Full wwPDB X-ray Structure Validation Report (i)

Jan 4, 2024 – 02:22 pm GMT

PDB ID	:	5LMM
Title	:	Structure of E coli Hydrogenase Hyd-1 mutant E28Q
Authors	:	Carr, S.B.; Phillips, S.E.V.; Evans, R.M.; Brooke, E.J.; Armstrong, F.A.
Deposited on	:	2016-08-01
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:

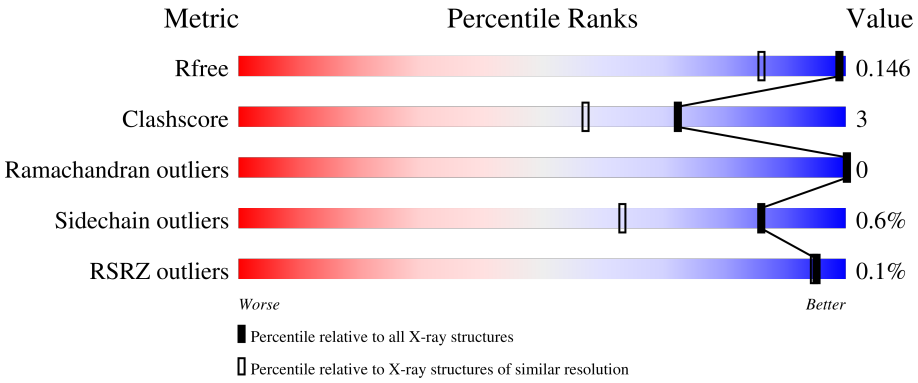
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
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	71% 6% • 21%
1	T	335	71% 7% • 21%
2	L	582	93% 6% •
2	M	582	94% 5% •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	SO4	T	407	-	-	X	-

2 Entry composition (i)

There are 14 unique types of molecules in this entry. The entry contains 15256 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	264	Total	C	N	O	S	0	17	0
			2145	1363	369	392	21			
1	T	264	Total	C	N	O	S	0	16	0
			2150	1365	375	389	21			

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

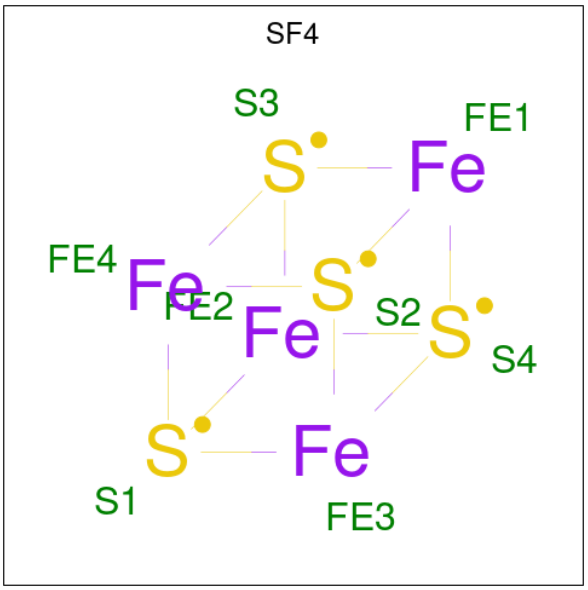
- Molecule 2 is a protein called Hydrogenase-1 large chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	581	Total	C	N	O	S	0	32	0
			4732	3008	826	870	28			
2	M	581	Total	C	N	O	S	0	24	0
			4678	2979	810	862	27			

There are 2 discrepancies between the modelled and reference sequences:

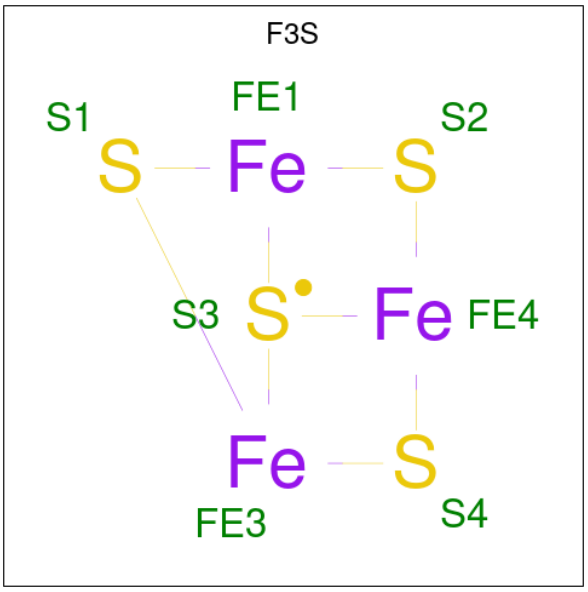
Chain	Residue	Modelled	Actual	Comment	Reference
L	28	GLN	GLU	conflict	UNP P0ACD8
M	28	GLN	GLU	conflict	UNP P0ACD8

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



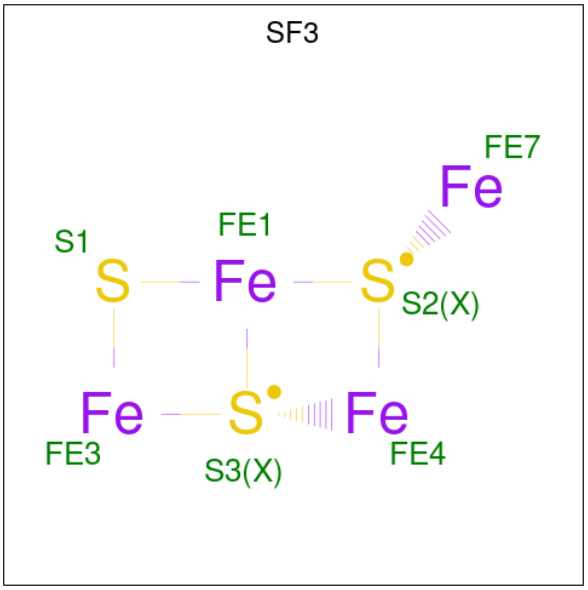
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	S	1	Total	Fe	S	0	0
			8	4	4		
3	T	1	Total	Fe	S	0	0
			8	4	4		

