wwPDB X-ray Structure Validation Summary Report (i)

Jan 7, 2024 – 10:50 pm GMT

PDB ID	:	6FPO
Title	:	High resolution structure of native Hydrogenase (Hyd-1)
Authors	:	Carr, S.B.; Armstrong, F.A.; Evans, R.M.
Deposited on	:	2018-02-11
Resolution	:	1.05 Å(reported)

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 ⓘ

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

The reported resolution of this entry is 1.05 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	Percentile Ranks	Value
Rfree		0.138
Clashscore		5
Ramachandran outliers		0.1%
Sidechain outliers		0.7%
RSRZ outliers		0.8%

Worse — *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
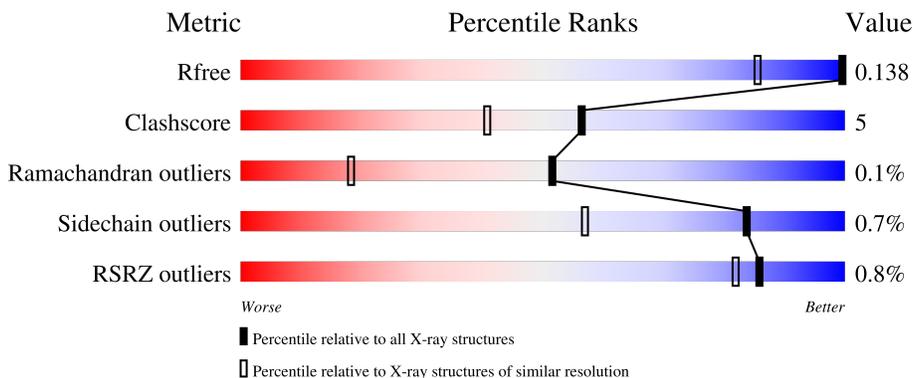
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	1202 (1.10-1.02)
Clashscore	141614	1252 (1.10-1.02)
Ramachandran outliers	138981	1204 (1.10-1.02)
Sidechain outliers	138945	1202 (1.10-1.02)
RSRZ outliers	127900	1178 (1.10-1.02)

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	70% 7% ·· 21%
1	T	335	71% 7% · 21%
2	L	582	91% 8% ·
2	M	582	90% 9% ·

2 Entry composition ⓘ

There are 13 unique types of molecules in this entry. The entry contains 15620 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	18	0
			2136	1358	365	393	20			
1	T	264	Total	C	N	O	S	0	20	0
			2162	1374	373	394	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	30	0
			4722	3009	823	861	29			
2	M	581	Total	C	N	O	S	0	36	0
			4739	3032	810	864	33			

WORLDWIDE PDB
PROTEIN DATA BANK

- Molecule 3 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).
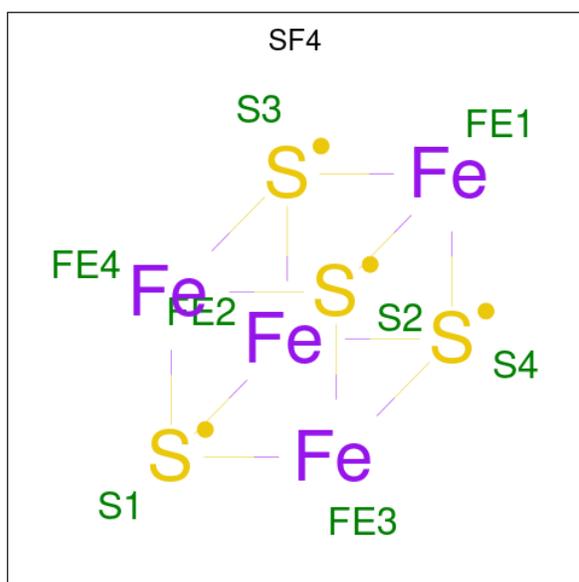
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	S	1	Total	Fe	S	0	0
			8	4	4		
3	T	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 4 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe_3S_4).
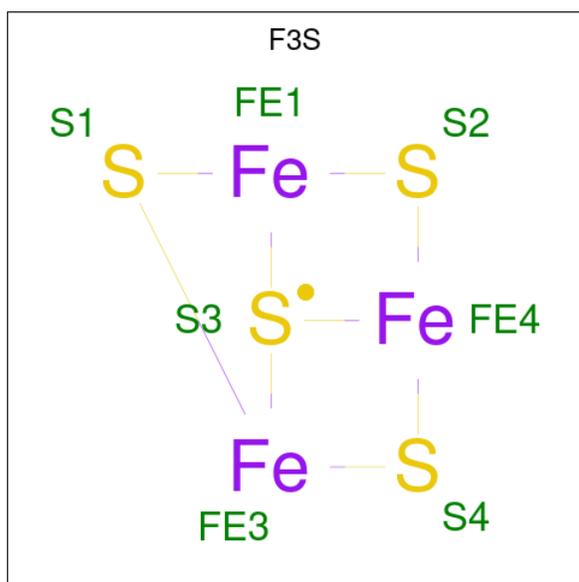
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	S	1	Total	Fe	S	0	0
			7	3	4		

