Full wwPDB X-ray Structure Validation Report (i)

May 15, 2020 – 11:08 am BST

PDB ID	:	3ZIU
Title	:	Crystal structure of Mycoplasma mobile Leucyl-tRNA Synthetase with Leu-AMS in the active site
Authors	:	Li, L.; Palencia, A.; Lukk, T.; Li, Z.; Luthey-Schulten, Z.A.; Cusack, S.; Martinis, S.A.; Boniecki, M.T.
Deposited on	:	2013-01-10
Resolution	:	2.07 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 following versions of software and data (see references (i)) were used in the production of this report:

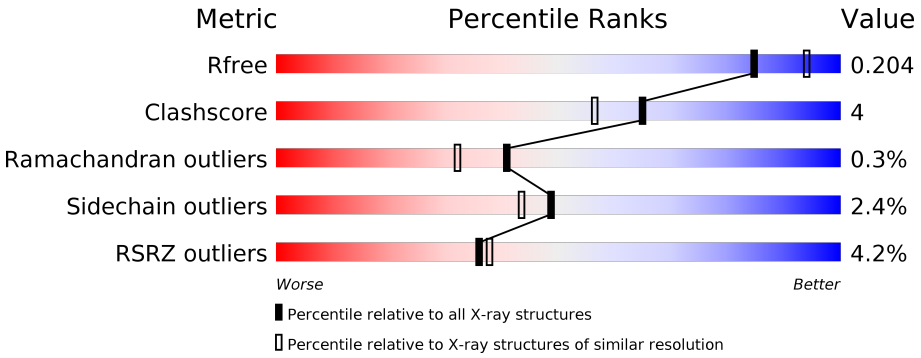
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.07 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	2684 (2.08-2.04)
Clashscore	141614	2801 (2.08-2.04)
Ramachandran outliers	138981	2768 (2.08-2.04)
Sidechain outliers	138945	2768 (2.08-2.04)
RSRZ outliers	127900	2646 (2.08-2.04)

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 on 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	A	637	7% 87% 10% ·
1	B	637	% 82% 8% · 10%

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
3	GOL	A	1640	-	-	X	-
3	GOL	A	1643	-	-	X	-
3	GOL	B	1581	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11142 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.

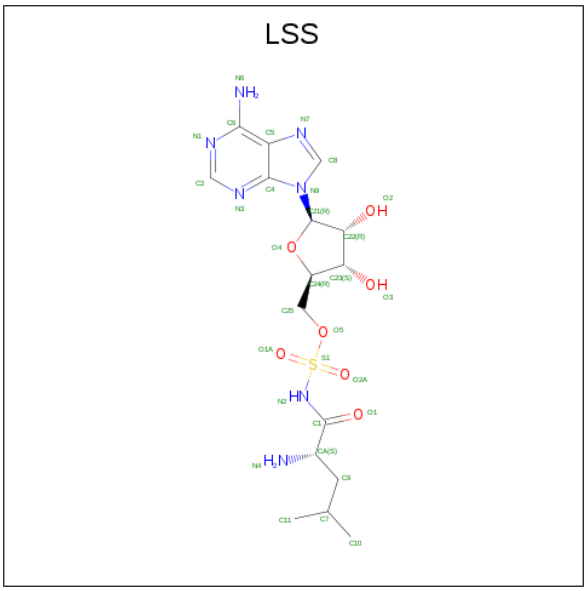
- Molecule 1 is a protein called LEUCYL-TRNA SYNTHETASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	621	Total	C	N	O	S	0	3	0
			5164	3357	848	941	18			
1	B	575	Total	C	N	O	S	0	8	0
			4844	3149	793	884	18			

There are 14 discrepancies between the modelled and reference sequences:

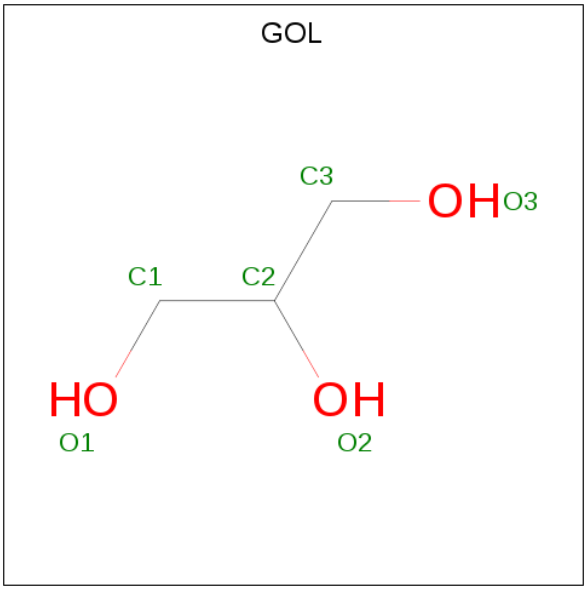
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	LEU	-	expression tag	UNP Q6KHA5
A	2	VAL	-	expression tag	UNP Q6KHA5
A	3	PRO	-	expression tag	UNP Q6KHA5
A	4	ARG	-	expression tag	UNP Q6KHA5
A	5	GLY	-	expression tag	UNP Q6KHA5
A	6	SER	-	expression tag	UNP Q6KHA5
A	7	HIS	-	expression tag	UNP Q6KHA5
B	1	LEU	-	expression tag	UNP Q6KHA5
B	2	VAL	-	expression tag	UNP Q6KHA5
B	3	PRO	-	expression tag	UNP Q6KHA5
B	4	ARG	-	expression tag	UNP Q6KHA5
B	5	GLY	-	expression tag	UNP Q6KHA5
B	6	SER	-	expression tag	UNP Q6KHA5
B	7	HIS	-	expression tag	UNP Q6KHA5