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



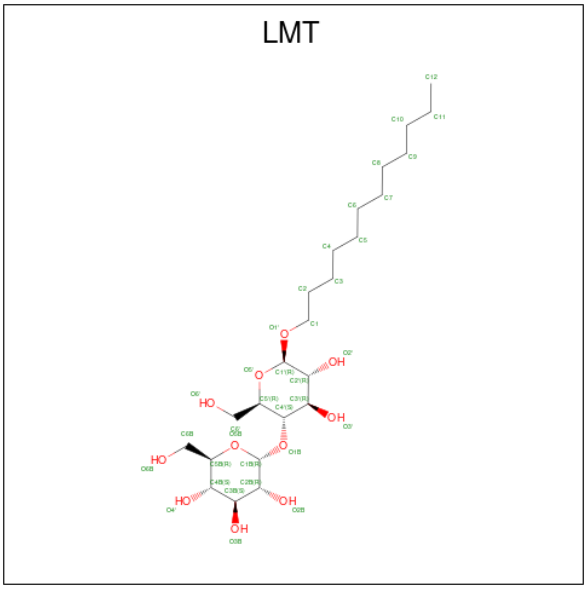
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	S	1	Total Fe S 7 3 4	0	0
4	T	1	Total Fe S 7 3 4	0	0

- 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 8 5 3	0	1
5	T	1	Total Fe S 8 5 3	0	1

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

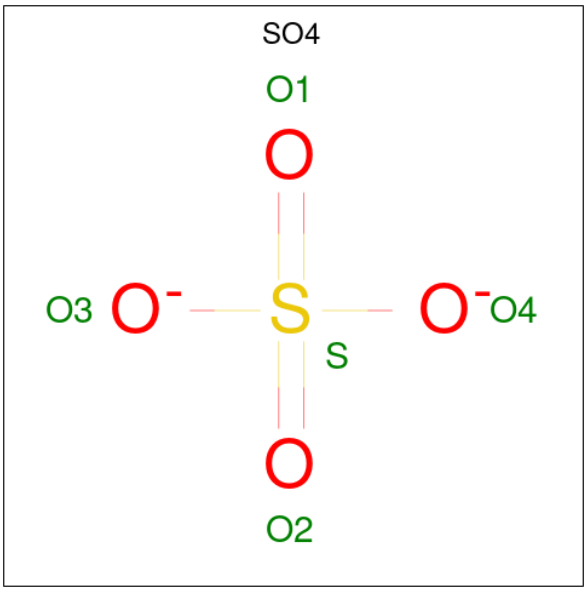


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	S	1	Total C O 14 13 1	0	0
6	T	1	Total C O 14 13 1	0	0

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

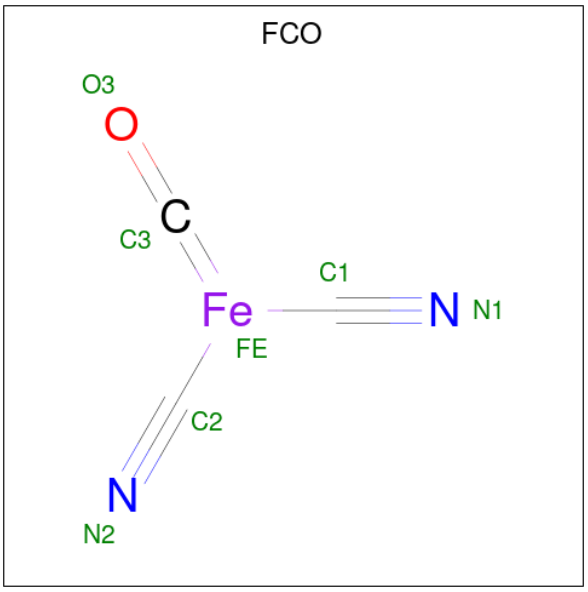
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	S	1	Total Cl 1 1	0	0
7	T	2	Total Cl 2 2	0	0

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	S	1	Total O S 5 4 1	0	0
8	L	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 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 7 3 1 2 1	0	0
9	M	1	Total C Fe N O 7 3 1 2 1	0	0

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

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

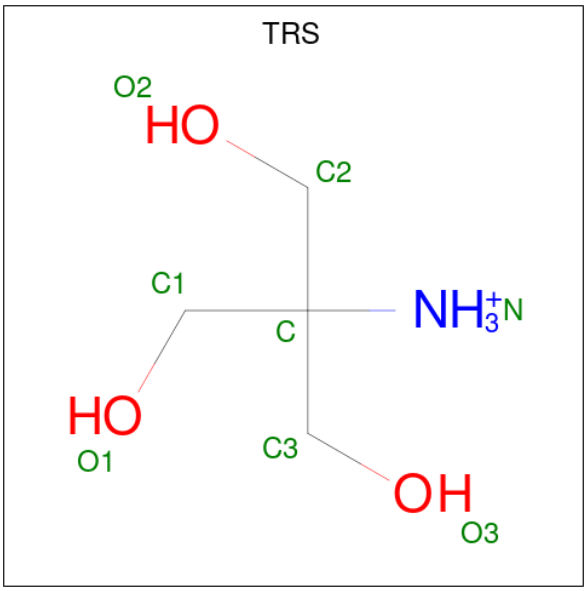
- Molecule 11 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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

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

- Molecule 13 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	M	1	Total C N O 8 4 1 3	0	0

- Molecule 14 is water.

