



# Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 03:52 am BST

PDB ID : 5AH5  
Title : Crystal structure of the ternary complex of Agrobacterium radiobacter K84 agnB2 LeuRS-tRNA-LeuAMS  
Authors : Palencia, A.; Chopra, S.; Virus, C.; Schulwitz, S.; Temple, B.R.; Cusack, S.; Reader, J.S.  
Deposited on : 2015-02-05  
Resolution : 2.10 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](mailto: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 following versions of software and data (see [references ⓘ](#)) 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

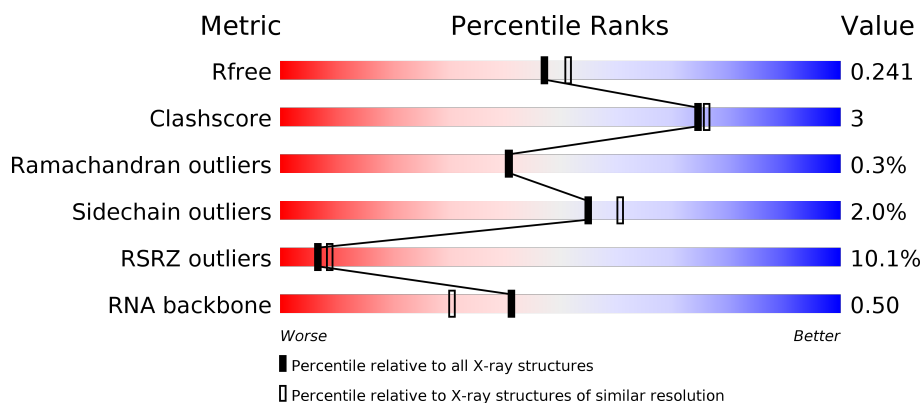
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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))
$R_{free}$	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)
RNA backbone	3102	1000 (2.54-1.66)

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  $\geq 3$ , 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	A	822	<div> <div>11%</div> <div> <div></div> <div>86%</div> <div>9%</div> <div>• •</div> </div> </div>
1	B	822	<div> <div>10%</div> <div> <div></div> <div>82%</div> <div>10%</div> <div>• 6%</div> </div> </div>
2	C	84	<div> <div>0%</div> <div> <div></div> <div>69%</div> <div>20%</div> <div>6%</div> <div>5%</div> </div> </div>
2	D	84	<div> <div>0%</div> <div> <div></div> <div>65%</div> <div>27%</div> <div>• •</div> </div> </div>

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 16819 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 LEUCINE-TRNA LIGASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	789	Total	C	N	O	S	0	5	0
			6288	3990	1093	1175	30			
1	B	771	Total	C	N	O	S	0	4	0
			6146	3899	1067	1150	30			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	815	LEU	-	expression tag	UNP B9JQP8
A	816	GLU	-	expression tag	UNP B9JQP8
A	817	HIS	-	expression tag	UNP B9JQP8
A	818	HIS	-	expression tag	UNP B9JQP8
A	819	HIS	-	expression tag	UNP B9JQP8
A	820	HIS	-	expression tag	UNP B9JQP8
A	821	HIS	-	expression tag	UNP B9JQP8
A	822	HIS	-	expression tag	UNP B9JQP8
B	815	LEU	-	expression tag	UNP B9JQP8
B	816	GLU	-	expression tag	UNP B9JQP8
B	817	HIS	-	expression tag	UNP B9JQP8
B	818	HIS	-	expression tag	UNP B9JQP8
B	819	HIS	-	expression tag	UNP B9JQP8
B	820	HIS	-	expression tag	UNP B9JQP8
B	821	HIS	-	expression tag	UNP B9JQP8
B	822	HIS	-	expression tag	UNP B9JQP8

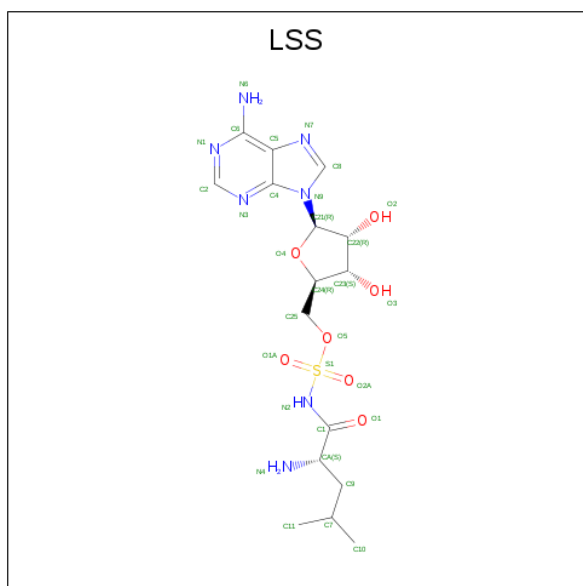
- Molecule 2 is a RNA chain called TRNA-LEU TAA ISOACCEPTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	80	Total	C	N	O	P	0	0	0
			1702	759	304	559	80			
2	D	81	Total	C	N	O	P	0	0	0
			1721	768	305	567	81			