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

- Molecule 5 is FE4-S3 CLUSTER (three-letter code: SF3) (formula: Fe_4S_3).
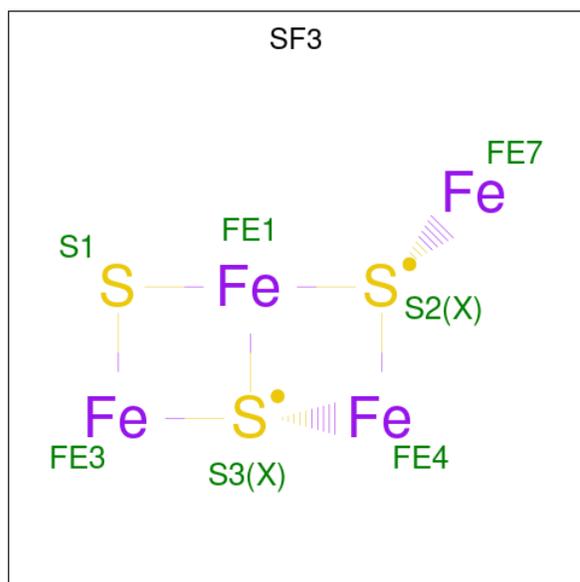
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	S	1	Total 7	Fe 4	S 3	0	0
5	T	1	Total 7	Fe 4	S 3	0	0

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

LMT
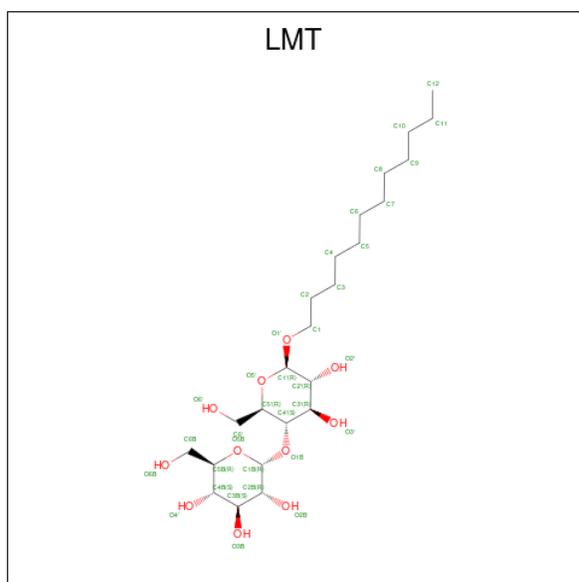
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	S	1	Total 24	C 18	O 6	0	0
6	T	1	Total 14	C 13	O 1	0	0

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

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

- Molecule 8 is CARBONMONOXIDE-(DICYANO) IRON (three-letter code: FCO) (formula: C_3FeN_2O).

