ-NH1	-5.05	117.78	120.30
1	S	168	ARG	NE-CZ-NH2	-5.02	117.79	120.30
1	S	234[A]	ARG	NE-CZ-NH2	5.01	122.80	120.30
1	S	234[B]	ARG	NE-CZ-NH2	5.01	122.80	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	2090	0	2039	5	0
1	T	2113	0	2067	9	0
2	L	4684	0	4603	9	0
2	M	4702	0	4638	25	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	14	0	25	0	0
6	T	14	0	25	0	0
7	S	1	0	0	0	0
7	T	1	0	0	0	0
8	L	5	0	0	0	0
8	M	5	0	0	0	0
8	S	5	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	M	1	0	0	0	0
13	L	481	0	0	4	0
13	M	521	0	0	5	0
13	S	226	0	0	3	0
13	T	200	0	0	3	0
All	All	15125	0	13397	47	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 (47) 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:434[B]:MET:HE1	2:M:457[B]:HIS:CD2	1.39	1.54
2:M:434[B]:MET:HE3	2:M:457[B]:HIS:CE1	1.61	1.33
2:M:434[B]:MET:CE	2:M:457[B]:HIS:NE2	1.96	1.28
2:M:434[B]:MET:CE	2:M:457[B]:HIS:CD2	2.18	1.25
2:M:434[B]:MET:CE	2:M:457[B]:HIS:CE1	2.35	1.04
1:T:70:LYS:NZ	13:T:501:HOH:O	1.92	1.02
2:M:434[B]:MET:HE1	2:M:457[B]:HIS:NE2	1.73	0.87
2:M:434[B]:MET:HE1	2:M:457[B]:HIS:CG	2.12	0.84
2:M:434[B]:MET:CE	2:M:457[B]:HIS:CG	2.65	0.79
2:L:488[B]:GLU:OE2	13:L:701:HOH:O	1.99	0.78
2:L:457[A]:HIS:ND1	13:L:702:HOH:O	2.20	0.74
2:M:434[B]:MET:HE3	2:M:457[B]:HIS:ND1	2.01	0.74
2:M:556:LYS:NZ	13:M:701:HOH:O	2.27	0.67
1:T:61[B]:GLU:OE2	1:T:101:ARG:NH2	2.30	0.64
2:L:52[B]:MET:HG2	13:L:1073:HOH:O	1.99	0.62
2:M:486[A]:SER:OG	2:M:488[A]:GLU:OE2	2.12	0.62
2:M:434[B]:MET:HE2	2:M:457[B]:HIS:NE2	2.10	0.62
2:M:52[B]:MET:HG2	13:M:1080:HOH:O	2.01	0.61
2:M:60[B]:LEU:HD11	2:M:72:VAL:CG1	2.34	0.58
2:L:169:ARG:O	2:L:172:LYS:HE3	2.04	0.57
2:M:254[B]:MET:HE2	2:M:254[B]:MET:HA	1.88	0.56
1:S:234[A]:ARG:NH2	1:S:244:GLN:HE22	2.04	0.55
1:S:61[A]:GLU:HG2	13:S:613:HOH:O	2.08	0.54
2:M:162:TYR:OH	2:M:208[B]:GLU:OE2	2.23	0.51
2:L:486:SER:OG	2:L:488[B]:GLU:OE1	2.13	0.49
1:T:76[B]:GLU:HG3	13:T:532:HOH:O	2.12	0.49
2:L:135:LEU:HD22	2:L:187:TRP:CD1	2.48	0.48
1:T:89:ILE:HG22	13:M:704:HOH:O	2.13	0.48
1:T:61[B]:GLU:CD	1:T:101:ARG:HH12	2.18	0.47
2:L:530:VAL:CG1	2:L:531:PRO:HD2	2.45	0.46
2:M:30:HIS:CD2	2:M:52[B]:MET:SD	3.09	0.46
2:L:169:ARG:NH1	13:L:708:HOH:O	2.45	0.45
1:T:217:TYR:HE1	1:T:267:VAL:HG12	1.81	0.45
2:M:280:LEU:HG	13:M:705:HOH:O	2.17	0.45
2:L:254[B]:MET:HA	2:L:254[B]:MET:HE2	1.99	0.44
2:M:30:HIS:CG	2:M:52[B]:MET:SD	3.11	0.44
1:T:186:ILE:HD11	1:T:228:ASN:HB3	2.00	0.44
1:S:76[B]:GLU:HG3	13:S:573:HOH:O	2.18	0.44
1:T:61[B]:GLU:HG2	13:T:578:HOH:O	2.17	0.43
2:M:434[B]:MET:HE3	2:M:457[B]:HIS:CG	2.39	0.43
1:S:234[A]:ARG:NH1	1:S:244:GLN:OE1	2.52	0.43
2:M:530:VAL:CG1	2:M:531:PRO:HD2	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:89:ILE:HB	2:M:51:THR:HB	2.01	0.42
2:M:457[B]:HIS:NE2	13:M:705:HOH:O	2.37	0.42
2:M:540:ASP:HB2	2:M:541:PRO:CD	2.50	0.41
1:S:101[B]:ARG:HD3	13:S:678:HOH:O	2.20	0.41
2:M:445:ILE:O	2:M:450:GLY:HA3	2.21	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	271/335 (81%)	259 (96%)	12 (4%)	0	100	100
1	T	273/335 (82%)	260 (95%)	13 (5%)	0	100	100
2	L	603/582 (104%)	588 (98%)	15 (2%)	0	100	100
2	M	606/582 (104%)	590 (97%)	16 (3%)	0	100	100
All	All	1753/1834 (96%)	1697 (97%)	56 (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	226/274 (82%)	225 (100%)	1 (0%)	91	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	T	228/274 (83%)	227 (100%)	1 (0%)	91	78
2	L	504/480 (105%)	501 (99%)	3 (1%)	86	70
2	M	507/480 (106%)	507 (100%)	0	100	100
All	All	1465/1508 (97%)	1460 (100%)	5 (0%)	91	81

