



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 25, 2026 – 02:08 pm BST

PDB ID : 5ADU / pdb_00005adu
Title : The Mechanism of Hydrogen Activation by NiFe-hydrogenases
Authors : Evans, R.; Brooke, E.J.; Wehlin, S.A.; Nomerotskaia, E.; Sargent, F.; Carr, S.B.; Phillips, S.E.V.; Armstrong, F.A.
Deposited on : 2015-08-24
Resolution : 1.10 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	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

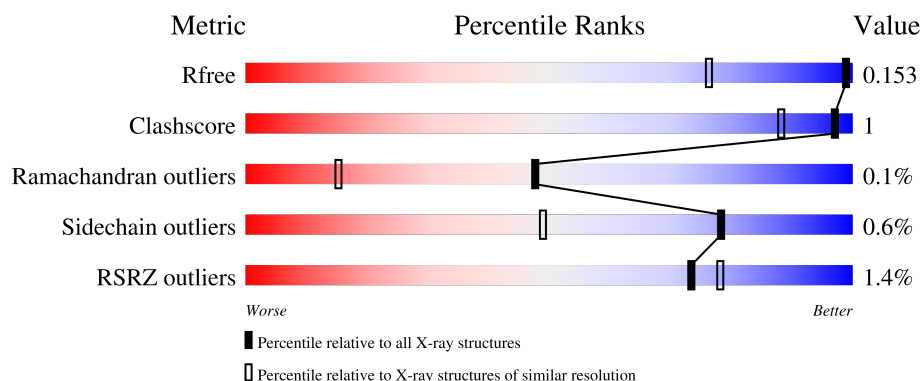
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.10 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}	180053	1625 (1.12-1.08)
Clashscore	190562	1656 (1.12-1.08)
Ramachandran outliers	187476	1616 (1.12-1.08)
Sidechain outliers	187428	1612 (1.12-1.08)
RSRZ outliers	180081	1625 (1.12-1.08)

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	L	582	<div> <div>2%</div> <div>97%</div> <div>.</div> </div>
1	M	582	<div> <div>%</div> <div>98%</div> <div>.</div> </div>
2	S	335	<div> <div>%</div> <div>75%</div> <div>.</div> <div>21%</div> </div>
2	T	335	<div> <div>%</div> <div>74%</div> <div>.</div> <div>21%</div> </div>

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 14757 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 large chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	581	Total	C	N	O	S	0	27	0
			4707	2991	825	862	29			
1	M	581	Total	C	N	O	S	0	21	0
			4662	2966	810	857	29			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	118	ASN	ASP	engineered mutation	UNP P0ACD8
L	574	ASN	ASP	engineered mutation	UNP P0ACD8
M	118	ASN	ASP	engineered mutation	UNP P0ACD8
M	574	ASN	ASP	engineered mutation	UNP P0ACD8

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	S	263	Total	C	N	O	S	0	10	0
			2089	1326	358	384	21			
2	T	264	Total	C	N	O	S	0	10	0
			2100	1334	362	383	21			

There are 16 discrepancies between the modelled and reference sequences:

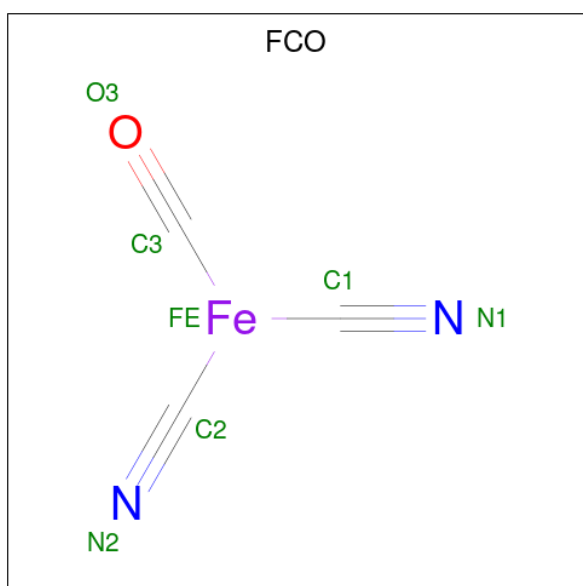
Chain	Residue	Modelled	Actual	Comment	Reference
S	328	ARG	-	expression tag	UNP P69739
S	329	SER	-	expression tag	UNP P69739
S	330	HIS	-	expression tag	UNP P69739
S	331	HIS	-	expression tag	UNP P69739
S	332	HIS	-	expression tag	UNP P69739
S	333	HIS	-	expression tag	UNP P69739
S	334	HIS	-	expression tag	UNP P69739
S	335	HIS	-	expression tag	UNP P69739

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Chain	Residue	Modelled	Actual	Comment	Reference
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 3 is CARBONMONOXIDE-(DICYANO) IRON (CCD ID: FCO) (formula: C_3FeN_2O).