FCO

O3
O

C3
C

C1
Fe ———— N   N1
FE

C2

N

N2
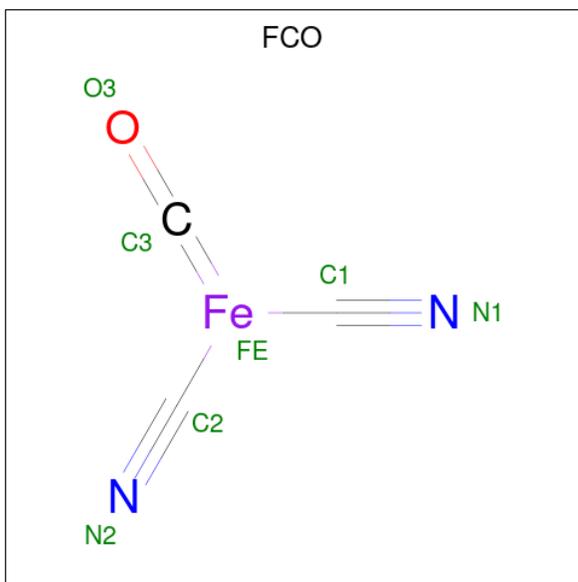
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	L	1	Total 7	C 3	Fe 1	N 2	O 1	0	0
8	M	1	Total 7	C 3	Fe 1	N 2	O 1	0	0

- Molecule 9 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

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

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

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

- Molecule 11 is LITHIUM ION (three-letter code: LI) (formula: Li).

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

- Molecule 12 is SULFATE ION (three-letter code: SO4) (formula: O_4S).
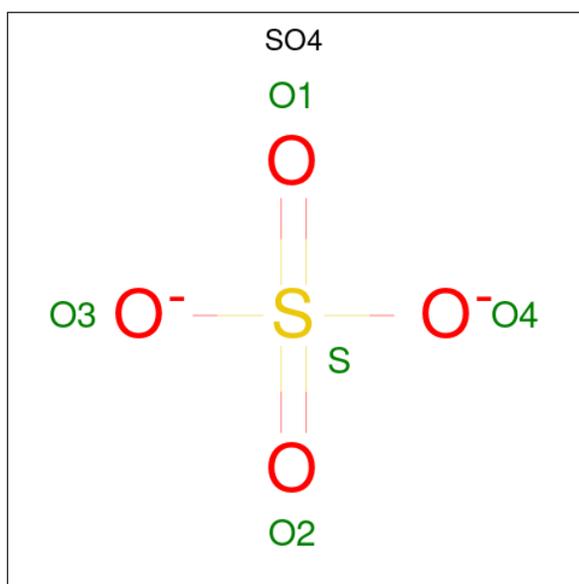
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	L	1	Total 5	O 4	S 1	0	0
12	M	1	Total 5	O 4	S 1	0	0

- Molecule 13 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	S	270	Total 270	O 270	0	0
13	L	594	Total 594	O 594	0	0
13	T	256	Total 256	O 256	0	0
13	M	628	Total 628	O 628	0	0

3 Residue-property plots ⓘ

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 ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	93.79Å 97.73Å 183.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	91.55 – 1.05 48.87 – 1.05	Depositor EDS
% Data completeness (in resolution range)	99.7 (91.55-1.05) 99.7 (48.87-1.05)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	1.52 (at 1.05Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.115 , 0.134 0.120 , 0.138	Depositor DCC
R_{free} test set	38607 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	9.4	Xtriage
Anisotropy	0.170	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 52.0	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	15620	wwPDB-VP
Average B, all atoms (Å^2)	12.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.96% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 ⓘ

5.1   Standard geometry ⓘ

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

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	0.91	4/2239 (0.2%)	1.09	17/3039 (0.6%)
1	T	0.92	4/2266 (0.2%)	1.09	16/3075 (0.5%)
2	L	0.90	10/4921 (0.2%)	0.97	26/6688 (0.4%)
2	M	0.88	10/4956 (0.2%)	1.01	24/6736 (0.4%)
All	All	0.90	28/14382 (0.2%)	1.02	83/19538 (0.4%)

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	2
2	L	0	1
2	M	0	1
All	All	0	6