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	S	191	TYR
2	L	172	LYS
2	L	433	ARG
2	L	524	ASP
1	T	191	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	M	61	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](#)

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	CSD	L	576	10,2	3,7,8	1.02	0	1,8,10	0.12	0
2	CSD	M	576	10,2	3,7,8	0.63	0	1,8,10	0.99	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CSD	L	576	10,2	-	0/2/6/8	-
2	CSD	M	576	10,2	-	0/2/6/8	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 7 are monoatomic - leaving 13 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	$\# Z > 2$
6	LMT	T	404	-	13,13,36	0.36	0	12,12,47	0.37	0
4	F3S	T	402	1	0,9,9	-	-	-		
4	F3S	S	402	1	0,9,9	-	-	-		
5	SF3	T	403	13,1	0,8,8	-	-	-		
8	SO4	S	406	-	4,4,4	0.37	0	6,6,6	0.26	0
9	FCO	M	601	13,2	0,6,6	-	-	-		
8	SO4	L	601	-	4,4,4	0.33	0	6,6,6	0.31	0
8	SO4	M	604	-	4,4,4	0.39	0	6,6,6	0.32	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	FCO	L	602	13,2	0,6,6	-	-	-		
3	SF4	S	401	1	0,12,12	-	-	-		
3	SF4	T	401	1	0,12,12	-	-	-		
6	LMT	S	404	-	13,13,36	0.43	0	12,12,47	0.60	0
5	SF3	S	403	13,1	0,8,8	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	LMT	T	404	-	-	0/11/11/61	-
4	F3S	S	402	1	-	-	0/3/3/3
4	F3S	T	402	1	-	-	0/3/3/3
5	SF3	T	403	13,1	-	-	0/2/2/2
5	SF3	S	403	13,1	-	-	0/2/2/2
3	SF4	S	401	1	-	-	0/6/5/5
3	SF4	T	401	1	-	-	0/6/5/5
6	LMT	S	404	-	-	2/11/11/61	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