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Zn	0	0
			1	1		
3	A	1	Total	Zn	0	0
			1	1		

- Molecule 4 is 5'-O-(L-leucylsulfamoyl)adenosine (three-letter code: LSS) (formula: C<sub>16</sub>H<sub>25</sub>N<sub>7</sub>O<sub>7</sub>S).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	1	Total	Mn	0	0
			1	1		
6	C	1	Total	Mn	0	0
			1	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	322	Total	O	0	0
			322	322		
7	B	384	Total	O	0	0
			384	384		

*Continued on next page...*

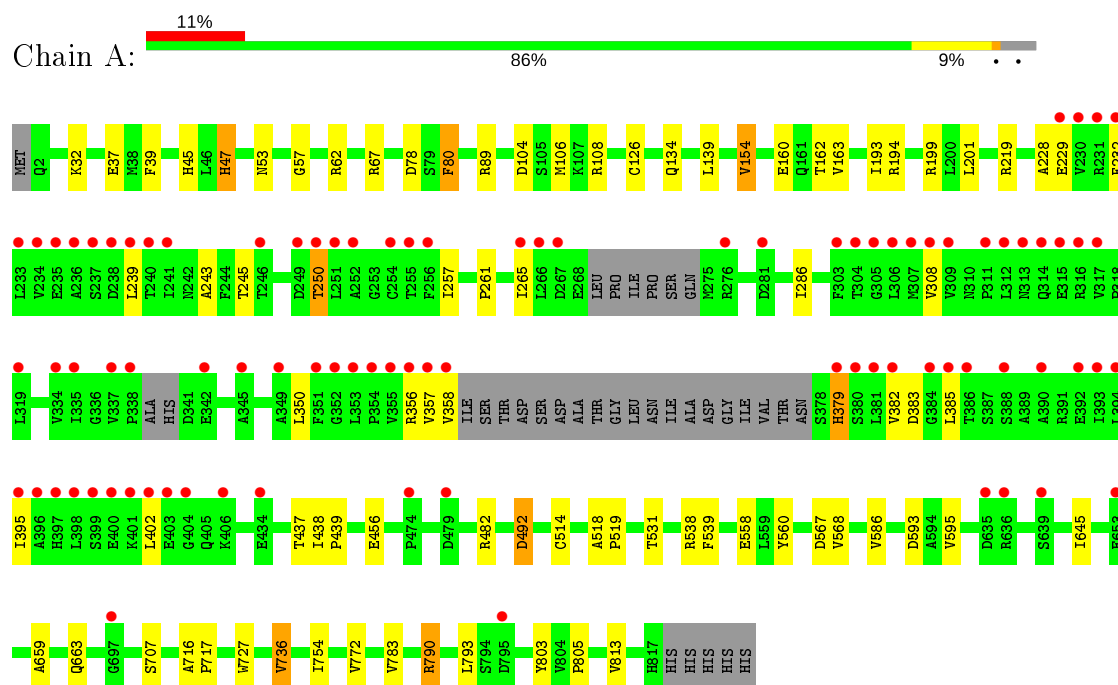
*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	C	89	Total	O	0	0
			89	89		
7	D	76	Total	O	0	0
			76	76		

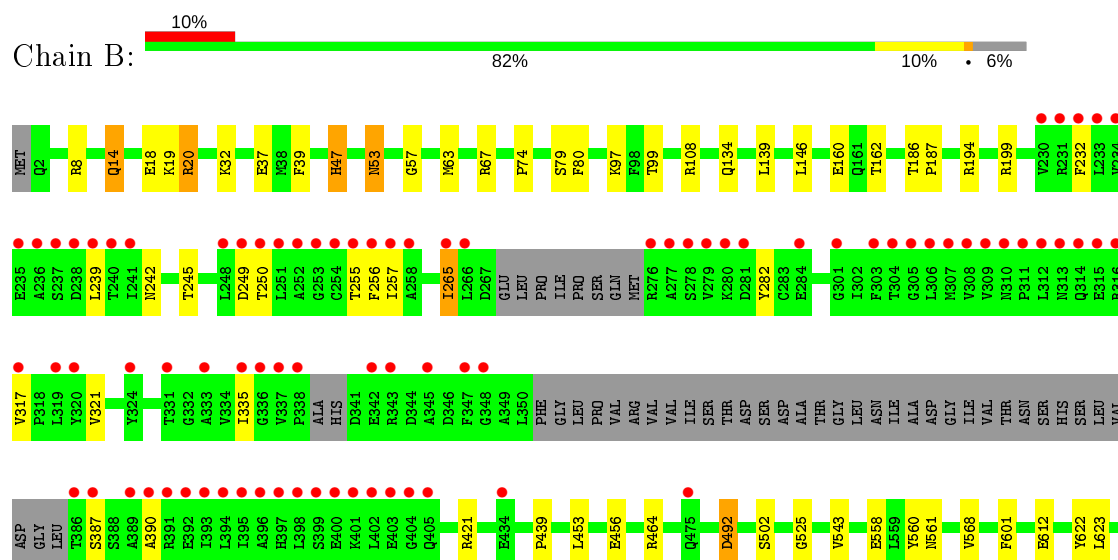
### 3 Residue-property plots [i](#)