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

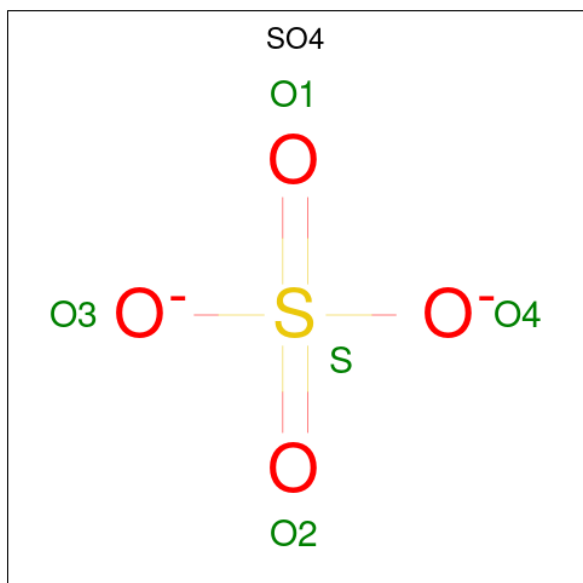
- Molecule 4 is NICKEL (II) ION (CCD ID: NI) (formula: Ni).

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

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

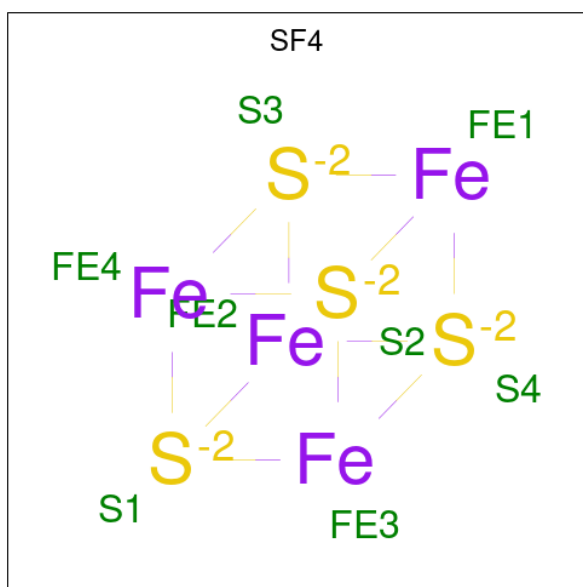
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	L	1	Total	Mg	0	0
			1	1		
5	M	1	Total	Mg	0	0
			1	1		

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



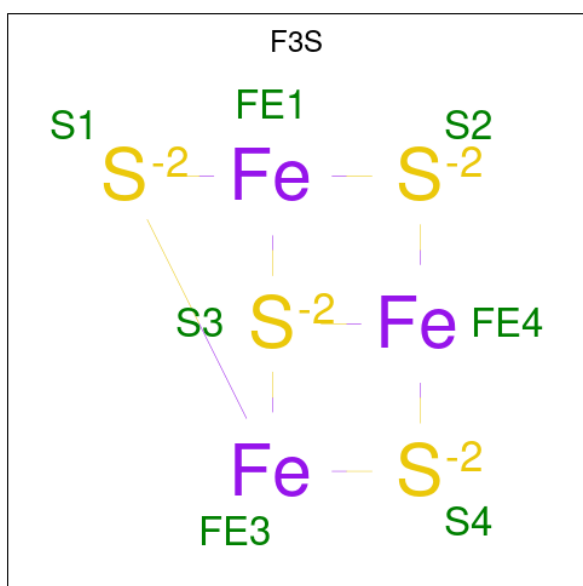
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	M	1	Total	O	S	0	0
			5	4	1		
6	S	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