- Molecule 2 is 5'-O-(L-leucylsulfamoyl)adenosine (three-letter code: LSS) (formula: $C_{16}H_{25}N_7O_7S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			31	16	7	7	1		
2	B	1	Total	C	N	O	S	0	0
			31	16	7	7	1		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O		0	0
			6	3	3			
3	A	1	Total	C	O		0	0
			6	3	3			

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0

- Molecule 4 is water.

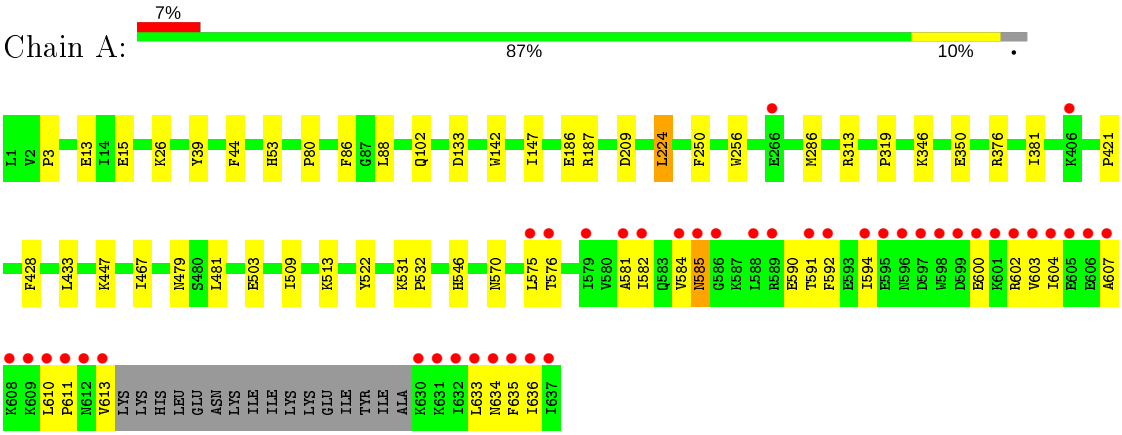
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	524	Total O 524 524	0	0
4	B	488	Total O 488 488	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

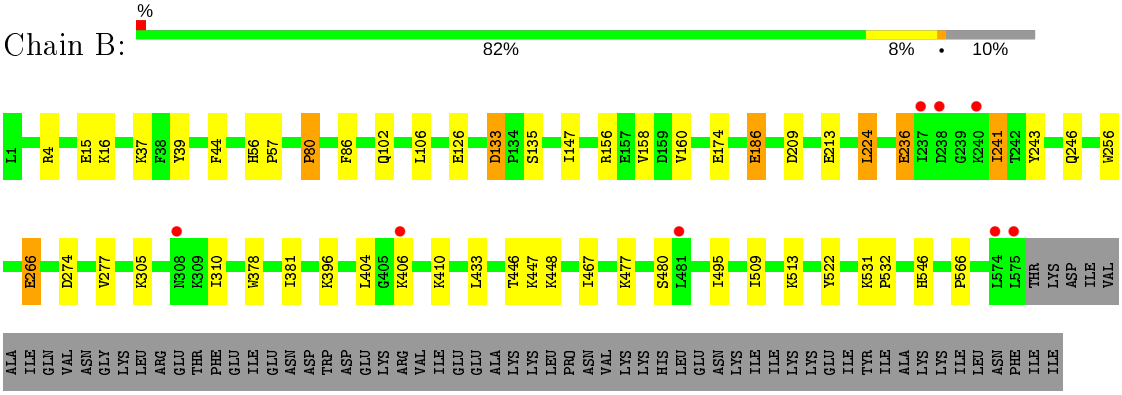
- Molecule 1: LEUCYL-TRNA SYNTHETASE

Chain A:



- Molecule 1: LEUCYL-TRNA SYNTHETASE

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α, β, γ	202.85Å 202.85Å 213.92Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	135.76 – 2.07 12.01 – 2.07	Depositor EDS
% Data completeness (in resolution range)	99.3 (135.76-2.07) 100.0 (12.01-2.07)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.74 (at 2.07Å)	Xtriage
Refinement program	REFMAC 5.6.0116	Depositor
R, R_{free}	0.160 , 0.199 0.167 , 0.204	Depositor DCC
R_{free} test set	5079 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	22.4	Xtriage
Anisotropy	0.054	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.42 , 61.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	11142	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.08% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, LSS

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	A	0.73	2/5308 (0.0%)	0.74	4/7175 (0.1%)
1	B	0.75	2/4992 (0.0%)	0.77	3/6753 (0.0%)
All	All	0.74	4/10300 (0.0%)	0.76	7/13928 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	378	TRP	CD2-CE2	6.39	1.49	1.41
1	A	142	TRP	CD2-CE2	5.52	1.48	1.41
1	B	256	TRP	CD2-CE2	5.24	1.47	1.41
1	A	256	TRP	CD2-CE2	5.10	1.47	1.41

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	224	LEU	CA-CB-CG	-6.90	99.43	115.30
1	A	376	ARG	NE-CZ-NH1	6.70	123.65	120.30
1	A	209	ASP	CB-CG-OD1	5.42	123.18	118.30
1	A	376	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	A	224	LEU	CA-CB-CG	-5.27	103.18	115.30
1	B	133[A]	ASP	CB-CG-OD1	5.06	122.85	118.30
1	B	133[B]	ASP	CB-CG-OD1	5.06	122.85	118.30

There are no chirality outliers.

There are no planarity outliers.

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	A	5164	0	5144	43	0
1	B	4844	0	4799	33	0
2	A	31	0	25	0	0
2	B	31	0	25	0	0
3	A	30	0	40	11	0
3	B	30	0	40	9	0
4	A	524	0	0	9	0
4	B	488	0	0	9	0
All	All	11142	0	10073	82	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 4.