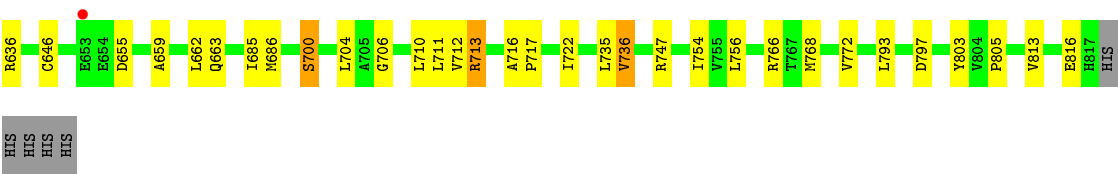
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: LEUCINE-TRNA LIGASE

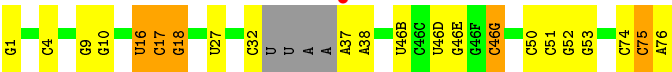


#### • Molecule 1: LEUCINE-TRNA LIGASE





● Molecule 2: TRNA-LEU TAA ISOACCEPTOR



● Molecule 2: TRNA-LEU TAA ISOACCEPTOR





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	169.91Å 50.32Å 170.52Å 90.00° 93.48° 90.00°	Depositor
Resolution (Å)	48.58 – 2.10 48.54 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.5 (48.58-2.10) 99.5 (48.54-2.10)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.92 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0131	Depositor
R, $R_{free}$	0.194 , 0.237 0.200 , 0.241	Depositor DCC
$R_{free}$ test set	8487 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	37.7	Xtriage
Anisotropy	0.085	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 43.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.014 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	16819	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.68% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MN, SO4, 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	0.83	0/6447	0.93	17/8760 (0.2%)
1	B	0.90	3/6299 (0.0%)	0.94	22/8559 (0.3%)
2	C	0.67	1/1899 (0.1%)	1.00	5/2953 (0.2%)
2	D	0.69	3/1920 (0.2%)	0.97	6/2985 (0.2%)
All	All	0.83	7/16565 (0.0%)	0.95	50/23257 (0.2%)

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	A	0	1
1	B	0	1
All	All	0	2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1	G	OP3-P	-10.10	1.49	1.61
2	C	1	G	OP3-P	-9.70	1.49	1.61
2	D	22	A	O3'-P	-6.16	1.53	1.61
2	D	23	C	O3'-P	-5.86	1.54	1.61
1	B	421	ARG	CD-NE	-5.30	1.37	1.46
1	B	816	GLU	CG-CD	5.29	1.59	1.51
1	B	502	SER	CB-OG	-5.18	1.35	1.42

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	194	ARG	NE-CZ-NH2	-10.88	114.86	120.30
1	B	421	ARG	NE-CZ-NH2	-10.76	114.92	120.30
1	B	713	ARG	NE-CZ-NH1	9.51	125.05	120.30
1	B	20	ARG	NE-CZ-NH1	9.20	124.90	120.30
2	C	4	C	O5'-P-OP2	-8.55	98.00	105.70
1	B	713	ARG	NE-CZ-NH2	-8.37	116.12	120.30
1	B	421	ARG	NE-CZ-NH1	8.28	124.44	120.30
1	B	67	ARG	NE-CZ-NH1	8.19	124.39	120.30
1	A	199	ARG	NE-CZ-NH2	-7.91	116.35	120.30
1	A	492	ASP	CB-CG-OD1	7.88	125.39	118.30
1	B	20	ARG	NE-CZ-NH2	-7.64	116.48	120.30
1	B	67	ARG	NE-CZ-NH2	-7.50	116.55	120.30
1	A	194	ARG	NE-CZ-NH1	7.34	123.97	120.30
1	B	199	ARG	NE-CZ-NH2	-7.15	116.72	120.30
2	D	21	A	O5'-P-OP2	-7.02	99.38	105.70
2	D	70	G	O5'-P-OP2	-7.01	99.39	105.70
2	C	16	U	O5'-P-OP2	6.90	118.98	110.70
1	B	63	MET	CG-SD-CE	6.62	110.79	100.20
2	D	46(E)	G	C2'-C3'-O3'	6.27	123.73	113.70
1	A	108	ARG	NE-CZ-NH1	6.24	123.42	120.30
1	B	736	VAL	CB-CA-C	-6.23	99.56	111.40
1	A	593	ASP	CB-CG-OD1	6.15	123.83	118.30
1	B	464	ARG	NE-CZ-NH2	-6.12	117.24	120.30
1	A	106	MET	CG-SD-CE	5.88	109.60	100.20
2	C	75	C	C2'-C3'-O3'	5.78	122.95	113.70
1	A	104	ASP	CB-CG-OD1	5.75	123.48	118.30
2	C	27	U	O5'-P-OP2	-5.74	100.53	105.70
1	A	78	ASP	CB-CG-OD1	5.67	123.40	118.30
1	B	766	ARG	NE-CZ-NH2	-5.65	117.47	120.30
1	A	194	ARG	CG-CD-NE	-5.61	100.02	111.80
2	D	62	C	O5'-P-OP2	-5.57	100.69	105.70
1	B	108	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	B	816	GLU	OE1-CD-OE2	-5.53	116.67	123.30
1	A	62	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	B	194	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	A	199	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	B	199	ARG	NE-CZ-NH1	5.33	122.96	120.30
1	B	797	ASP	CB-CG-OD1	5.31	123.08	118.30
1	B	747	ARG	NE-CZ-NH1	5.23	122.91	120.30
1	A	790	ARG	NE-CZ-NH2	-5.21	117.69	120.30
1	B	492	ASP	CB-CG-OD1	5.20	122.98	118.30
1	A	482	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	A	67	ARG	NE-CZ-NH1	5.13	122.87	120.30