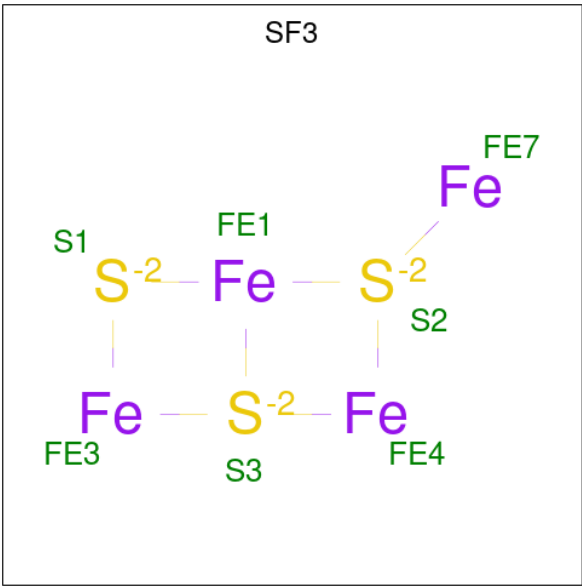
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	S	1	Total	Fe	S	0	0
			8	4	4		
7	T	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 8 is FE3-S4 CLUSTER (CCD ID: F3S) (formula: Fe_3S_4).



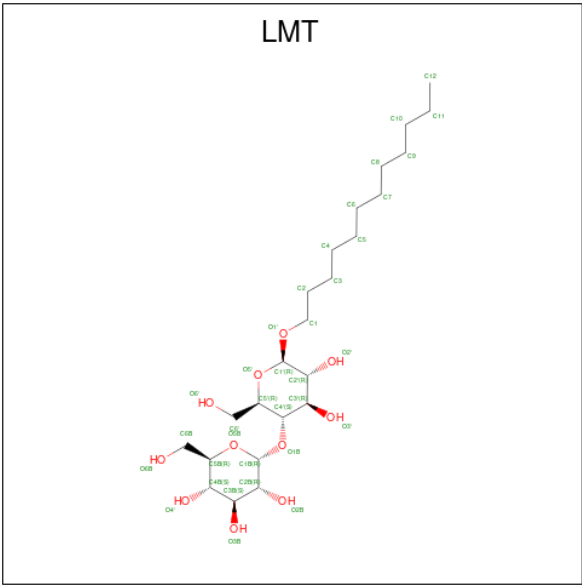
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	S	1	Total	Fe	S	0	0
			7	3	4		
8	T	1	Total	Fe	S	0	0
			7	3	4		

- Molecule 9 is FE4-S3 CLUSTER (CCD ID: SF3) (formula: Fe₄S₃).



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

- Molecule 10 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



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

- Molecule 11 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	L	411	Total	O	0	0
			411	411		
12	M	418	Total	O	0	0
			418	418		
12	S	145	Total	O	0	0
			145	145		
12	T	119	Total	O	0	0
			119	119		

- Molecule 1: Hydrogenase-1 large chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	94.86Å 98.98Å 185.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	92.78 – 1.10 92.60 – 1.10	Depositor EDS
% Data completeness (in resolution range)	95.3 (92.78-1.10) 95.3 (92.60-1.10)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.71 (at 1.10Å)	Xtriage
Refinement program	REFMAC 5.8.0131	Depositor
R, R_{free}	0.126 , 0.142 0.139 , 0.153	Depositor DCC
R_{free} test set	33299 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	7.8	Xtriage
Anisotropy	0.032	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 35.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.012 for k,h,-l	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	14757	wwPDB-VP
Average B, all atoms (Å ²)	10.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.28% 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, LMT, MG, SF3, CL, F3S, CSO, SF4, SO4, FCO

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	L	1.06	1/4893 (0.0%)	0.82	1/6649 (0.0%)
1	M	1.08	1/4839 (0.0%)	0.82	1/6576 (0.0%)
2	S	1.15	3/2171 (0.1%)	0.88	1/2945 (0.0%)
2	T	1.14	3/2182 (0.1%)	0.87	1/2959 (0.0%)
All	All	1.09	8/14085 (0.1%)	0.84	4/19129 (0.0%)

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	S	0	1
2	T	0	1
All	All	0	2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	276	ILE	CA-CB	7.57	1.58	1.54
2	T	188	ASP	CG-OD2	-6.02	1.14	1.25
2	S	260	ARG	CZ-NH1	5.87	1.41	1.32
2	S	197	ASP	CB-CG	5.74	1.66	1.52
2	T	260	ARG	CZ-NH1	5.32	1.40	1.32
1	L	276	ILE	CA-C	5.11	1.57	1.52
2	S	197	ASP	CG-OD2	5.07	1.34	1.25
2	T	134	ILE	CA-CB	5.04	1.60	1.54