All (82) 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)
1:A:133[B]:ASP:OD1	4:A:2177:HOH:O	1.89	0.91
1:B:106:LEU:HD22	4:B:2127:HOH:O	1.72	0.89
1:A:600:GLU:O	1:A:604:ILE:HD12	1.87	0.75
1:B:186[A]:GLU:HG3	4:B:2231:HOH:O	1.89	0.73
1:A:479:ASN:HD21	1:A:481:LEU:HD12	1.55	0.71
1:B:277:VAL:HG22	3:B:1579:GOL:H11	1.74	0.67
1:A:250:PHE:O	1:A:319:PRO:HD3	1.95	0.67
3:B:1581:GOL:H31	4:B:2122:HOH:O	1.95	0.65
1:B:305:LYS:HG2	1:B:310:ILE:CD1	2.26	0.65
1:A:102:GLN:OE1	3:A:1643:GOL:H11	1.97	0.64
1:B:406:LYS:HA	1:B:448:LYS:HE3	1.82	0.62
1:A:286:MET:HE2	4:A:2333:HOH:O	1.99	0.62
1:B:433:LEU:HD23	1:B:433:LEU:C	2.19	0.61
3:B:1577:GOL:H12	4:B:2348:HOH:O	2.02	0.59
1:A:187:ARG:HD3	4:A:2242:HOH:O	2.03	0.58
3:B:1579:GOL:H31	4:B:2296:HOH:O	2.03	0.58
1:A:102:GLN:OE1	3:A:1643:GOL:C1	2.54	0.55
1:B:186[B]:GLU:HG3	4:B:2214:HOH:O	2.07	0.55
1:B:102:GLN:OE1	3:B:1581:GOL:H11	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:346:LYS:NZ	1:A:350:GLU:OE2	2.40	0.54
1:B:209:ASP:OD1	1:B:243:TYR:OH	2.21	0.54
1:B:396:LYS:NZ	3:B:1577:GOL:O1	2.35	0.54
1:A:607:ALA:O	1:A:613:VAL:HG21	2.07	0.54
1:B:236:GLU:HG3	1:B:241:ILE:HD13	1.89	0.54
3:A:1640:GOL:C3	4:A:2375:HOH:O	2.56	0.53
1:A:313:ARG:HH22	3:A:1641:GOL:H32	1.73	0.52
1:B:133[A]:ASP:OD2	1:B:135:SER:OG	2.27	0.52
3:A:1640:GOL:H32	4:A:2375:HOH:O	2.09	0.52
1:A:582:ILE:HD11	1:A:592:PHE:CE1	2.45	0.52
1:B:266:GLU:H	1:B:266:GLU:CD	2.12	0.52
1:B:305:LYS:HG2	1:B:310:ILE:HD13	1.91	0.51
1:A:186:GLU:HG3	4:A:2223:HOH:O	2.11	0.51
1:B:446:THR:HG22	4:B:2372:HOH:O	2.10	0.51
1:A:147:ILE:HG12	1:A:381:ILE:HD13	1.93	0.51
1:B:106:LEU:CD2	4:B:2127:HOH:O	2.45	0.51
1:A:594:ILE:HD12	1:A:594:ILE:O	2.12	0.50
1:A:503:GLU:OE1	3:A:1640:GOL:H12	2.12	0.50
1:B:236:GLU:CG	1:B:241:ILE:HD13	2.41	0.50
1:B:102:GLN:HG3	3:B:1581:GOL:O1	2.12	0.49
1:B:509:ILE:HG22	1:B:513:LYS:NZ	2.27	0.49
1:A:102:GLN:HG3	3:A:1643:GOL:O1	2.12	0.49
1:A:467:ILE:HB	1:A:522:TYR:CE1	2.47	0.49
1:B:467:ILE:HB	1:B:522:TYR:CE1	2.47	0.49
1:A:13:GLU:HB2	4:A:2030:HOH:O	2.12	0.49
1:A:286:MET:CE	4:A:2333:HOH:O	2.58	0.49
1:B:495:ILE:HD13	1:B:566:PRO:HB2	1.96	0.48
1:A:581:ALA:HA	1:A:591:THR:HG22	1.96	0.48
1:B:509:ILE:HG22	1:B:513:LYS:HZ3	1.78	0.47
1:B:509:ILE:CG2	1:B:513:LYS:NZ	2.78	0.47
1:A:503:GLU:OE1	3:A:1640:GOL:C1	2.63	0.47
3:A:1643:GOL:H31	4:A:2136:HOH:O	2.14	0.47
1:A:584:VAL:O	1:A:584:VAL:HG12	2.14	0.47
1:A:603:VAL:HG12	1:A:603:VAL:O	2.15	0.47
1:A:633:LEU:HD12	1:A:635:PHE:CE2	2.50	0.46
3:B:1579:GOL:C3	4:B:2296:HOH:O	2.63	0.46
1:B:15:GLU:HG2	1:B:546:HIS:CG	2.52	0.45
1:A:634:ASN:HD21	1:A:636:ILE:HD11	1.81	0.45
1:A:3:PRO:HD3	1:A:428:PHE:CE1	2.52	0.45
1:A:15:GLU:HG2	1:A:546:HIS:CG	2.52	0.44
1:A:585:ASN:HA	1:A:636:ILE:HD13	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:174:GLU:HA	1:B:186[B]:GLU:HG2	2.00	0.43
1:A:433:LEU:HD23	1:A:433:LEU:C	2.39	0.42
1:A:531:LYS:N	1:A:532:PRO:HD2	2.35	0.42
1:B:404:LEU:HD23	1:B:410:LYS:HA	2.02	0.42
1:A:503:GLU:O	3:A:1640:GOL:O2	2.37	0.42
1:A:509:ILE:HG22	1:A:513:LYS:NZ	2.35	0.42
1:A:602:ARG:NH2	1:A:603:VAL:HG22	2.34	0.42
1:A:88:LEU:HD12	3:A:1642:GOL:H31	2.01	0.42
1:B:147:ILE:HG12	1:B:381:ILE:HD13	2.02	0.42
1:B:56:HIS:N	1:B:57:PRO:HD2	2.35	0.41
1:A:590:GLU:HG2	1:A:610:LEU:HD22	2.02	0.41
1:A:582:ILE:HD13	1:A:607:ALA:HB1	2.03	0.41
1:B:158:VAL:HG23	1:B:160:VAL:CG1	2.50	0.41
1:B:102:GLN:OE1	3:B:1581:GOL:C1	2.69	0.41
1:A:634:ASN:ND2	1:A:636:ILE:HD11	2.35	0.41
1:B:531:LYS:N	1:B:532:PRO:CD	2.84	0.41
1:B:156:ARG:HG3	1:B:158:VAL:HG13	2.03	0.41
1:A:590:GLU:CG	1:A:610:LEU:HD22	2.51	0.40
1:A:633:LEU:CD1	1:A:635:PHE:CE2	3.04	0.40
1:A:53:HIS:HA	1:A:421:PRO:HD3	2.02	0.40
1:A:26:LYS:NZ	1:B:126[A]:GLU:OE1	2.48	0.40
1:A:610:LEU:HA	1:A:611:PRO:HD3	2.01	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	A	620/637 (97%)	604 (97%)	14 (2%)	2 (0%)	41	32
1	B	581/637 (91%)	569 (98%)	11 (2%)	1 (0%)	47	39
All	All	1201/1274 (94%)	1173 (98%)	25 (2%)	3 (0%)	41	39

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	575	LEU
1	B	80	PRO
1	A	80	PRO

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	A	564/580 (97%)	556 (99%)	8 (1%)	67	64
1	B	530/580 (91%)	511 (96%)	19 (4%)	35	28
All	All	1094/1160 (94%)	1067 (98%)	27 (2%)	49	41