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	783	VAL	CG1-CB-CG2	-5.12	102.70	110.90
2	C	50	C	O5'-P-OP2	-5.11	101.11	105.70
2	D	60	U	O5'-P-OP2	-5.10	101.11	105.70
2	D	75	C	C2'-C3'-O3'	5.08	121.83	113.70
1	B	8	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	A	538	ARG	NE-CZ-NH2	-5.03	117.79	120.30
1	B	766	ARG	NE-CZ-NH1	5.01	122.81	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	531	THR	Peptide
1	B	265	ILE	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	A	6288	0	6179	39	0
1	B	6146	0	6030	47	0
2	C	1702	0	868	6	0
2	D	1721	0	876	4	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	31	0	25	1	0
4	B	31	0	25	0	0
5	A	5	0	0	0	0
5	B	10	0	0	0	0
5	C	5	0	0	0	0
5	D	5	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
7	A	322	0	0	5	0
7	B	384	0	0	6	0
7	C	89	0	0	1	0
7	D	76	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	16819	0	14003	95	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 (95) 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:B:646:CYS:SG	7:B:2316:HOH:O	2.26	0.93
1:A:47[A]:HIS:HB2	7:A:2045:HOH:O	1.85	0.76
1:B:713:ARG:HD2	7:B:2343:HOH:O	1.87	0.75
1:A:257:ILE:HD12	1:A:308:VAL:HG11	1.73	0.70
1:B:754:ILE:HD12	1:B:772:VAL:HG22	1.74	0.69
1:B:232:PHE:CE2	1:B:257:ILE:HD11	2.28	0.68
2:D:7:A:O2'	2:D:49:G:OP2	2.11	0.68
2:C:46(G):C:H6	2:C:46(G):C:H5"	1.60	0.65
1:A:727:TRP:CD2	1:A:736:VAL:HG13	2.31	0.65
1:A:793:LEU:HD22	1:A:813:VAL:HG11	1.77	0.65
1:B:662:LEU:HD23	1:B:710:LEU:HD23	1.79	0.64
2:C:53:G:O6	7:C:2066:HOH:O	2.13	0.63
1:B:97[B]:LYS:NZ	7:B:2099:HOH:O	2.26	0.63
1:A:437:THR:O	1:A:438:ILE:HD12	2.01	0.61
1:B:756:LEU:HD23	1:B:768:MET:CE	2.31	0.60
1:B:97[B]:LYS:CE	7:B:2099:HOH:O	2.49	0.59
1:B:793:LEU:HD22	1:B:813:VAL:HG11	1.84	0.59
1:A:154:VAL:HG13	1:A:163:VAL:HG13	1.86	0.57
1:B:601:PHE:CZ	1:B:686:MET:HE1	2.39	0.57
1:A:89[B]:ARG:NH2	7:A:2074:HOH:O	2.34	0.55
1:A:382:VAL:HG12	1:A:385:LEU:HD12	1.90	0.54
1:B:793:LEU:CD2	1:B:813:VAL:HG11	2.38	0.54
1:B:239:LEU:HD23	1:B:265:ILE:HD11	1.89	0.53
1:B:20:ARG:NH2	7:B:2027:HOH:O	2.37	0.52
1:A:250:THR:HG23	1:A:358:VAL:HG21	1.91	0.52
1:B:662:LEU:CD2	1:B:710:LEU:HD23	2.39	0.52
1:A:261:PRO:HG2	1:A:286:ILE:HG21	1.91	0.52
1:A:201:LEU:HD11	1:A:219:ARG:HG3	1.93	0.51
1:B:558:GLU:HG2	1:B:560:TYR:CE2	2.45	0.51
1:B:601:PHE:CE1	1:B:686:MET:HE1	2.46	0.51
1:B:686:MET:HE1	2:D:23:C:O2'	2.10	0.51
1:B:601:PHE:CE1	1:B:686:MET:CE	2.94	0.51
1:B:37:GLU:OE2	1:B:57:GLY:HA3	2.11	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:47[A]:HIS:HB2	7:B:2065:HOH:O	2.11	0.50
2:C:46(G):C:C5'	2:C:46(G):C:H6	2.22	0.50
1:B:160:GLU:HB3	1:B:162:THR:HG22	1.94	0.50
1:A:645:ILE:HD11	1:A:707:SER:OG	2.11	0.50
1:A:229:GLU:HA	1:A:243:ALA:O	2.13	0.49
1:B:803:TYR:CZ	1:B:805:PRO:HA	2.48	0.48
1:B:636:ARG:HD2	1:B:704:LEU:HD23	1.96	0.48
1:A:803:TYR:CZ	1:A:805:PRO:HA	2.49	0.48
1:B:14:GLN:NE2	1:B:18:GLU:OE1	2.46	0.48
1:B:387:SER:O	1:B:390:ALA:HB3	2.14	0.47
1:B:134:GLN:OE1	1:B:492:ASP:HA	2.14	0.47
1:B:53:ASN:C	1:B:53:ASN:HD22	2.17	0.47
1:A:245:THR:OG1	7:A:2158:HOH:O	2.20	0.47
2:C:17:C:C2'	2:C:18:G:OP1	2.63	0.47
1:B:256:PHE:HA	1:B:317:VAL:HG12	1.96	0.47
1:A:45:HIS:CE1	7:A:2042:HOH:O	2.68	0.47
1:B:622:TYR:CE1	1:B:686:MET:HG2	2.50	0.46
1:A:793:LEU:CD2	1:A:813:VAL:HG11	2.43	0.46
2:C:46(G):C:C5'	2:C:46(G):C:C6	2.99	0.46
1:A:37:GLU:OE2	1:A:57:GLY:HA3	2.16	0.45
1:B:249:ASP:OD1	1:B:250:THR:HG23	2.16	0.45
1:B:659:ALA:O	1:B:663:GLN:HG2	2.16	0.45
1:A:193:ILE:HG13	1:A:539:PHE:CG	2.51	0.45
1:A:239:LEU:CD2	1:A:265:ILE:HD11	2.46	0.45
1:A:160:GLU:HB3	1:A:162:THR:HG22	1.99	0.45
1:A:139:LEU:HD22	1:A:439:PRO:HB3	1.98	0.45
1:A:357:VAL:O	1:A:379:HIS:NE2	2.46	0.45
2:D:8:U:H5'	2:D:49:G:OP2	2.16	0.45
1:B:186:THR:HG22	1:B:187:PRO:HD2	1.99	0.44
1:B:685:ILE:HG23	1:B:711:LEU:CD1	2.48	0.44
1:B:623:LEU:HB3	1:B:722:ILE:HD13	2.00	0.44
1:A:518:ALA:HB1	1:A:519:PRO:HA	2.00	0.43
1:A:790:ARG:NH1	7:A:2312:HOH:O	2.43	0.43
1:B:655:ASP:OD2	1:B:700:SER:OG	2.35	0.43
1:A:80:PHE:CE2	1:A:126:CYS:HA	2.54	0.43
1:B:146:LEU:HD13	1:B:543:VAL:HG13	1.99	0.42
1:B:525:GLY:O	1:B:561:ASN:HA	2.19	0.42
1:B:139:LEU:HD22	1:B:439:PRO:HB3	2.01	0.42
1:B:282:TYR:HE2	1:B:321:VAL:HG12	1.83	0.42
1:A:659:ALA:O	1:A:663:GLN:HG2	2.19	0.42
1:B:706:GLY:O	1:B:710:LEU:HB2	2.19	0.42