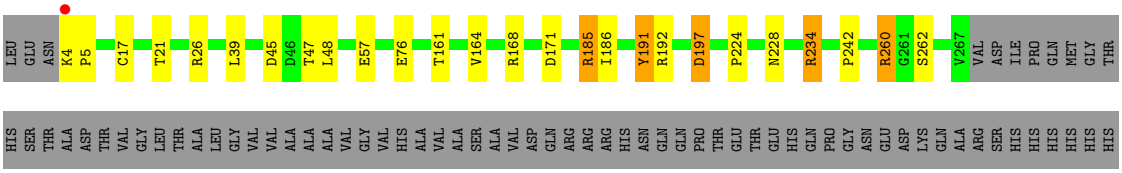
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	S	228	Total O 228 228	0	0
14	L	480	Total O 480 480	0	0
14	T	211	Total O 211 211	0	0
14	M	507	Total O 507 507	0	0

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.

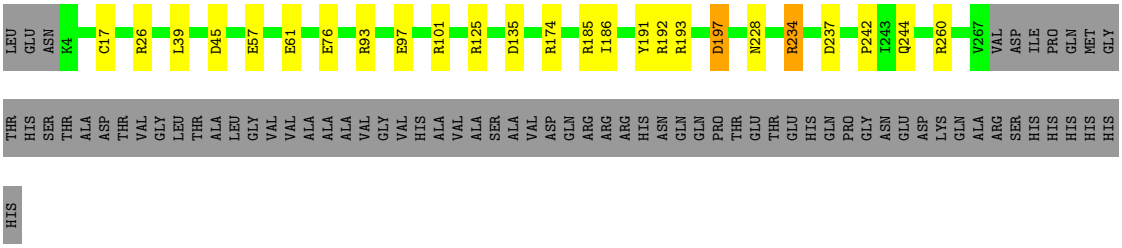
• Molecule 1: Hydrogenase-1 small chain

Chain S:



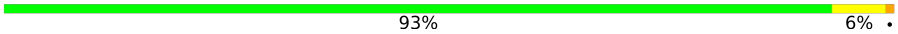
• Molecule 1: Hydrogenase-1 small chain

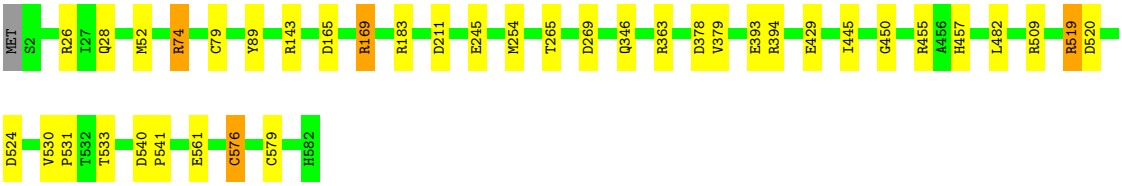
Chain T:



• Molecule 2: Hydrogenase-1 large chain

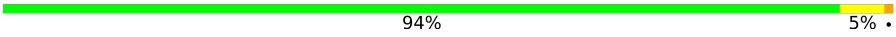
Chain L:

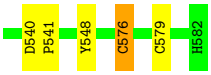




• Molecule 2: Hydrogenase-1 large chain

Chain M:




D540
P541
Y548
C576
C579
H582

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	93.98Å 97.80Å 183.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	91.74 – 1.20 83.65 – 1.20	Depositor EDS
% Data completeness (in resolution range)	97.7 (91.74-1.20) 97.7 (83.65-1.20)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.65 (at 1.20Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.118 , 0.146 0.119 , 0.146	Depositor DCC
R_{free} test set	25987 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	11.0	Xtriage
Anisotropy	0.188	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 47.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	15256	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 6.75% 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: F3S, SF4, SF3, CSO, LI, NI, FCO, TRS, SO4, CL, MG, 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	0.86	3/2236 (0.1%)	1.05	13/3033 (0.4%)
1	T	0.86	2/2238 (0.1%)	1.09	13/3035 (0.4%)
2	L	0.80	5/4931 (0.1%)	0.90	15/6703 (0.2%)
2	M	0.79	1/4859 (0.0%)	0.91	19/6607 (0.3%)
All	All	0.81	11/14264 (0.1%)	0.96	60/19378 (0.3%)

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
2	L	0	1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	T	260	ARG	CZ-NH1	9.03	1.44	1.33
2	L	561	GLU	CD-OE1	8.95	1.35	1.25
1	S	57	GLU	CD-OE2	-7.68	1.17	1.25
1	S	262	SER	CB-OG	7.26	1.51	1.42
2	L	561	GLU	CG-CD	7.18	1.62	1.51
1	S	260	ARG	CZ-NH1	6.92	1.42	1.33
1	T	57	GLU	CD-OE2	-6.22	1.18	1.25
2	L	379	VAL	C-O	5.62	1.34	1.23
2	L	245	GLU	CD-OE1	5.57	1.31	1.25
2	L	429	GLU	CD-OE2	-5.36	1.19	1.25
2	M	215	GLU	CD-OE2	-5.24	1.19	1.25