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	TYR
1	A	44	PHE
1	A	86	PHE
1	A	224	LEU
1	A	447	LYS
1	A	570	ASN
1	A	576	THR
1	A	585	ASN
1	B	4	ARG
1	B	16	LYS
1	B	37	LYS
1	B	39	TYR
1	B	44	PHE
1	B	80	PRO
1	B	86	PHE
1	B	186[A]	GLU
1	B	186[B]	GLU
1	B	213	GLU
1	B	224	LEU
1	B	236	GLU

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Mol	Chain	Res	Type
1	B	241	ILE
1	B	246	GLN
1	B	266	GLU
1	B	274	ASP
1	B	447	LYS
1	B	477	LYS
1	B	480	SER

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

Mol	Chain	Res	Type
1	A	479	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

12 ligands 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	$\#\|Z\| > 2$
3	GOL	B	1581	-	5,5,5	0.48	0	5,5,5	0.83	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	GOL	B	1579	-	5,5,5	0.43	0	5,5,5	1.41	0
3	GOL	A	1640	-	5,5,5	0.57	0	5,5,5	1.04	0
3	GOL	B	1577	-	5,5,5	0.27	0	5,5,5	0.43	0
3	GOL	B	1580	-	5,5,5	0.43	0	5,5,5	0.36	0
3	GOL	A	1643	-	5,5,5	0.37	0	5,5,5	0.77	0
2	LSS	B	1576	-	30,33,33	1.16	4 (13%)	33,49,49	1.43	5 (15%)
3	GOL	A	1639	-	5,5,5	0.23	0	5,5,5	0.52	0
2	LSS	A	1638	-	30,33,33	1.40	4 (13%)	33,49,49	1.65	5 (15%)
3	GOL	B	1578	-	5,5,5	0.35	0	5,5,5	0.75	0
3	GOL	A	1642	-	5,5,5	0.69	0	5,5,5	0.68	0
3	GOL	A	1641	-	5,5,5	0.49	0	5,5,5	0.87	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
3	GOL	B	1581	-	-	2/4/4/4	-
3	GOL	B	1579	-	-	2/4/4/4	-
3	GOL	A	1640	-	-	2/4/4/4	-
3	GOL	B	1577	-	-	4/4/4/4	-
3	GOL	B	1580	-	-	2/4/4/4	-
3	GOL	A	1643	-	-	2/4/4/4	-
2	LSS	B	1576	-	-	0/18/39/39	0/3/3/3
3	GOL	A	1639	-	-	2/4/4/4	-
2	LSS	A	1638	-	-	1/18/39/39	0/3/3/3
3	GOL	B	1578	-	-	2/4/4/4	-
3	GOL	A	1642	-	-	2/4/4/4	-
3	GOL	A	1641	-	-	1/4/4/4	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1638	LSS	O2A-S1	3.56	1.45	1.42
2	A	1638	LSS	S1-N2	-3.43	1.53	1.59
2	A	1638	LSS	O1A-S1	3.16	1.45	1.42
2	B	1576	LSS	O5-S1	-2.77	1.53	1.59
2	B	1576	LSS	O2A-S1	2.75	1.44	1.42
2	A	1638	LSS	O5-S1	-2.63	1.54	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1576	LSS	S1-N2	-2.41	1.55	1.59
2	B	1576	LSS	C2-N3	2.19	1.35	1.32

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1638	LSS	O2A-S1-O1A	-6.11	111.23	120.76
2	B	1576	LSS	O2A-S1-O1A	-3.91	114.67	120.76
2	A	1638	LSS	N3-C2-N1	-3.61	123.04	128.68
2	B	1576	LSS	N3-C2-N1	-3.02	123.96	128.68
2	A	1638	LSS	C1-N2-S1	-2.93	119.86	124.61
2	B	1576	LSS	O4-C21-C22	-2.90	102.68	106.93
2	A	1638	LSS	O5-S1-N2	2.75	113.28	105.60
2	B	1576	LSS	O5-S1-N2	2.68	113.08	105.60
2	B	1576	LSS	C9-CA-N4	2.23	115.28	110.32
2	A	1638	LSS	C21-N9-C4	-2.02	123.09	126.64

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1579	GOL	C1-C2-C3-O3
3	B	1577	GOL	O1-C1-C2-C3
3	B	1577	GOL	C1-C2-C3-O3
3	A	1639	GOL	O1-C1-C2-O2
3	A	1639	GOL	O1-C1-C2-C3
3	B	1578	GOL	O1-C1-C2-C3
3	A	1642	GOL	O1-C1-C2-O2
3	B	1581	GOL	C1-C2-C3-O3
3	B	1580	GOL	O1-C1-C2-C3
3	A	1643	GOL	C1-C2-C3-O3
3	A	1642	GOL	O1-C1-C2-C3
3	B	1577	GOL	O1-C1-C2-O2
3	B	1580	GOL	O1-C1-C2-O2
3	A	1643	GOL	O2-C2-C3-O3
3	B	1581	GOL	O2-C2-C3-O3
3	B	1579	GOL	O2-C2-C3-O3
3	B	1577	GOL	O2-C2-C3-O3
3	B	1578	GOL	O1-C1-C2-O2
3	A	1640	GOL	O2-C2-C3-O3
3	A	1640	GOL	C1-C2-C3-O3
2	A	1638	LSS	N2-C1-CA-N4