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:PHE:HB3	1:A:308:VAL:HG22	2.01	0.42
2:D:13:A:O2'	2:D:14:A:H5'	2.18	0.42
1:A:716:ALA:N	1:A:717:PRO:CD	2.83	0.42
1:B:716:ALA:HB3	1:B:717:PRO:HD3	2.02	0.42
1:A:567:ASP:C	1:A:567:ASP:OD1	2.58	0.42
1:A:201:LEU:HD11	1:A:219:ARG:CG	2.50	0.41
1:A:53:ASN:ND2	4:A:1818:LSS:O3	2.53	0.41
1:B:79:SER:HB2	1:B:99:THR:HG21	2.01	0.41
1:A:754:ILE:HG13	1:A:772:VAL:HG22	2.02	0.41
1:A:586:VAL:HG12	1:A:595:VAL:HG22	2.02	0.41
1:B:568:VAL:HG12	1:B:612:GLU:HG2	2.00	0.41
1:A:134:GLN:OE1	1:A:492:ASP:HA	2.21	0.41
1:A:228:ALA:HB1	1:A:395:ILE:HD13	2.02	0.41
1:A:558:GLU:HG2	1:A:560:TYR:CE2	2.55	0.41
1:B:754:ILE:CD1	1:B:772:VAL:HG22	2.47	0.41
1:A:586:VAL:HG12	1:A:595:VAL:CG2	2.51	0.41
1:B:685:ILE:HG23	1:B:711:LEU:HD11	2.03	0.41
1:B:19:LYS:HG3	1:B:735:LEU:HD12	2.02	0.41
2:C:51:C:H2'	2:C:52:G:O4'	2.21	0.40
1:A:727:TRP:CE3	1:A:736:VAL:HG13	2.57	0.40
1:B:601:PHE:CZ	1:B:686:MET:CE	3.03	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	786/822 (96%)	751 (96%)	33 (4%)	2 (0%)	41	41
1	B	767/822 (93%)	735 (96%)	30 (4%)	2 (0%)	41	41
All	All	1553/1644 (94%)	1486 (96%)	63 (4%)	4 (0%)	41	41