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	530	VAL	N-CA-CB	-6.97	107.02	111.83
1	M	530	VAL	N-CA-CB	-6.23	107.53	111.83
2	S	187	HIS	CA-CB-CG	5.25	119.05	113.80
2	T	187	HIS	CA-CB-CG	5.24	119.04	113.80

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	S	26	ARG	Sidechain
2	T	26	ARG	Sidechain

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	L	4707	0	4653	8	0
1	M	4662	0	4601	6	0
2	S	2089	0	2039	5	0
2	T	2100	0	2058	8	0
3	L	7	0	0	0	0
3	M	7	0	0	0	0
4	L	1	0	0	0	0
4	M	1	0	0	0	0
5	L	1	0	0	0	0
5	M	1	0	0	0	0
6	M	5	0	0	0	0
6	S	5	0	0	0	0
7	S	8	0	0	0	0
7	T	8	0	0	0	0
8	S	7	0	0	0	0
8	T	7	0	0	0	0
9	S	8	0	0	0	0
9	T	8	0	0	0	0
10	S	14	0	25	1	0
10	T	14	0	25	2	0
11	S	2	0	0	0	0
11	T	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	L	411	0	0	0	0
12	M	418	0	0	2	0
12	S	145	0	0	0	0
12	T	119	0	0	1	0
All	All	14757	0	13401	25	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 1.

All (25) 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:S:61[B]:GLU:OE2	2:S:101[B]:ARG:NH1	1.80	1.15
2:S:234[A]:ARG:HD3	2:T:234[A]:ARG:NH1	1.71	1.05
1:M:175[B]:GLU:HG3	12:M:2149:HOH:O	1.77	0.83
1:M:486[A]:SER:OG	1:M:488[A]:GLU:OE2	2.03	0.76
1:M:275[B]:MET:HE2	1:M:456:ALA:HA	1.70	0.72
1:M:243:ILE:HG23	1:M:254[B]:MET:HG2	1.73	0.70
1:L:79:CSO:OD	1:L:79:CSO:N	2.24	0.70
1:M:79:CSO:OD	1:M:79:CSO:N	2.27	0.68
2:S:234[A]:ARG:CD	2:T:234[A]:ARG:NH1	2.54	0.66
1:L:275[B]:MET:HE2	1:L:456:ALA:HA	1.77	0.65
2:T:61[B]:GLU:HG2	12:T:2020:HOH:O	2.04	0.57
1:L:254[B]:MET:HA	1:L:254[B]:MET:HE2	1.89	0.54
1:M:429[B]:GLU:HG3	12:M:2350:HOH:O	2.08	0.53
2:S:175[B]:MET:HA	2:S:175[B]:MET:HE2	1.91	0.52
2:T:255:ASN:O	2:T:260:ARG:NH2	2.36	0.52
1:L:135:LEU:HD22	1:L:187:TRP:CD1	2.45	0.51
1:L:378:ASP:OD1	1:L:379[A]:VAL:O	2.32	0.47
2:T:217:TYR:HE1	2:T:267:VAL:HG12	1.80	0.47
2:T:163:MET:HE3	10:T:404:LMT:H72	1.96	0.47
1:L:519[B]:ARG:HG2	1:L:520:ASP:OD2	2.16	0.44
2:S:163:MET:HE3	10:S:404:LMT:H72	2.00	0.44
1:L:380[A]:LYS:O	1:L:387:GLN:HB2	2.20	0.42
2:T:7:ILE:HG21	10:T:404:LMT:H62	2.02	0.41
1:L:530:VAL:CG1	1:L:531:PRO:HD2	2.51	0.40
2:T:186:ILE:HD11	2: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	L	606/582 (104%)	587 (97%)	17 (3%)	2 (0%)	36	13
1	M	600/582 (103%)	586 (98%)	14 (2%)	0	100	100
2	S	271/335 (81%)	259 (96%)	12 (4%)	0	100	100
2	T	272/335 (81%)	259 (95%)	13 (5%)	0	100	100
All	All	1749/1834 (95%)	1691 (97%)	56 (3%)	2 (0%)	48	15

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	381[A]	GLY
1	L	381[B]	GLY

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	L	506/480 (105%)	505 (100%)	1 (0%)	87	64
1	M	501/480 (104%)	498 (99%)	3 (1%)	78	49
2	S	226/274 (82%)	222 (98%)	4 (2%)	51	15
2	T	227/274 (83%)	223 (98%)	4 (2%)	51	15
All	All	1460/1508 (97%)	1448 (99%)	12 (1%)	78	40