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	T	260	ARG	NE-CZ-NH2	-15.36	112.62	120.30
1	T	260	ARG	NE-CZ-NH1	13.17	126.88	120.30
1	S	185[A]	ARG	NE-CZ-NH1	9.65	125.13	120.30
1	S	185[B]	ARG	NE-CZ-NH1	9.65	125.13	120.30
1	S	260	ARG	NE-CZ-NH2	-8.12	116.24	120.30
1	T	234[A]	ARG	NE-CZ-NH2	-7.62	116.49	120.30
1	T	234[B]	ARG	NE-CZ-NH2	-7.62	116.49	120.30
2	M	433[A]	ARG	NE-CZ-NH1	7.57	124.08	120.30
2	M	433[B]	ARG	NE-CZ-NH1	7.57	124.08	120.30
1	T	185[A]	ARG	NE-CZ-NH1	7.43	124.01	120.30
1	T	185[B]	ARG	NE-CZ-NH1	7.43	124.01	120.30
2	L	509	ARG	NE-CZ-NH1	7.31	123.96	120.30
1	T	197[A]	ASP	CB-CG-OD1	7.23	124.81	118.30
1	T	197[B]	ASP	CB-CG-OD1	7.23	124.81	118.30
1	T	26	ARG	NE-CZ-NH2	-7.21	116.69	120.30
2	L	74	ARG	NE-CZ-NH2	-7.20	116.70	120.30
1	T	237	ASP	CB-CG-OD2	-7.19	111.83	118.30
2	M	169	ARG	NE-CZ-NH1	7.02	123.81	120.30
2	M	433[A]	ARG	NE-CZ-NH2	-7.01	116.80	120.30
2	M	433[B]	ARG	NE-CZ-NH2	-7.01	116.80	120.30
2	L	482	LEU	CB-CG-CD1	7.00	122.89	111.00
2	M	74	ARG	NE-CZ-NH2	-6.94	116.83	120.30
1	S	197[A]	ASP	CB-CG-OD1	6.90	124.51	118.30
1	S	197[B]	ASP	CB-CG-OD1	6.90	124.51	118.30
2	M	32	ARG	NE-CZ-NH1	6.83	123.72	120.30
2	L	89	TYR	CB-CG-CD2	-6.73	116.96	121.00
2	M	363	ARG	NE-CZ-NH1	6.66	123.63	120.30
1	S	260	ARG	CG-CD-NE	-6.62	97.90	111.80
2	L	89	TYR	CB-CG-CD1	6.29	124.77	121.00
2	L	363[A]	ARG	NE-CZ-NH2	-6.17	117.21	120.30
2	L	363[B]	ARG	NE-CZ-NH2	-6.17	117.21	120.30
1	T	135	ASP	CB-CG-OD1	6.05	123.75	118.30
1	S	191	TYR	CB-CG-CD1	6.01	124.61	121.00
2	L	74	ARG	NE-CZ-NH1	5.99	123.30	120.30
1	T	192	ARG	NE-CZ-NH2	-5.99	117.31	120.30
1	S	168	ARG	NE-CZ-NH1	5.84	123.22	120.30
2	M	576	CYS	CA-CB-SG	-5.79	103.58	114.00
2	M	82	VAL	CG1-CB-CG2	5.78	120.14	110.90
2	M	455	ARG	NE-CZ-NH2	-5.72	117.44	120.30
2	M	269[A]	ASP	CB-CG-OD1	5.64	123.38	118.30
2	M	269[B]	ASP	CB-CG-OD1	5.64	123.38	118.30
2	L	378	ASP	CB-CG-OD1	5.61	123.35	118.30
2	L	394	ARG	NE-CZ-NH2	-5.55	117.52	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	S	234[A]	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	S	234[B]	ARG	NE-CZ-NH2	-5.54	117.53	120.30
2	M	143	ARG	NE-CZ-NH1	5.54	123.07	120.30
2	L	455	ARG	NE-CZ-NH2	-5.52	117.54	120.30
2	M	74	ARG	NE-CZ-NH1	5.50	123.05	120.30
2	L	26	ARG	NE-CZ-NH1	5.49	123.05	120.30
1	S	26	ARG	NE-CZ-NH2	-5.43	117.58	120.30
1	T	45	ASP	CB-CG-OD1	5.36	123.12	118.30
2	M	54	ARG	NE-CZ-NH2	-5.34	117.63	120.30
2	L	211	ASP	CB-CG-OD1	5.33	123.09	118.30
2	M	338	ASP	CB-CG-OD1	5.32	123.09	118.30
2	M	548	TYR	CB-CG-CD1	5.29	124.17	121.00
2	L	576	CYS	CA-CB-SG	-5.26	104.53	114.00
1	S	57	GLU	OE1-CD-OE2	-5.18	117.08	123.30
2	M	89	TYR	CB-CG-CD2	-5.17	117.90	121.00
1	S	192	ARG	NE-CZ-NH2	-5.10	117.75	120.30
2	L	169	ARG	NE-CZ-NH2	-5.03	117.79	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	L	74	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	2145	0	2110	21	0
1	T	2150	0	2112	24	0
2	L	4732	0	4673	31	0
2	M	4678	0	4612	27	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	8	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	T	8	0	0	0	0
6	S	14	0	25	1	0
6	T	14	0	25	0	0
7	S	1	0	0	0	0
7	T	2	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
8	T	5	0	0	2	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
12	M	1	0	0	0	0
13	M	8	0	12	1	0
14	L	480	0	0	22	0
14	M	507	0	0	13	0
14	S	228	0	0	4	0
14	T	211	0	0	5	0
All	All	15256	0	13569	93	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 (93) 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	14:L:705:HOH:O	1.63	1.26
2:M:28:GLN:CD	14:M:701:HOH:O	1.69	1.25
1:T:93[B]:ARG:CZ	1:T:97:GLU:OE1	1.88	1.21
2:L:457[A]:HIS:ND1	14:L:703:HOH:O	1.72	1.21
2:M:28:GLN:CG	14:M:701:HOH:O	1.86	1.19
2:L:28:GLN:CG	14:L:705:HOH:O	1.83	1.13
2:L:143[B]:ARG:HG3	14:L:717:HOH:O	1.57	1.01
1:T:174[B]:ARG:HG3	8:T:407:SO4:O1	1.63	0.99
2:M:393[B]:GLU:HG2	14:M:863:HOH:O	1.61	0.99
2:M:28:GLN:NE2	14:M:701:HOH:O	1.82	0.98
1:S:161[B]:THR:HG23	14:S:686:HOH:O	1.62	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:346[A]:GLN:OE1	14:L:704:HOH:O	1.79	0.98
1:S:234[A]:ARG:NH2	1:T:234[A]:ARG:NH2	2.12	0.98
2:L:393[B]:GLU:HG2	14:L:868:HOH:O	1.65	0.96