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	402	LEU
1	A	356	ARG
1	B	74	PRO
1	B	335	ILE

### 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	684/707 (97%)	670 (98%)	14 (2%)	55	60
1	B	667/707 (94%)	652 (98%)	15 (2%)	52	57
All	All	1351/1414 (96%)	1322 (98%)	29 (2%)	55	59

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	LYS
1	A	39	PHE
1	A	47[A]	HIS
1	A	47[B]	HIS
1	A	80	PHE
1	A	154	VAL
1	A	250	THR
1	A	350	LEU
1	A	379	HIS
1	A	383	ASP
1	A	456	GLU
1	A	514	CYS
1	A	568	VAL
1	A	736	VAL
1	B	14	GLN
1	B	32	LYS
1	B	39	PHE
1	B	47[A]	HIS
1	B	47[B]	HIS

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	B	53	ASN
1	B	80	PHE
1	B	242	ASN
1	B	245	THR
1	B	255	THR
1	B	453	LEU
1	B	456	GLU
1	B	700	SER
1	B	712	VAL
1	B	736	VAL

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	53	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	C	79/84 (94%)	12 (15%)	7 (8%)
2	D	79/84 (94%)	12 (15%)	3 (3%)
All	All	158/168 (94%)	24 (15%)	10 (6%)

All (24) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	C	10	G
2	C	16	U
2	C	17	C
2	C	18	G
2	C	32	C
2	C	38	A
2	C	46(D)	U
2	C	46(E)	G
2	C	46(G)	C
2	C	74	C
2	C	75	C
2	C	76	A
2	D	10	G
2	D	16	U

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	D	17	C
2	D	18	G
2	D	32	C
2	D	33	U
2	D	46(D)	U
2	D	46(E)	G
2	D	48	U
2	D	74	C
2	D	75	C
2	D	76	A

All (10) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	C	9	G
2	C	16	U
2	C	17	C
2	C	37	A
2	C	46(B)	U
2	C	46(G)	C
2	C	75	C
2	D	9	G
2	D	46(B)	U
2	D	75	C

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 4 are monoatomic - leaving 7 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	LSS	A	1818	-	30,33,33	1.56	5 (16%)	33,49,49	1.85	8 (24%)
5	SO4	B	1819	-	4,4,4	0.41	0	6,6,6	0.26	0
5	SO4	C	1078	-	4,4,4	0.44	0	6,6,6	0.45	0
5	SO4	B	1820	-	4,4,4	0.48	0	6,6,6	0.52	0
4	LSS	B	1818	-	30,33,33	1.92	6 (20%)	33,49,49	1.89	6 (18%)
5	SO4	A	1819	-	4,4,4	0.53	0	6,6,6	0.60	0
5	SO4	D	1078	-	4,4,4	0.43	0	6,6,6	0.37	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
4	LSS	A	1818	-	-	0/18/39/39	0/3/3/3
4	LSS	B	1818	-	-	0/18/39/39	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1818	LSS	O1A-S1	5.85	1.47	1.42
4	B	1818	LSS	S1-N2	-5.68	1.49	1.59
4	A	1818	LSS	S1-N2	-5.28	1.50	1.59
4	B	1818	LSS	O2A-S1	3.21	1.45	1.42
4	A	1818	LSS	C1-N2	-3.10	1.31	1.37
4	B	1818	LSS	C22-C21	-2.91	1.49	1.53
4	B	1818	LSS	C1-N2	-2.64	1.32	1.37
4	A	1818	LSS	C22-C21	-2.55	1.49	1.53
4	A	1818	LSS	O2A-S1	2.52	1.44	1.42
4	A	1818	LSS	O2-C22	-2.33	1.37	1.43
4	B	1818	LSS	C2-N3	2.14	1.35	1.32

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1818	LSS	O2A-S1-O1A	-7.59	108.94	120.76
4	A	1818	LSS	O2A-S1-O1A	-4.58	113.62	120.76
4	A	1818	LSS	N3-C2-N1	-4.23	122.06	128.68