The worst 5 of 28 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	T	57	GLU	CD-OE1	-8.98	1.15	1.25
2	L	197[A]	GLU	CD-OE2	8.34	1.34	1.25
2	L	197[B]	GLU	CD-OE2	8.34	1.34	1.25
2	L	183[A]	ARG	CZ-NH2	8.20	1.43	1.33
2	L	183[B]	ARG	CZ-NH2	8.20	1.43	1.33

The worst 5 of 83 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	M	363	ARG	NE-CZ-NH2	14.83	127.72	120.30
2	M	500	ARG	NE-CZ-NH2	-14.76	112.92	120.30
2	M	433	ARG	NE-CZ-NH1	10.25	125.42	120.30
1	S	234	ARG	NE-CZ-NH1	-9.79	115.40	120.30
2	M	433	ARG	NE-CZ-NH2	-9.65	115.47	120.30

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	L	74	ARG	Sidechain
1	S	186	ILE	Mainchain
1	S	26	ARG	Sidechain
1	T	26	ARG	Sidechain
1	T	266	ARG	Peptide

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	2136	0	2102	27	0
1	T	2162	0	2130	27	0
2	L	4722	0	4688	46	1
2	M	4739	0	4731	49	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	24	0	35	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	7	0	0	0	0
8	M	7	0	0	0	0
9	L	1	0	0	0	0
9	M	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	L	1	0	0	0	0
10	M	1	0	0	0	0
11	L	1	0	0	0	0
12	L	5	0	0	0	0
12	M	5	0	0	0	0
13	L	594	0	0	24	2
13	M	628	0	0	18	2
13	S	270	0	0	12	0
13	T	256	0	0	13	1
All	All	15620	0	13711	138	3

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 5.

The worst 5 of 138 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:457[A]:HIS:CD2	13:L:990:HOH:O	1.82	1.30
1:T:39[B]:LEU:HD11	13:T:730:HOH:O	1.21	1.29
1:S:39[A]:LEU:HD11	13:S:740:HOH:O	1.34	1.27
2:M:434[B]:MET:HE1	13:M:1167:HOH:O	1.06	1.22
2:L:346[B]:GLN:OE1	13:L:702:HOH:O	1.67	1.11

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:363[B]:ARG:NH1	13:M:714:HOH:O[2_575]	1.89	0.31
13:L:998:HOH:O	13:M:1265:HOH:O[2_675]	2.07	0.13
13:L:1231:HOH:O	13:T:734:HOH:O[2_575]	2.13	0.07

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	S	280/335 (84%)	263 (94%)	16 (6%)	1 (0%)	34	11
1	T	282/335 (84%)	267 (95%)	15 (5%)	0	100	100
2	L	609/582 (105%)	590 (97%)	19 (3%)	0	100	100
2	M	615/582 (106%)	598 (97%)	17 (3%)	0	100	100
All	All	1786/1834 (97%)	1718 (96%)	67 (4%)	1 (0%)	51	18

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	S	187	HIS

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	S	234/274 (85%)	230 (98%)	4 (2%)	60	23
1	T	236/274 (86%)	234 (99%)	2 (1%)	81	52
2	L	510/480 (106%)	506 (99%)	4 (1%)	81	52
2	M	516/480 (108%)	514 (100%)	2 (0%)	91	73
All	All	1496/1508 (99%)	1484 (99%)	12 (1%)	84	52

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	L	524	ASP
1	T	191	TYR
2	M	478	LYS
1	T	242	PRO
1	S	191	TYR

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

Mol	Chain	Res	Type
1	S	13	HIS
2	L	332	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	8,9,2	3,6,7	0.70	0	0,6,8	-	-
2	CSO	M	79	9,2	3,6,7	0.99	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	8,9,2	-	0/1/5/7	-
2	CSO	M	79	9,2	-	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 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	L	79	CSO	2	0
2	M	79	CSO	3	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 19 ligands modelled in this entry, 7 are monoatomic - leaving 12 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	$\#|Z| > 2$
4	F3S	S	402	1	0,9,9	-	-	-		
6	LMT	S	404	-	24,24,36	0.88	1 (4%)	29,29,47	2.38	7 (24%)
3	SF4	S	401	1	0,12,12	-	-	-		
5	SF3	T	403	13,1	0,8,8	-	-	-		
4	F3S	T	402	1	0,9,9	-	-	-		
12	SO4	L	605	-	4,4,4	0.35	0	6,6,6	0.51	0
8	FCO	L	601	13,2	0,6,6	-	-	-		
8	FCO	M	601	13,2	0,6,6	-	-	-		
12	SO4	M	604	-	4,4,4	0.32	0	6,6,6	0.61	0
5	SF3	S	403	13,1	0,8,8	-	-	-		
3	SF4	T	401	1	0,12,12	-	-	-		
6	LMT	T	404	-	13,13,36	0.71	0	12,12,47	1.62	3 (25%)