2:L:28:GLN:NE2	14:L:705:HOH:O	1.85	0.94
1:T:93[B]:ARG:NH2	1:T:97:GLU:OE1	2.02	0.93
1:S:45:ASP:OD1	1:S:47[A]:THR:HG22	1.76	0.85
2:L:28:GLN:HG3	14:L:705:HOH:O	1.54	0.83
2:M:28:GLN:HG3	14:M:701:HOH:O	1.60	0.82
1:T:125[B]:ARG:NH1	14:T:502:HOH:O	2.12	0.82
1:S:234[A]:ARG:HH21	1:T:234[A]:ARG:NH2	1.78	0.82
1:S:234[A]:ARG:NH2	1:T:234[A]:ARG:HH21	1.78	0.80
2:L:165[B]:ASP:OD1	14:L:706:HOH:O	1.99	0.80
2:L:269[B]:ASP:OD1	14:L:707:HOH:O	1.99	0.79
1:S:234[A]:ARG:HH21	1:T:234[A]:ARG:HH21	1.29	0.78
2:L:79:CSO:OD	2:L:79:CSO:N	2.20	0.75
1:S:171[B]:ASP:OD1	14:S:502:HOH:O	2.05	0.74
1:T:61[B]:GLU:HG2	14:T:587:HOH:O	1.88	0.74
2:M:269[B]:ASP:OD1	14:M:702:HOH:O	2.07	0.71
1:S:21:THR:HG21	1:S:47[A]:THR:HG21	1.72	0.71
2:M:393[B]:GLU:HG3	13:M:606:TRS:O2	1.91	0.71
2:M:79:CSO:OD	2:M:79:CSO:N	2.24	0.70
1:T:93[B]:ARG:NE	1:T:97:GLU:OE1	2.24	0.69
1:T:76[B]:GLU:HG3	14:T:555:HOH:O	1.94	0.66
1:S:234[B]:ARG:NH1	1:T:234[B]:ARG:HD3	2.11	0.66
2:M:377:GLY:HA3	2:M:393[B]:GLU:OE1	1.99	0.63
1:S:234[A]:ARG:CZ	1:T:234[A]:ARG:NH2	2.62	0.62
2:M:421[A]:HIS:HE1	14:M:948:HOH:O	1.82	0.62
1:S:76[B]:GLU:HG3	14:S:526:HOH:O	2.00	0.61
2:L:576:CYS:CB	14:L:1030:HOH:O	2.48	0.61
2:L:254[B]:MET:HA	2:L:254[B]:MET:HE2	1.83	0.59
1:S:234[A]:ARG:NH2	1:T:234[A]:ARG:CZ	2.65	0.58
6:S:404:LMT:C1'	14:S:678:HOH:O	2.51	0.58
2:L:530[B]:VAL:HG22	2:L:533:THR:OG1	2.03	0.58
2:M:60[B]:LEU:HD11	2:M:72:VAL:CG1	2.33	0.57
2:L:530[B]:VAL:HG21	2:L:579:CYS:O	2.03	0.57
2:L:183[B]:ARG:NH2	14:L:701:HOH:O	0.74	0.57
2:M:576:CYS:CB	14:M:994:HOH:O	2.51	0.57
1:S:234[A]:ARG:CZ	1:T:234[A]:ARG:CZ	2.82	0.56
2:L:52:MET:HG2	14:L:1014:HOH:O	2.05	0.56
14:L:1157:HOH:O	1:T:39[A]:LEU:HD11	2.06	0.56
1:S:161[B]:THR:HG22	2:M:254:MET:CE	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:530[B]:VAL:HG21	2:L:579:CYS:C	2.27	0.55
2:M:52:MET:HG2	14:M:927:HOH:O	2.08	0.54
2:M:208[B]:GLU:OE1	14:M:703:HOH:O	2.18	0.54
2:M:429[B]:GLU:HG3	14:M:748:HOH:O	2.08	0.53
2:L:169:ARG:NH1	14:L:711:HOH:O	2.34	0.52
1:T:193[A]:ARG:NH2	14:T:505:HOH:O	2.43	0.50
1:S:4:LYS:HG3	1:S:5:PRO:HD2	1.93	0.50
2:L:519[B]:ARG:HG2	2:L:520:ASP:OD2	2.11	0.50
2:L:457[A]:HIS:CG	14:L:703:HOH:O	2.44	0.49
2:M:245:GLU:CD	14:M:926:HOH:O	2.50	0.49
1:S:161[B]:THR:HG22	2:M:254:MET:HE2	1.94	0.49
2:L:457[A]:HIS:HE1	14:L:1120:HOH:O	1.95	0.49
1:T:234[B]:ARG:NH2	1:T:244:GLN:HE22	2.10	0.48
1:T:186:ILE:HD11	1:T:228:ASN:HB3	1.96	0.48
2:L:265[B]:THR:HG21	14:L:971:HOH:O	2.14	0.48
1:T:174[B]:ARG:HG3	8:T:407:SO4:S	2.55	0.47
1:S:47[A]:THR:HG23	1:S:48:LEU:HG	1.96	0.46
2:L:143[B]:ARG:NH1	14:L:717:HOH:O	2.48	0.46
2:M:393[B]:GLU:HG2	2:M:394:ARG:H	1.79	0.46
1:S:186:ILE:HD11	1:S:228:ASN:HB3	1.98	0.46
2:M:530:VAL:CG1	2:M:531:PRO:HD2	2.46	0.46
1:S:197[B]:ASP:OD1	1:T:197[B]:ASP:OD1	2.35	0.45
2:L:540:ASP:HB2	2:L:541:PRO:CD	2.47	0.45
2:M:60[B]:LEU:HD11	2:M:72:VAL:HG13	1.99	0.45
2:L:576:CYS:HB2	14:L:1030:HOH:O	2.17	0.44
1:T:101:ARG:HG2	1:T:101:ARG:HH11	1.83	0.44
2:L:530[A]:VAL:CG1	2:L:531:PRO:HD2	2.49	0.43
2:L:530[A]:VAL:HG11	2:L:579:CYS:HB3	2.00	0.42
1:S:185[A]:ARG:HD2	1:S:224:PRO:O	2.19	0.42
2:L:169:ARG:NH2	14:L:721:HOH:O	2.53	0.42
1:S:39[B]:LEU:HG	1:S:164:VAL:HG21	2.02	0.42
2:L:445:ILE:O	2:L:450:GLY:HA3	2.19	0.41
1:T:125[B]:ARG:NH1	14:T:508:HOH:O	2.52	0.41
2:L:393[B]:GLU:CG	14:L:868:HOH:O	2.45	0.41
1:T:61[B]:GLU:OE1	1:T:101:ARG:NH1	2.52	0.41
2:M:433[B]:ARG:HH11	2:M:433[B]:ARG:HD3	1.74	0.41
2:M:393[B]:GLU:CG	14:M:863:HOH:O	2.40	0.40
2:M:530:VAL:HG11	2:M:579:CYS:HB3	2.02	0.40
2:M:162:TYR:OH	2:M:208[B]:GLU:OE2	2.36	0.40
2:M:540:ASP:HB2	2:M:541:PRO:CD	2.51	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	279/335 (83%)	265 (95%)	14 (5%)	0	100	100
1	T	278/335 (83%)	265 (95%)	13 (5%)	0	100	100
2	L	610/582 (105%)	594 (97%)	16 (3%)	0	100	100
2	M	602/582 (103%)	589 (98%)	13 (2%)	0	100	100
All	All	1769/1834 (96%)	1713 (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	234/274 (85%)	230 (98%)	4 (2%)	60	24
1	T	232/274 (85%)	229 (99%)	3 (1%)	69	33
2	L	511/480 (106%)	508 (99%)	3 (1%)	86	63
2	M	503/480 (105%)	503 (100%)	0	100	100
All	All	1480/1508 (98%)	1470 (99%)	10 (1%)	86	59