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

Mol	Chain	Res	Type
1	L	524	ASP
1	M	380[A]	LYS
1	M	380[B]	LYS
1	M	524	ASP
2	S	16[A]	GLU
2	S	16[B]	GLU
2	S	168	ARG
2	S	242	PRO
2	T	16[A]	GLU
2	T	16[B]	GLU
2	T	242	PRO
2	T	267	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	328	ASN
1	L	392	GLN
1	M	4	GLN
1	M	392	GLN
1	M	460	GLN
2	S	55	GLN
2	T	255	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	$\# Z > 2$
1	CSO	M	79	4,3,1	3,6,7	0.88	0	0,6,8	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	CSO	L	79	4,3,1	3,6,7	0.87	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
1	CSO	M	79	4,3,1	-	0/1/5/7	-
1	CSO	L	79	4,3,1	-	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
1	M	79	CSO	1	0
1	L	79	CSO	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 22 ligands modelled in this entry, 8 are monoatomic - leaving 14 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
10	LMT	S	404	-	13,13,36	0.52	0	12,12,47	0.86	0
10	LMT	T	404	-	13,13,36	0.43	0	12,12,47	0.59	0
9	SF3	S	403[B]	2	0,8,8	-	-	-		
6	SO4	M	604	-	4,4,4	0.56	0	6,6,6	0.36	0
9	SF3	T	403[C]	2	0,8,8	-	-	-		
7	SF4	T	401	2	0,12,12	-	-	-		
8	F3S	T	402	2	0,9,9	-	-	-		
3	FCO	M	601	12,1	1,6,6	0.92	0	-		
9	SF3	T	403[B]	2	0,8,8	-	-	-		
7	SF4	S	401	2	0,12,12	-	-	-		
3	FCO	L	601	12,1	1,6,6	1.72	0	-		
9	SF3	S	403[C]	2	0,8,8	-	-	-		
8	F3S	S	402	2	0,9,9	-	-	-		
6	SO4	S	407	-	4,4,4	0.45	0	6,6,6	0.60	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
10	LMT	S	404	-	-	4/11/11/61	-
10	LMT	T	404	-	-	6/11/11/61	-
9	SF3	S	403[B]	2	-	-	0/2/2/2
9	SF3	T	403[C]	2	-	-	0/2/2/2
7	SF4	T	401	2	-	-	0/6/5/5
8	F3S	T	402	2	-	-	0/3/3/3
9	SF3	T	403[B]	2	-	-	0/2/2/2
7	SF4	S	401	2	-	-	0/6/5/5
9	SF3	S	403[C]	2	-	-	0/2/2/2
8	F3S	S	402	2	-	-	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	T	404	LMT	O1'-C1-C2-C3
10	S	404	LMT	O1'-C1-C2-C3

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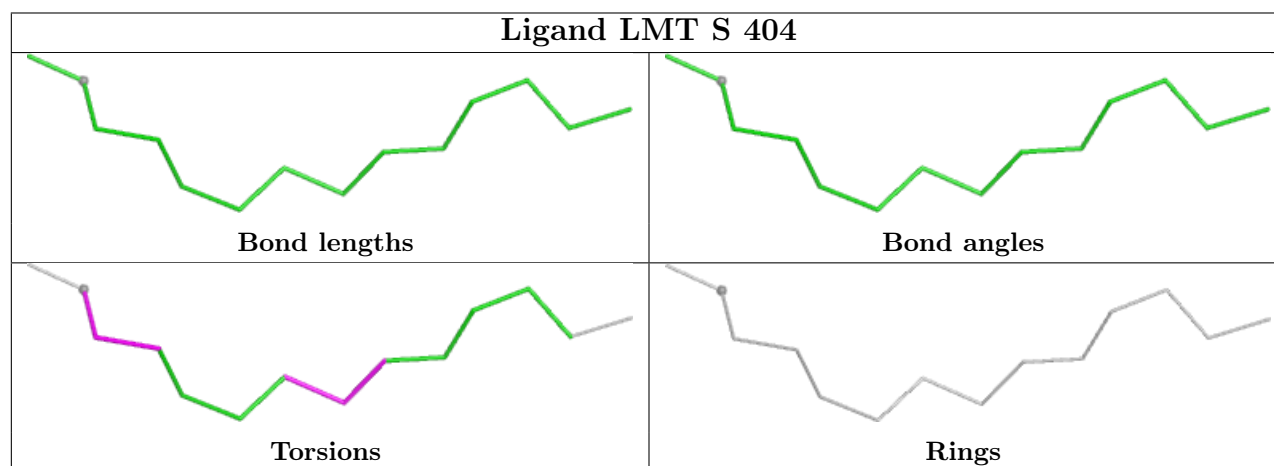
Mol	Chain	Res	Type	Atoms
10	T	404	LMT	C2-C1-O1'-C1'
10	T	404	LMT	C4-C5-C6-C7
10	S	404	LMT	C4-C5-C6-C7
10	T	404	LMT	C1-C2-C3-C4
10	S	404	LMT	C5-C6-C7-C8
10	T	404	LMT	C2-C3-C4-C5
10	T	404	LMT	C11-C10-C9-C8
10	S	404	LMT	C2-C1-O1'-C1'