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
4	F3S	S	402	1	-	-	0/3/3/3
6	LMT	S	404	-	-	3/15/35/61	0/1/1/2

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	S	404	LMT	O1'-C1'	2.84	1.45	1.40

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	S	404	LMT	C1-O1'-C1'	9.39	129.41	113.84
6	S	404	LMT	C3-C2-C1	4.14	131.81	113.49
6	T	404	LMT	C4-C3-C2	-3.68	95.76	114.42
6	S	404	LMT	C3'-C4'-C5'	-3.17	104.58	110.24
6	T	404	LMT	C5-C4-C3	-2.86	99.92	114.42

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

| Mol	Chain	Res	Type	Atoms
6	S	404	LMT	C2-C1-O1'-C1'
6	S	404	LMT	O1'-C1-C2-C3
6	T	404	LMT	O1'-C1-C2-C3
6	T	404	LMT	C2-C1-O1'-C1'
6	T	404	LMT	C2-C3-C4-C5

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 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 S 404	
Bond lengths
Bond angles
Torsions |
Rings |

Ligand LMT T 404	
Bond lengths
Bond angles
Torsions |
Rings |
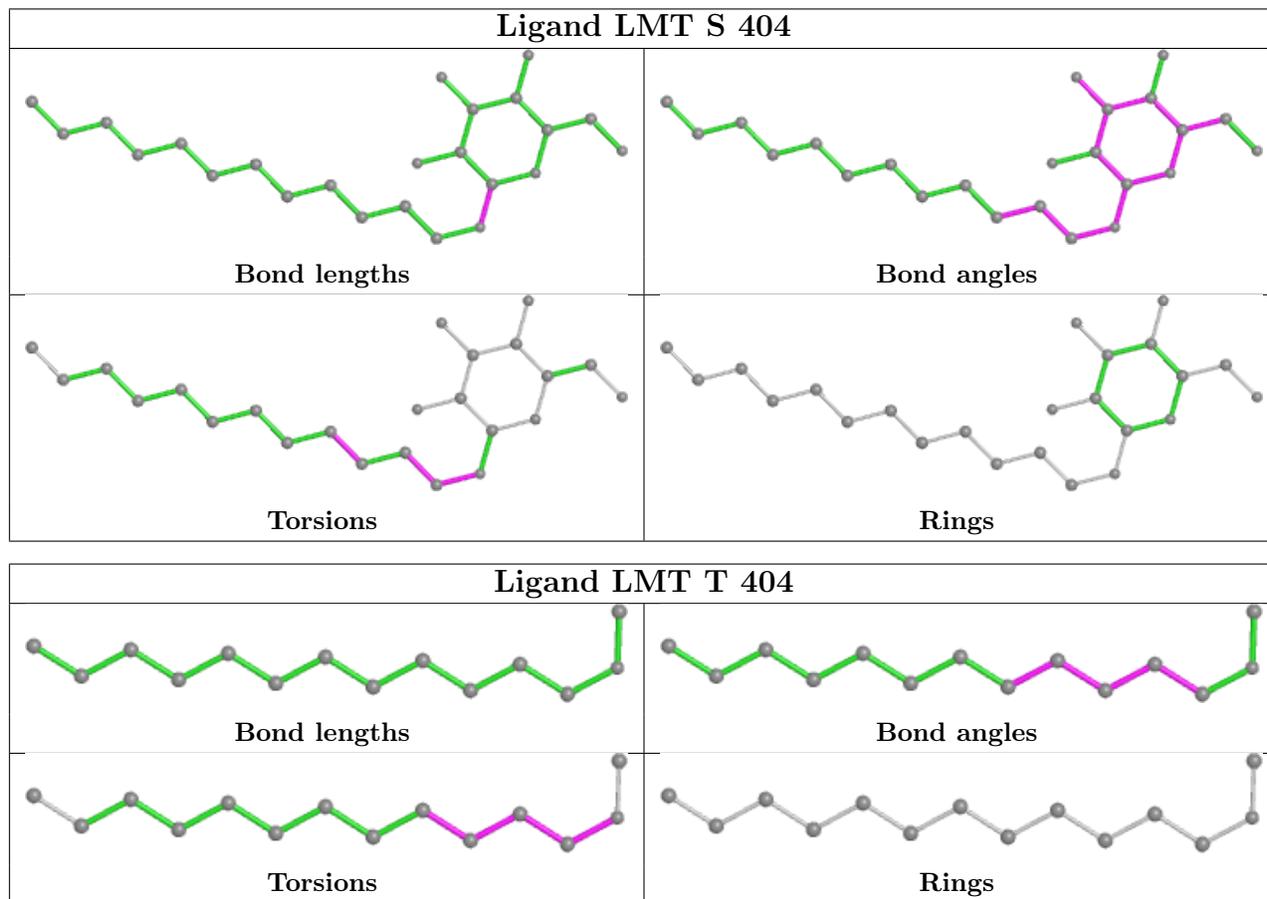
5.7 Other polymers ⓘ