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

Mol	Chain	Res	Type
1	S	17	CYS
1	S	191	TYR

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Mol	Chain	Res	Type
1	S	242	PRO
1	S	260	ARG
2	L	519[A]	ARG
2	L	519[B]	ARG
2	L	524	ASP
1	T	17	CYS
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
2	M	61	GLN
2	M	387	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	CSO	L	79	2,10,9	3,6,7	0.65	0	0,6,8	-	-
2	CSO	M	79	2,10,9	3,6,7	0.60	0	0,6,8	-	-

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
2	CSO	L	79	2,10,9	-	0/1/5/7	-
2	CSO	M	79	2,10,9	-	0/1/5/7	-

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.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	L	79	CSO	1	0
2	M	79	CSO	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 26 ligands modelled in this entry, 9 are monoatomic - leaving 17 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	$\#\|Z\| > 2$
9	FCO	L	602	14,2	0,6,6	-	-	-		
5	SF3	T	403[C]	14,1	0,8,8	-	-	-		
4	F3S	S	402	1	0,9,9	-	-	-		
8	SO4	L	601	-	4,4,4	0.33	0	6,6,6	0.38	0
9	FCO	M	601	14,2	0,6,6	-	-	-		
4	F3S	T	402	1	0,9,9	-	-	-		
13	TRS	M	606	-	7,7,7	0.59	0	9,9,9	0.59	0
5	SF3	T	403[B]	14,1	0,8,8	-	-	-		
3	SF4	S	401	1	0,12,12	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	SF3	S	403[C]	14,1	0,8,8	-	-	-		
3	SF4	T	401	1	0,12,12	-	-	-		
8	SO4	S	406	-	4,4,4	1.16	1 (25%)	6,6,6	0.93	0
8	SO4	T	407	-	4,4,4	0.33	0	6,6,6	1.03	1 (16%)
5	SF3	S	403[B]	14,1	0,8,8	-	-	-		
6	LMT	S	404	-	13,13,36	0.49	0	12,12,47	0.55	0
8	SO4	M	604	-	4,4,4	0.32	0	6,6,6	0.68	0
6	LMT	T	404	-	13,13,36	0.38	0	12,12,47	0.73	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
5	SF3	T	403[C]	14,1	-	-	0/2/2/2
4	F3S	S	402	1	-	-	0/3/3/3
4	F3S	T	402	1	-	-	0/3/3/3
13	TRS	M	606	-	-	1/9/9/9	-
5	SF3	T	403[B]	14,1	-	-	0/2/2/2
3	SF4	S	401	1	-	-	0/6/5/5
5	SF3	S	403[C]	14,1	-	-	0/2/2/2
3	SF4	T	401	1	-	-	0/6/5/5
6	LMT	S	404	-	-	3/11/11/61	-
5	SF3	S	403[B]	14,1	-	-	0/2/2/2
6	LMT	T	404	-	-	3/11/11/61	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	S	406	SO4	O1-S	2.23	1.58	1.46

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	T	407	SO4	O4-S-O1	-2.14	98.16	109.31

There are no chirality outliers.

All (7) torsion outliers are listed below:

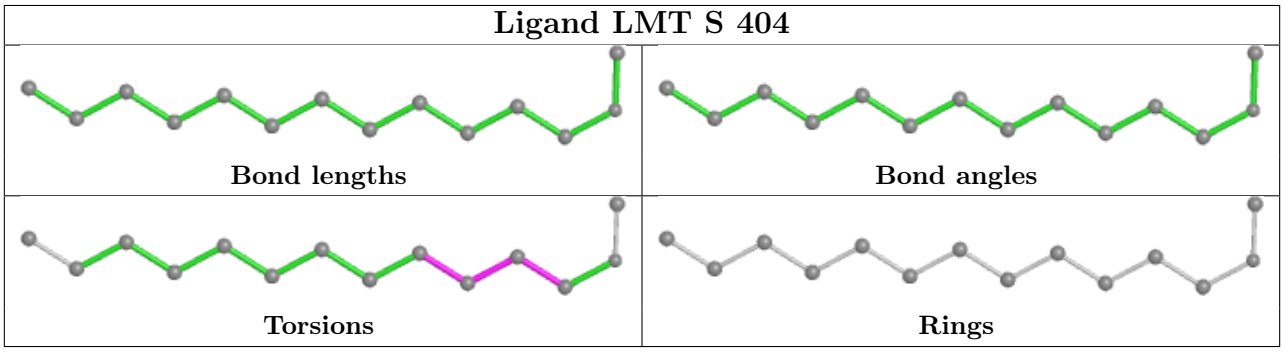
Mol	Chain	Res	Type	Atoms
6	T	404	LMT	C4-C5-C6-C7
6	T	404	LMT	C1-C2-C3-C4
6	S	404	LMT	O1'-C1-C2-C3
6	S	404	LMT	C1-C2-C3-C4
6	S	404	LMT	C2-C3-C4-C5
13	M	606	TRS	C1-C-C2-O2
6	T	404	LMT	C11-C10-C9-C8