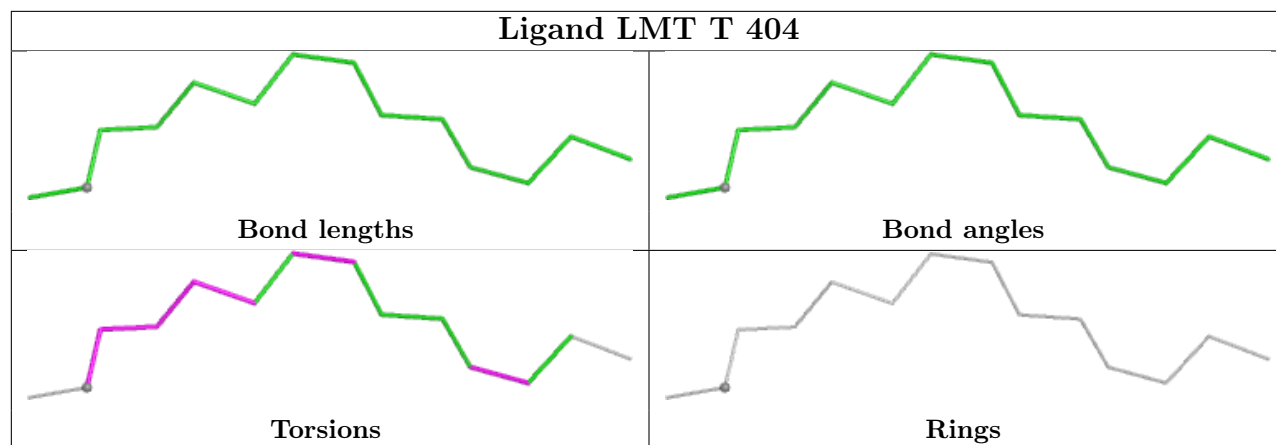
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	S	404	LMT	1	0
10	T	404	LMT	2	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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	L	580/582 (99%)	-0.25	9 (1%) 70 74	3, 9, 20, 45	27 (4%)
1	M	580/582 (99%)	-0.31	8 (1%) 73 78	3, 9, 17, 31	21 (3%)
2	S	263/335 (78%)	-0.32	2 (0%) 82 86	4, 8, 15, 46	10 (3%)
2	T	264/335 (78%)	-0.24	4 (1%) 72 76	4, 8, 17, 46	10 (3%)
All	All	1687/1834 (91%)	-0.28	23 (1%) 73 78	3, 9, 18, 46	68 (4%)

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	T	267	VAL	5.7
1	L	380[A]	LYS	4.4
1	L	285	PHE	4.0
1	L	379[A]	VAL	3.7
2	T	4	LYS	3.1
2	S	260	ARG	2.9
1	M	285	PHE	2.7
1	L	176	GLY	2.6
2	T	260	ARG	2.6
2	T	197	ASP	2.6
1	L	430	SER	2.5
1	M	174	VAL	2.4
2	S	4	LYS	2.4
1	M	143	ARG	2.3
1	L	437	ALA	2.3
1	L	426	ALA	2.2
1	L	433	ARG	2.1
1	M	433[A]	ARG	2.1
1	L	3	THR	2.1
1	M	280	LEU	2.1
1	M	176	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	M	2	SER	2.0
1	M	15	ALA	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
1	CSO	L	79	7/8	0.98	0.06	5,6,8,17	0
1	CSO	M	79	7/8	0.99	0.05	6,6,9,17	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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.