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1818	LSS	O5-C25-C24	3.89	114.88	107.62
4	A	1818	LSS	O4-C21-C22	-3.84	101.31	106.93
4	B	1818	LSS	N3-C2-N1	-3.64	123.00	128.68
4	B	1818	LSS	O5-C25-C24	3.34	113.85	107.62
4	A	1818	LSS	C22-C23-C24	-2.52	97.75	102.64
4	A	1818	LSS	C2-N1-C6	2.51	123.05	118.75
4	A	1818	LSS	C23-C22-C21	2.37	104.55	100.98
4	B	1818	LSS	O4-C24-C25	-2.15	102.29	109.37
4	B	1818	LSS	C21-N9-C4	-2.12	122.91	126.64
4	B	1818	LSS	O4-C24-C23	2.05	109.18	105.11
4	A	1818	LSS	O4-C24-C23	2.03	109.13	105.11

There are no chirality outliers.

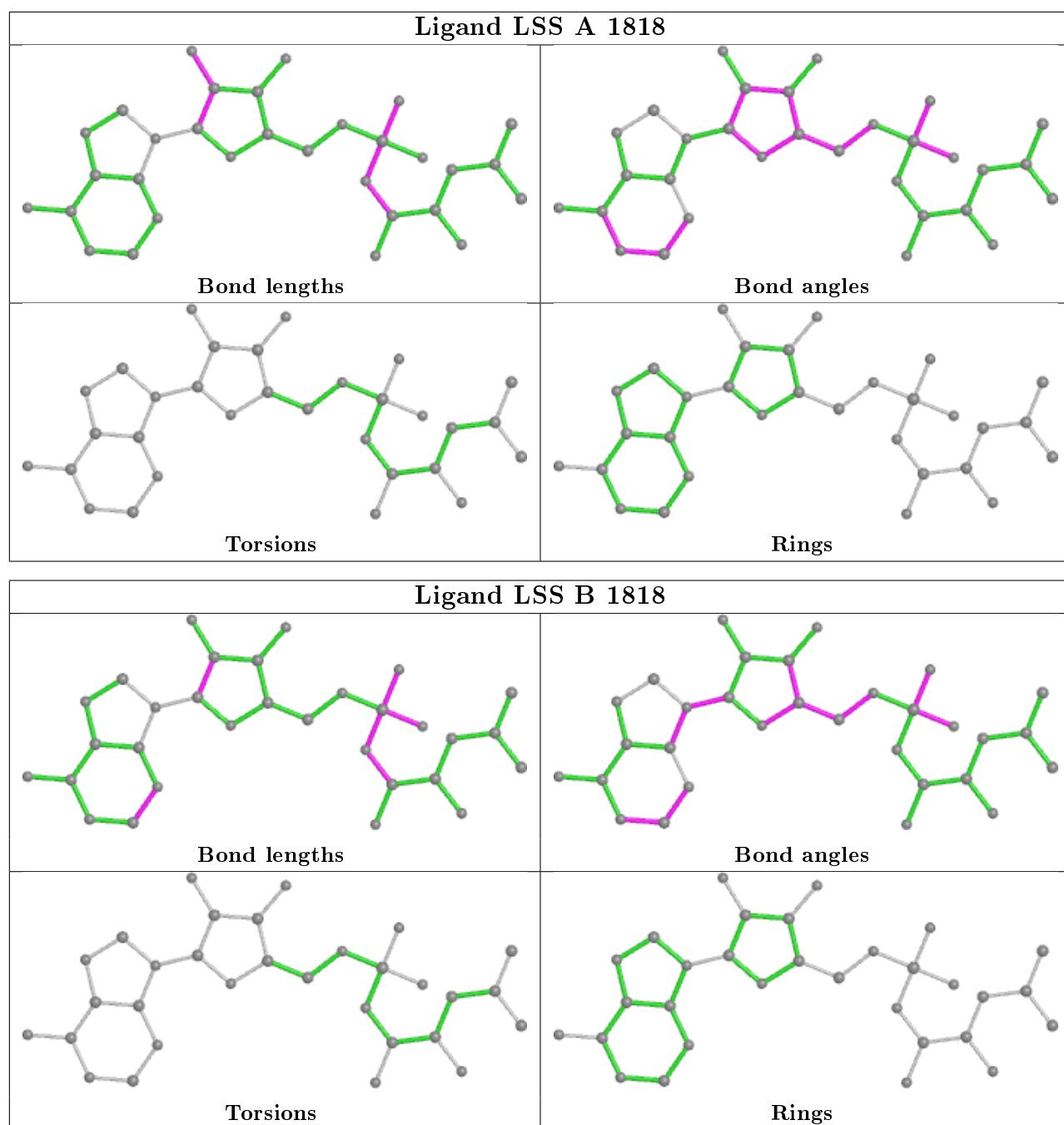
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1818	LSS	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 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	789/822 (95%)	0.47	88 (11%) 5 6	24, 42, 115, 147	0
1	B	771/822 (93%)	0.46	84 (10%) 5 7	21, 38, 119, 146	0
2	C	80/84 (95%)	-0.51	1 (1%) 77 80	31, 52, 106, 141	0
2	D	81/84 (96%)	-0.57	1 (1%) 79 82	29, 48, 82, 136	0
All	All	1721/1812 (94%)	0.37	174 (10%) 7 9	21, 41, 115, 147	0