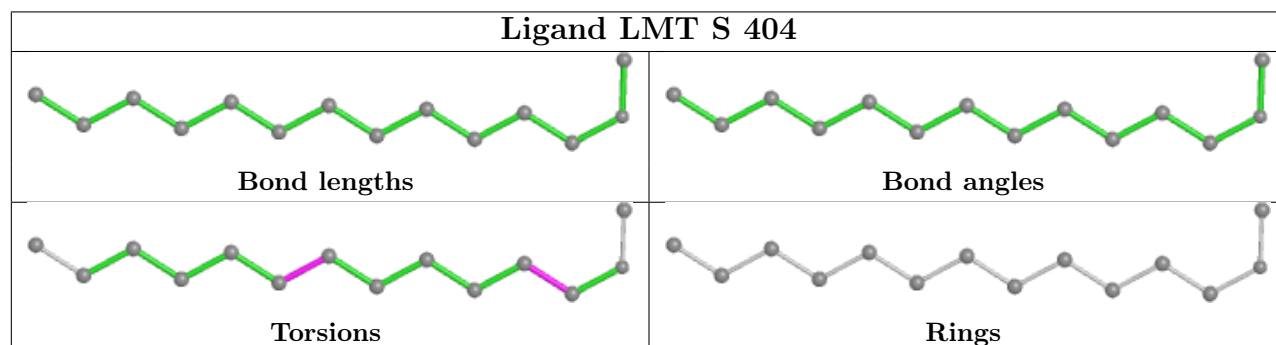
Mol	Chain	Res	Type	Atoms
6	S	404	LMT	O1'-C1-C2-C3
6	S	404	LMT	C5-C6-C7-C8

There are no ring outliers.

No monomer is involved in short contacts.

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	263/335 (78%)	-0.46	2 (0%) 86 84	7, 10, 17, 27	0
1	T	263/335 (78%)	-0.38	1 (0%) 92 91	7, 11, 19, 30	0
2	L	580/582 (99%)	-0.48	4 (0%) 87 86	7, 11, 23, 38	0
2	M	580/582 (99%)	-0.50	4 (0%) 87 86	7, 11, 19, 35	0
All	All	1686/1834 (91%)	-0.47	11 (0%) 87 86	7, 11, 20, 38	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	T	267	VAL	5.3
1	S	267	VAL	3.0
2	L	439[A]	ASN	2.7
2	M	2	SER	2.6
2	M	143	ARG	2.5
2	M	285	PHE	2.5
2	L	433	ARG	2.4
2	M	3	THR	2.2
2	L	2	SER	2.2
2	L	285	PHE	2.2
1	S	5	PRO	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
2	CSD	L	576	8/9	0.98	0.07	8,9,10,11	2

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	CSD	M	576	8/9	0.99	0.06	8,9,10,11	2