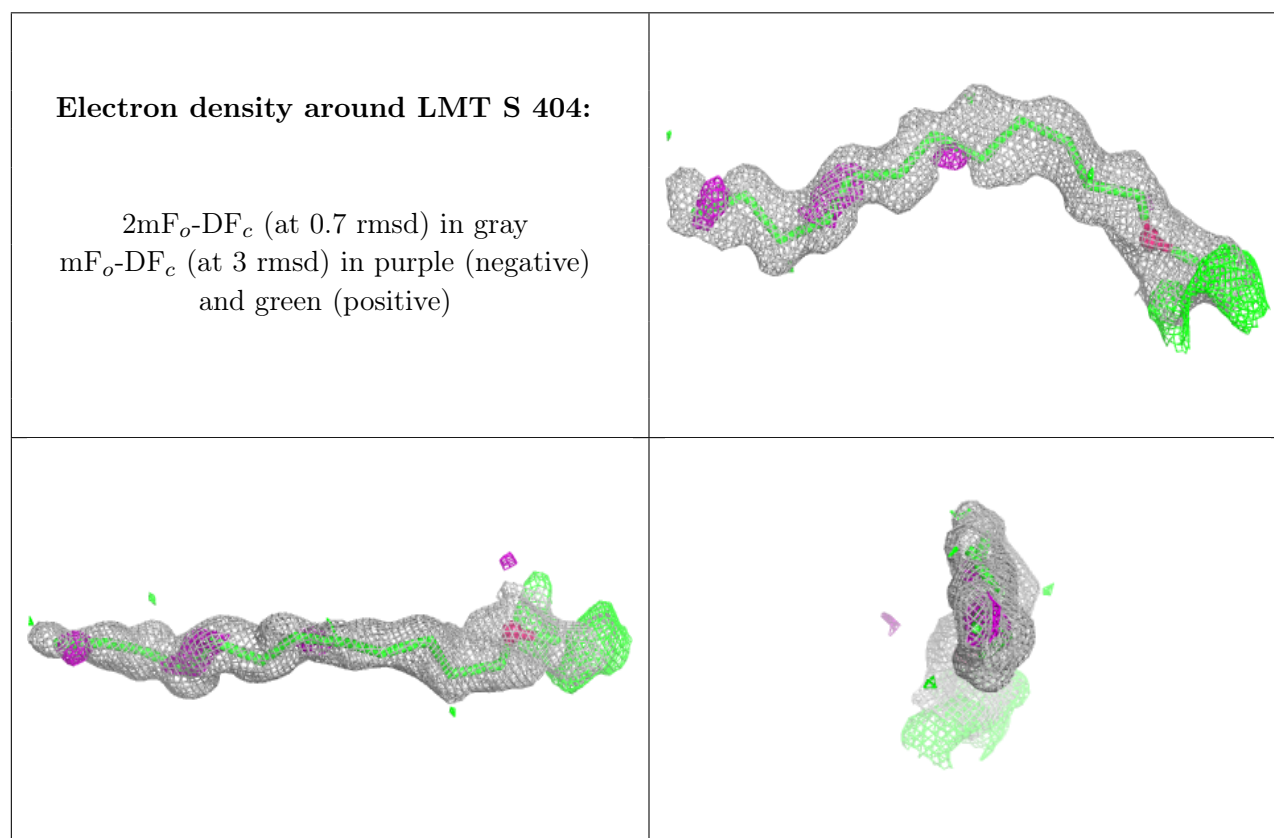
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
10	LMT	S	404	14/35	0.83	0.15	15,26,34,37	0
6	SO4	M	604	5/5	0.86	0.13	38,39,52,57	0
10	LMT	T	404	14/35	0.86	0.14	18,26,33,35	0
6	SO4	S	407	5/5	0.97	0.08	17,17,22,23	0
5	MG	L	603	1/1	1.00	0.01	4,4,4,4	0
5	MG	M	603	1/1	1.00	0.02	4,4,4,4	0
3	FCO	L	601	7/7	1.00	0.02	5,6,7,7	0
3	FCO	M	601	7/7	1.00	0.02	5,6,7,7	0
7	SF4	S	401	8/8	1.00	0.01	5,5,5,5	0
7	SF4	T	401	8/8	1.00	0.01	5,5,5,5	0
8	F3S	S	402	7/7	1.00	0.02	5,5,6,6	0
8	F3S	T	402	7/7	1.00	0.02	5,5,6,6	0
9	SF3	S	403[B]	7/7	1.00	0.01	5,6,6,6	1
9	SF3	S	403[C]	7/7	1.00	0.01	5,6,6,17	1