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, 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	264/335 (78%)	-0.32	4 (1%)	73	67	6, 9, 18, 44	0
1	T	264/335 (78%)	-0.28	2 (0%)	86	82	7, 10, 19, 37	1 (0%)
2	L	580/582 (99%)	-0.39	3 (0%)	91	88	6, 10, 22, 38	2 (0%)
2	M	580/582 (99%)	-0.42	4 (0%)	87	84	6, 10, 20, 43	1 (0%)
All	All	1688/1834 (92%)	-0.37	13 (0%)	86	82	6, 10, 20, 44	4 (0%)

The worst 5 of 13 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	T	267	VAL	11.1
1	S	267	VAL	6.3
2	M	114[A]	LEU	5.6
1	S	19	CYS	5.3
1	T	19	CYS	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, 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	CSO	M	79	7/8	0.69	0.22	8,9,12,13	1
2	CSO	L	79	7/8	0.99	0.06	8,9,12,14	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, 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
6	LMT	T	404	14/35	0.88	0.15	20,25,40,43	0
12	SO4	M	604	5/5	0.92	0.11	23,25,29,29	5
6	LMT	S	404	24/35	0.93	0.09	16,22,29,38	10
12	SO4	L	605	5/5	0.98	0.10	15,15,18,21	5
11	LI	L	604	1/1	0.98	0.36	14,14,14,14	0
9	NI	M	602	1/1	0.99	0.04	14,14,14,14	1
5	SF3	S	403	7/7	0.99	0.04	6,8,10,12	7
5	SF3	T	403	7/7	0.99	0.04	7,8,11,12	7
9	NI	L	602	1/1	0.99	0.04	14,14,14,14	1
7	CL	T	405	1/1	1.00	0.03	13,13,13,13	0
8	FCO	L	601	7/7	1.00	0.04	7,8,8,8	0
8	FCO	M	601	7/7	1.00	0.04	7,8,8,8	0
3	SF4	S	401	8/8	1.00	0.03	7,7,7,7	0
3	SF4	T	401	8/8	1.00	0.03	7,7,7,7	0
10	MG	L	603	1/1	1.00	0.04	6,6,6,6	0
10	MG	M	603	1/1	1.00	0.05	6,6,6,6	0
4	F3S	S	402	7/7	1.00	0.03	7,7,8,8	0
4	F3S	T	402	7/7	1.00	0.03	7,8,8,8	0
7	CL	S	405	1/1	1.00	0.02	11,11,11,11	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 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)

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)

6.5 Other polymers ⓘ

There are no such residues in this entry.