6.3 Carbohydrates [i](#)

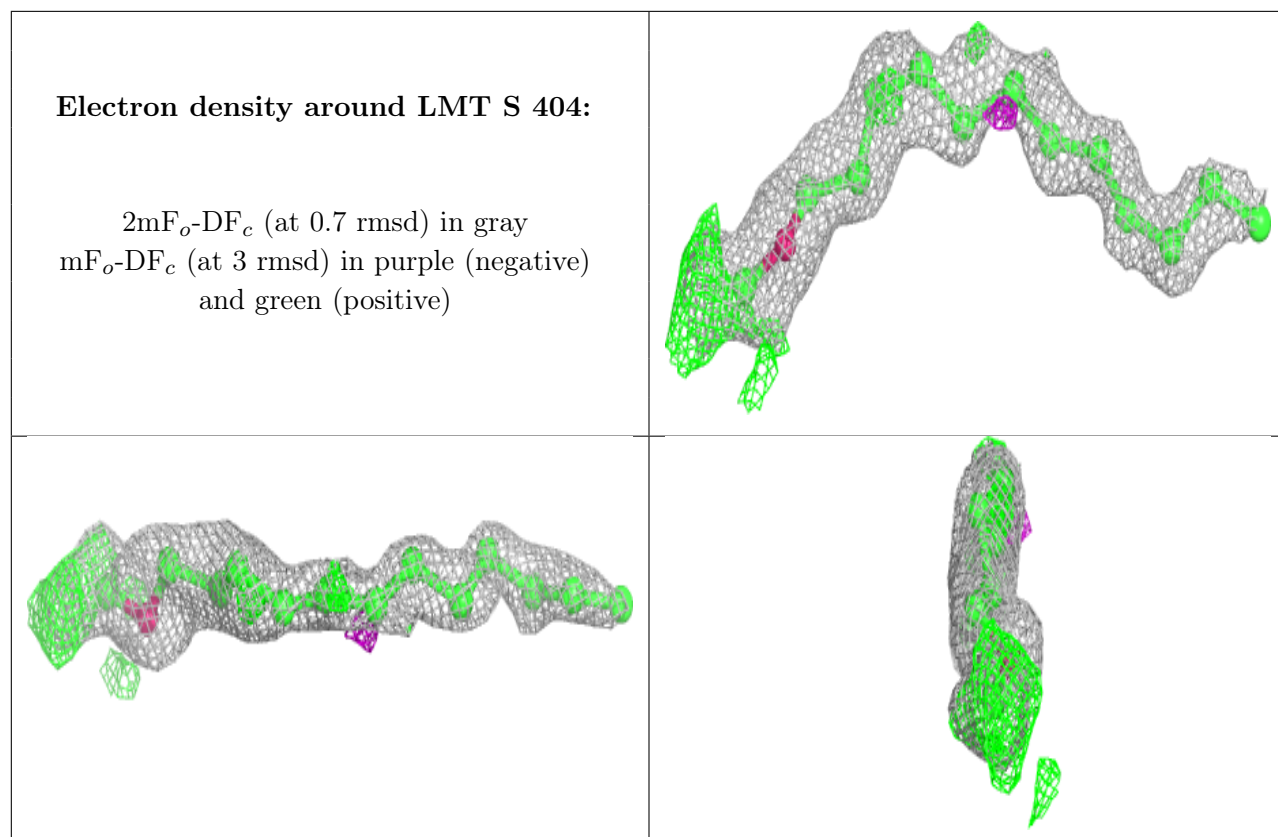
There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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(\AA^2)	Q<0.9
6	LMT	S	404	14/35	0.80	0.15	25,27,32,32	0
6	LMT	T	404	14/35	0.81	0.17	27,29,39,40	0
8	SO4	M	604	5/5	0.82	0.19	33,34,35,35	5
8	SO4	S	406	5/5	0.87	0.30	60,63,65,67	0
12	LI	M	605	1/1	0.95	0.16	13,13,13,13	0
8	SO4	L	601	5/5	0.97	0.07	14,15,17,17	5
5	SF3	S	403	7/7	0.99	0.04	9,11,12,16	0
5	SF3	T	403	7/7	0.99	0.04	10,11,13,17	0
7	CL	S	405	1/1	0.99	0.04	14,14,14,14	0
7	CL	T	405	1/1	0.99	0.04	14,14,14,14	0
4	F3S	S	402	7/7	1.00	0.04	8,8,9,9	0
4	F3S	T	402	7/7	1.00	0.04	8,9,9,10	0
3	SF4	S	401	8/8	1.00	0.03	7,7,7,8	0
9	FCO	L	602	7/7	1.00	0.05	7,7,7,8	0
9	FCO	M	601	7/7	1.00	0.05	7,7,8,8	0
10	NI	L	603	1/1	1.00	0.03	11,11,11,11	0
10	NI	M	602	1/1	1.00	0.03	11,11,11,11	0
11	MG	L	604	1/1	1.00	0.11	3,3,3,3	0
11	MG	M	603	1/1	1.00	0.12	3,3,3,3	0
3	SF4	T	401	8/8	1.00	0.03	7,7,7,8	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.