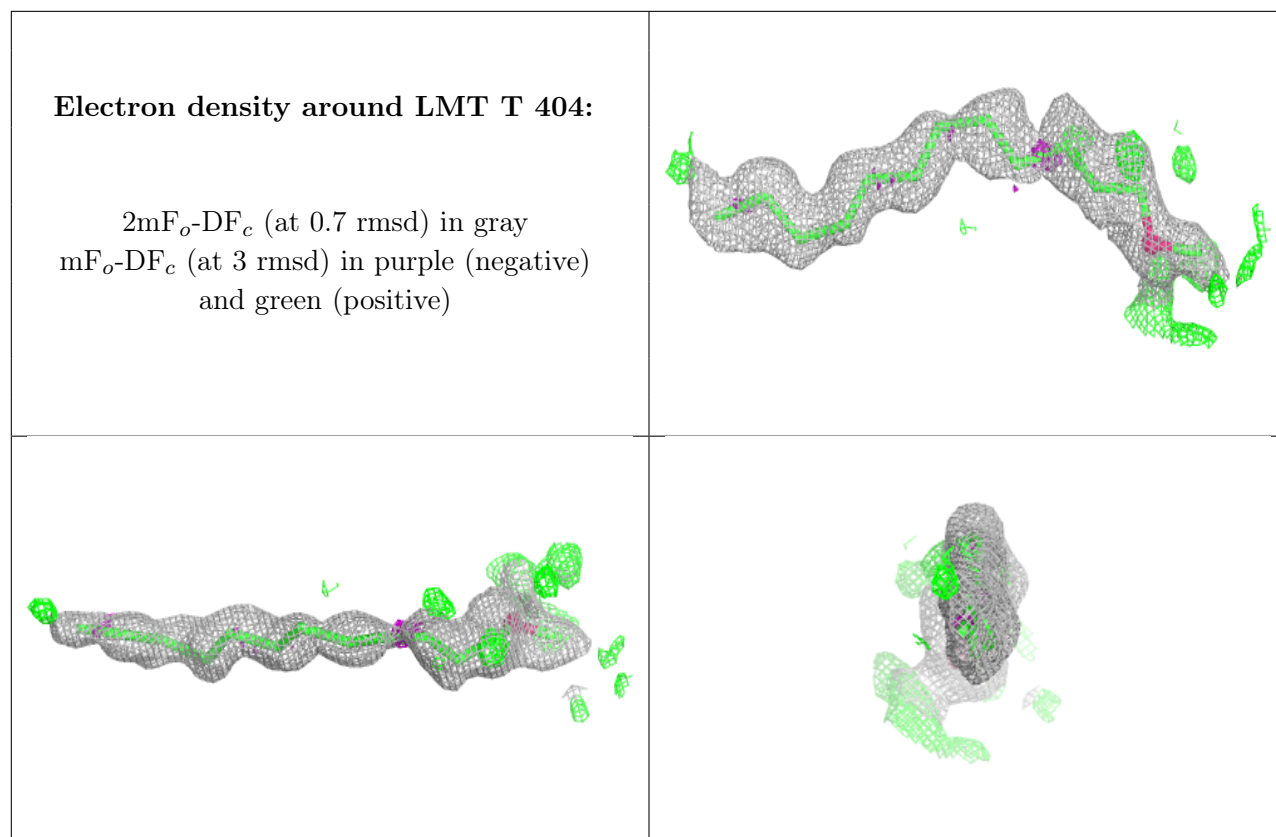
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
9	SF3	T	403[B]	7/7	1.00	0.02	5,6,6,6	1
9	SF3	T	403[C]	7/7	1.00	0.02	5,6,6,17	1
4	NI	L	602	1/1	1.00	0.08	14,14,14,14	0
4	NI	M	602	1/1	1.00	0.09	14,14,14,14	0
11	CL	S	405	1/1	1.00	0.02	9,9,9,9	0
11	CL	S	406	1/1	1.00	0.09	15,15,15,15	0
11	CL	T	405	1/1	1.00	0.03	10,10,10,10	0
11	CL	T	406	1/1	1.00	0.12	17,17,17,17	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.