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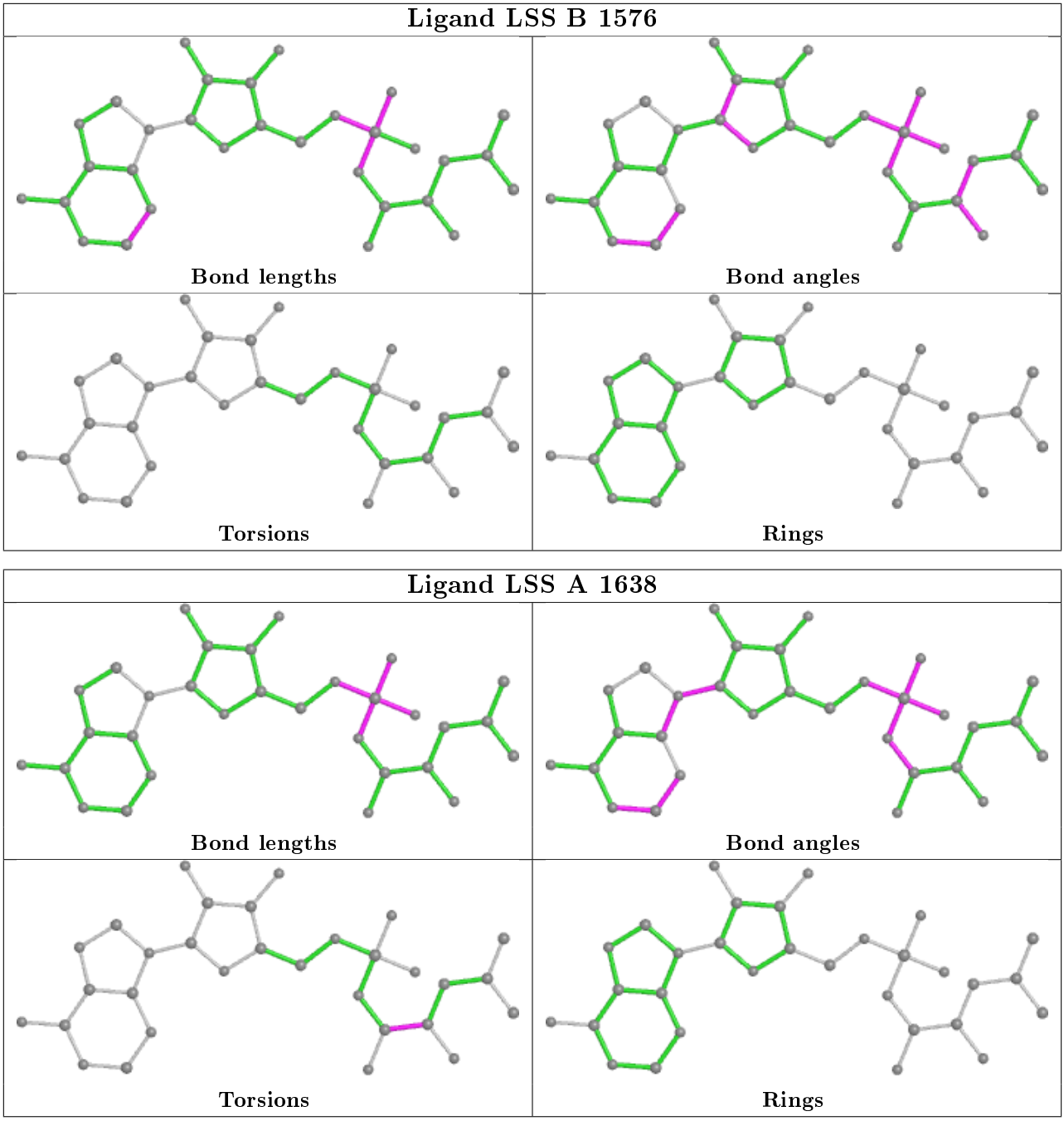
Mol	Chain	Res	Type	Atoms
3	A	1641	GOL	C1-C2-C3-O3

There are no ring outliers.