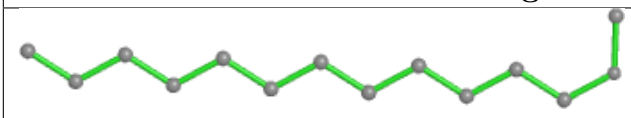
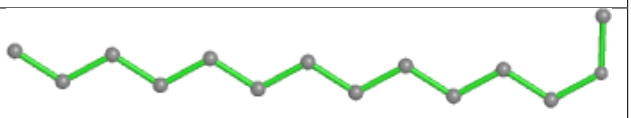
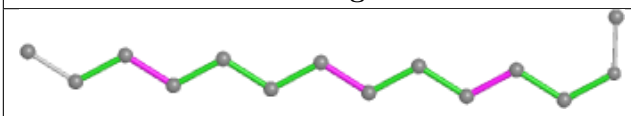
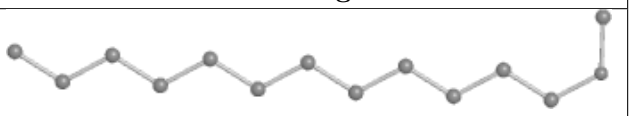
There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	M	606	TRS	1	0
8	T	407	SO4	2	0
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.



Ligand LMT T 404	
 Bond lengths	 Bond angles
 Torsions	 Rings

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	264/335 (78%)	-0.69	1 (0%) 92 92	7, 11, 19, 52	0
1	T	264/335 (78%)	-0.66	0 100 100	8, 12, 20, 40	0
2	L	580/582 (99%)	-0.71	0 100 100	8, 12, 25, 48	1 (0%)
2	M	580/582 (99%)	-0.71	0 100 100	8, 12, 22, 35	1 (0%)
All	All	1688/1834 (92%)	-0.70	1 (0%) 95 95	7, 12, 23, 52	2 (0%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	S	4	LYS	4.2

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

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
2	CSO	L	79	7/8	0.99	0.05	10,10,15,16	1
2	CSO	M	79	7/8	0.99	0.06	10,10,14,17	1

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands (i)

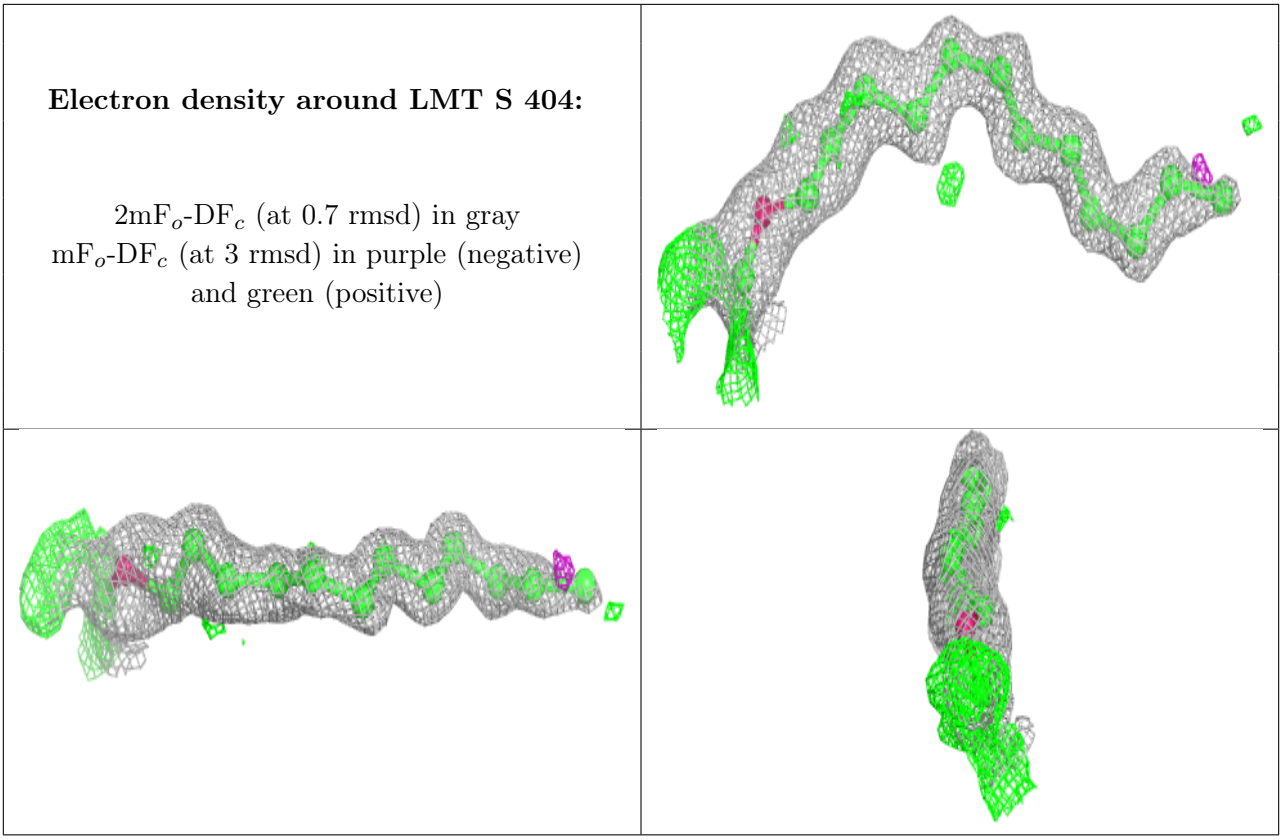
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	14/35	0.83	0.13	20,25,40,40	0
13	TRS	M	606	8/8	0.84	0.21	23,23,26,27	0
8	SO4	S	406	5/5	0.85	0.16	14,17,31,34	5
8	SO4	T	407	5/5	0.90	0.12	18,25,28,34	5
6	LMT	T	404	14/35	0.90	0.12	15,20,33,36	14
8	SO4	M	604	5/5	0.91	0.14	24,24,28,29	5
12	LI	L	605	1/1	0.93	0.39	21,21,21,21	0
12	LI	M	605	1/1	0.97	0.11	20,20,20,20	0
8	SO4	L	601	5/5	0.99	0.06	13,14,17,17	5
5	SF3	T	403[C]	7/7	0.99	0.04	9,10,12,17	1
5	SF3	S	403[B]	7/7	0.99	0.05	8,9,10,11	1
5	SF3	S	403[C]	7/7	0.99	0.05	8,10,11,16	1
7	CL	T	406	1/1	0.99	0.13	27,27,27,27	0
5	SF3	T	403[B]	7/7	0.99	0.04	9,10,12,12	1
3	SF4	S	401	8/8	1.00	0.05	8,8,9,9	0
3	SF4	T	401	8/8	1.00	0.05	8,8,9,9	0
7	CL	S	405	1/1	1.00	0.04	14,14,14,14	0
9	FCO	L	602	7/7	1.00	0.05	8,9,10,10	0
9	FCO	M	601	7/7	1.00	0.05	8,9,10,10	0
10	NI	L	603	1/1	1.00	0.03	14,14,14,14	0
10	NI	M	602	1/1	1.00	0.03	14,14,14,14	0
11	MG	L	604	1/1	1.00	0.08	6,6,6,6	0
11	MG	M	603	1/1	1.00	0.10	6,6,6,6	0
7	CL	T	405	1/1	1.00	0.03	14,14,14,14	0
4	F3S	S	402	7/7	1.00	0.04	9,9,10,10	0
4	F3S	T	402	7/7	1.00	0.04	9,10,10,10	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.