7 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1581	GOL	4	0
3	B	1579	GOL	3	0
3	A	1640	GOL	5	0
3	B	1577	GOL	2	0
3	A	1643	GOL	4	0
3	A	1642	GOL	1	0
3	A	1641	GOL	1	0

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



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	621/637 (97%)	-0.21	42 (6%) 17 18	12, 21, 89, 150	0
1	B	575/637 (90%)	-0.58	8 (1%) 75 76	11, 20, 44, 82	0
All	All	1196/1274 (93%)	-0.39	50 (4%) 36 38	11, 21, 53, 150	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	595	GLU	12.2
1	A	602	ARG	10.6
1	A	637	ILE	10.6
1	A	598	TRP	9.7
1	A	596	ASN	8.6
1	A	610	LEU	8.5
1	A	636	ILE	8.0
1	A	601	LYS	7.6
1	A	611	PRO	7.5
1	A	576	THR	7.2
1	A	603	VAL	7.1
1	A	609	LYS	6.5
1	A	600	GLU	6.1
1	A	597	ASP	6.1
1	B	237	ILE	5.6
1	A	575	LEU	5.4
1	A	599	ASP	5.4
1	A	605	GLU	5.3
1	A	612	ASN	5.3
1	B	238	ASP	5.0
1	A	613	VAL	4.6
1	B	575	LEU	4.4
1	A	635	PHE	4.4
1	A	604	ILE	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	581	ALA	4.3
1	A	584	VAL	4.2
1	A	633	LEU	4.2
1	A	608	LYS	4.0
1	A	632	ILE	3.9
1	A	631	LYS	3.8
1	B	308	ASN	3.6
1	A	582	ILE	3.5
1	A	607	ALA	3.5
1	A	594	ILE	3.2
1	A	585	ASN	3.1
1	A	634	ASN	2.8
1	A	588	LEU	2.8
1	A	406	LYS	2.8
1	B	481	LEU	2.7
1	B	240	LYS	2.6
1	A	589	ARG	2.6
1	A	630	LYS	2.5
1	A	591	THR	2.5
1	B	406	LYS	2.3
1	A	606	GLU	2.2
1	A	586	GLY	2.2
1	B	574	LEU	2.1
1	A	579	ILE	2.0
1	A	592	PHE	2.0
1	A	266	GLU	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

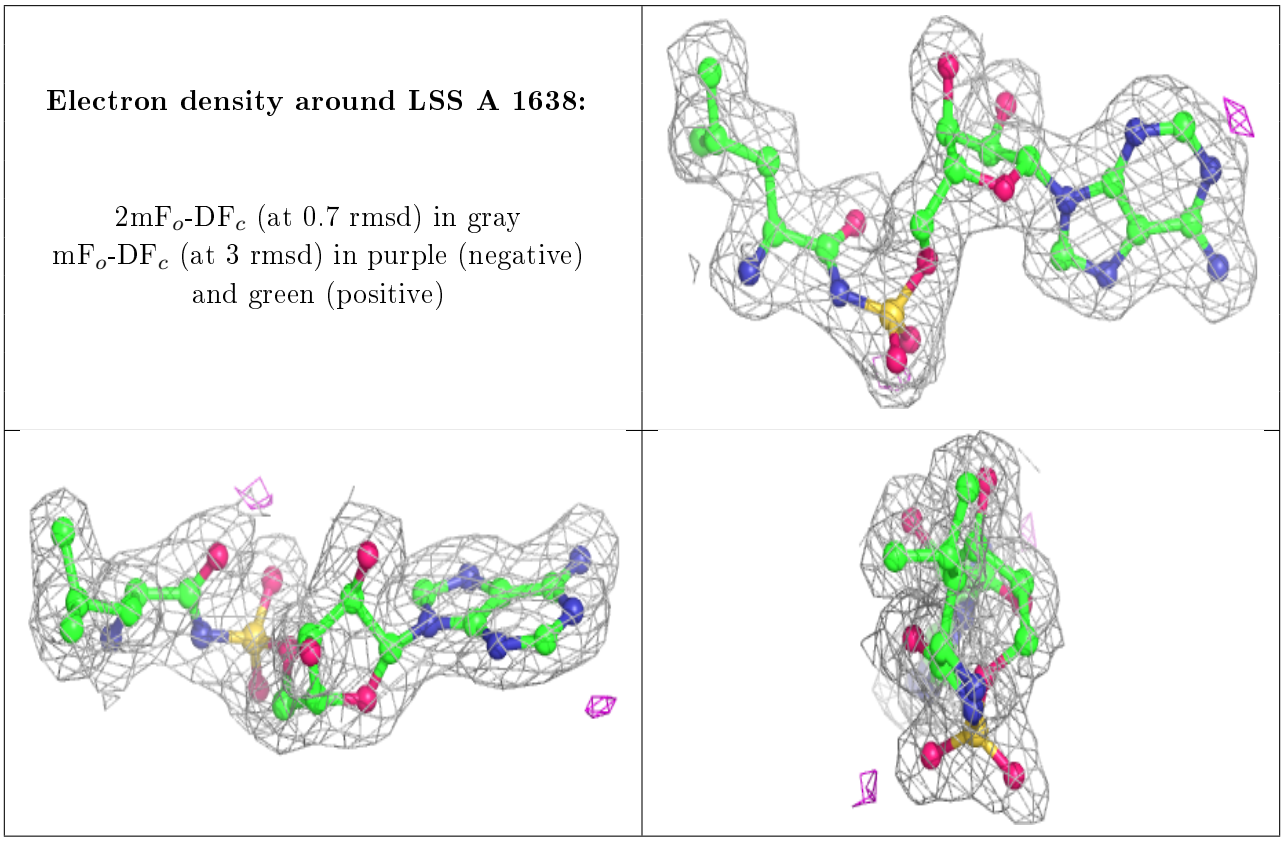
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
3	GOL	A	1639	6/6	0.77	0.15	33,38,39,43	0
3	GOL	B	1578	6/6	0.77	0.15	34,39,39,43	0
3	GOL	A	1641	6/6	0.80	0.23	31,40,42,47	0
3	GOL	B	1581	6/6	0.84	0.16	31,37,43,46	0
3	GOL	A	1640	6/6	0.87	0.11	35,41,44,47	0
3	GOL	A	1643	6/6	0.88	0.17	35,40,44,45	0
3	GOL	B	1579	6/6	0.89	0.16	28,33,34,38	0
3	GOL	A	1642	6/6	0.91	0.12	23,31,32,32	0
3	GOL	B	1577	6/6	0.93	0.09	43,45,46,47	0
3	GOL	B	1580	6/6	0.95	0.08	20,26,27,28	0
2	LSS	A	1638	31/31	0.98	0.07	10,13,14,15	0
2	LSS	B	1576	31/31	0.99	0.07	9,13,14,14	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.

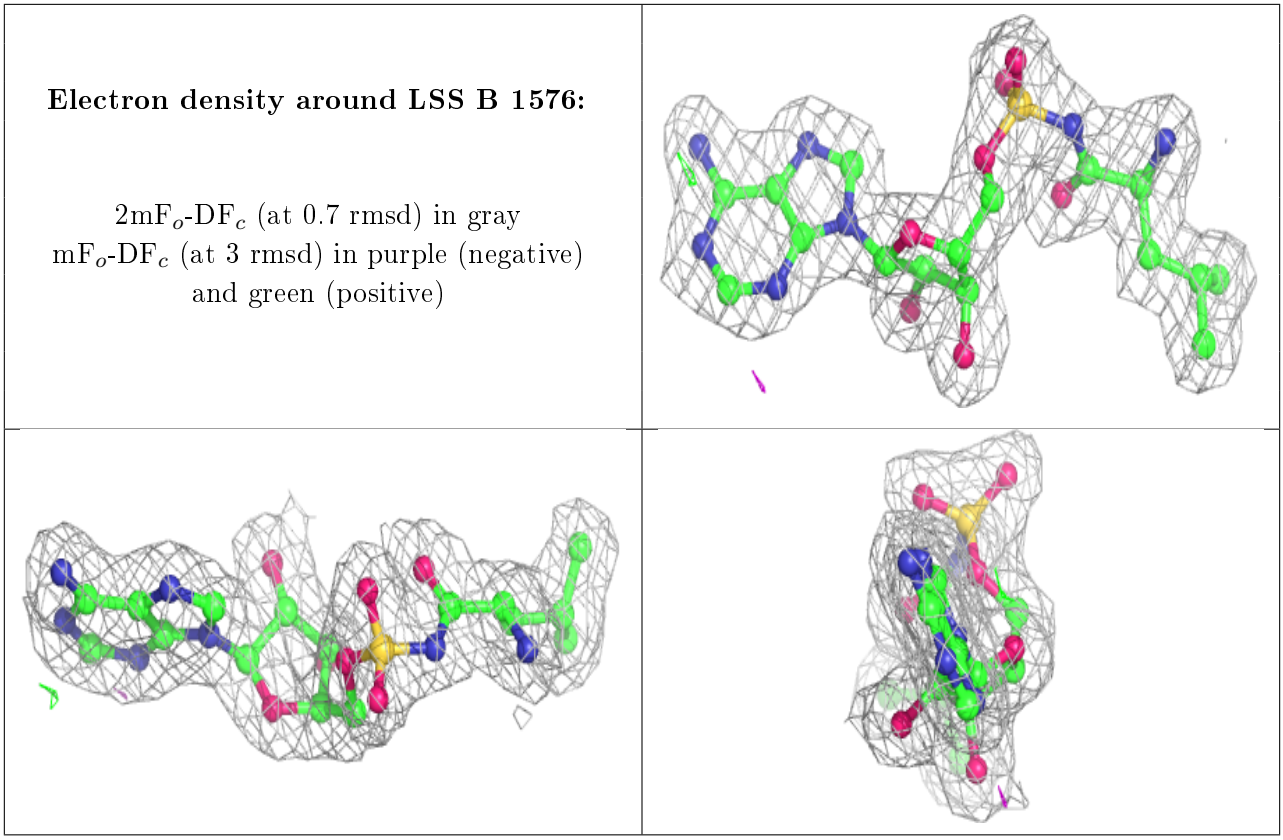
Electron density around LSS A 1638:

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



Electron density around LSS B 1576:

$2mF_o$-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.