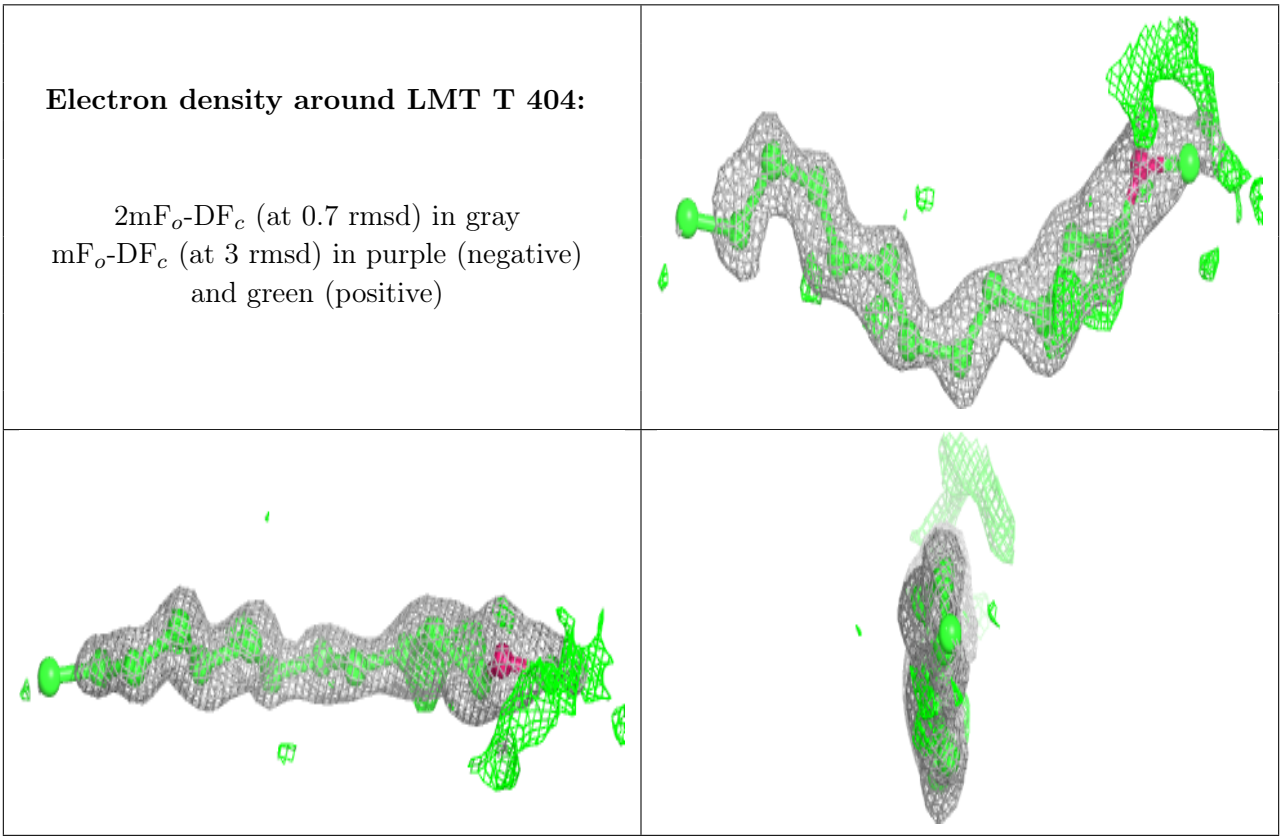
Electron density around LMT S 404:

$2mF_o$-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.