All (174) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	393	ILE	9.9
1	B	316	ARG	8.6
1	B	309	VAL	8.6
1	A	380	SER	7.9
1	B	312	LEU	7.8
1	A	312	LEU	7.5
1	B	233	LEU	7.4
1	A	358	VAL	7.3
1	B	337	VAL	7.0
1	B	390	ALA	6.6
1	B	252	ALA	6.6
1	B	236	ALA	6.5
1	B	335	ILE	6.5
1	A	402	LEU	6.4
1	A	357	VAL	6.3
1	A	239	LEU	6.2
1	B	239	LEU	6.2
1	B	400	GLU	6.1
1	B	234	VAL	5.8
1	A	306	LEU	5.7
1	B	256	PHE	5.7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	401	LYS	5.6
1	A	316	ARG	5.6
1	A	309	VAL	5.4
1	B	238	ASP	5.4
1	A	230	VAL	5.3
1	B	230	VAL	5.2
1	A	355	VAL	5.2
1	A	379	HIS	5.2
1	A	233	LEU	5.1
1	B	305	GLY	5.0
1	A	314	GLN	5.0
1	A	395	ILE	5.0
1	A	255	THR	5.0
1	A	397	HIS	5.0
1	A	393	ILE	4.9
1	B	404	GLY	4.9
1	B	317	VAL	4.9
1	A	236	ALA	4.9
1	B	241	ILE	4.9
1	A	403	GLU	4.9
1	B	306	LEU	4.9
1	A	384	GLY	4.8
1	B	394	LEU	4.8
1	A	251	LEU	4.6
1	A	390	ALA	4.6
1	B	308	VAL	4.5
1	B	303	PHE	4.5
1	B	320	TYR	4.5
1	B	395	ILE	4.5
1	B	237	SER	4.4
1	A	381	LEU	4.4
1	A	392	GLU	4.4
1	B	401	LYS	4.4
1	A	385	LEU	4.4
1	B	304	THR	4.4
1	A	238	ASP	4.3
1	B	389	ALA	4.3
1	B	397	HIS	4.3
1	A	234	VAL	4.3
1	A	352	GLY	4.2
1	A	308	VAL	4.1
1	B	386	THR	4.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	252	ALA	4.1
1	B	336	GLY	4.0
1	B	240	THR	4.0
1	A	400	GLU	4.0
1	B	277	ALA	3.9
1	A	305	GLY	3.8
1	B	254	CYS	3.8
1	B	392	GLU	3.8
1	A	307	MET	3.8
1	B	396	ALA	3.7
1	A	276	ARG	3.7
1	A	232	PHE	3.7
1	B	249	ASP	3.7
1	A	237	SER	3.6
1	B	251	LEU	3.6
1	A	256	PHE	3.5
1	B	232	PHE	3.5
1	B	250	THR	3.5
1	B	314	GLN	3.5
1	A	399	SER	3.4
1	A	254	CYS	3.4
1	A	267	ASP	3.4
1	A	404	GLY	3.4
1	A	345	ALA	3.3
1	A	388	SER	3.3
1	B	319	LEU	3.3
1	B	253	GLY	3.3
1	A	266	LEU	3.2
1	A	337	VAL	3.2
1	A	354	PRO	3.2
1	A	356	ARG	3.2
1	B	399	SER	3.0
1	A	303	PHE	3.0
1	A	335	ILE	3.0
1	B	257	ILE	3.0
1	A	250	THR	3.0
1	B	387	SER	3.0
1	A	396	ALA	2.9
1	A	353	LEU	2.9
1	B	311	PRO	2.9
1	B	258	ALA	2.9
1	B	255	THR	2.9

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	653	GLU	2.9
1	A	315	GLU	2.9
1	B	403	GLU	2.9
1	B	405	GLN	2.8
1	B	231	ARG	2.8
1	B	281	ASP	2.8
1	A	334	VAL	2.8
1	A	304	THR	2.8
1	A	639	SER	2.8
1	A	229	GLU	2.7
1	A	394	LEU	2.7
1	B	434	GLU	2.7
1	A	398	LEU	2.7
1	B	301	GLY	2.7
1	A	313	ASN	2.7
1	B	278	SER	2.7
1	B	348	GLY	2.7
1	B	276	ARG	2.7
1	B	235	GLU	2.7
1	B	345	ALA	2.6
1	A	281	ASP	2.6
1	A	319	LEU	2.6
1	A	249	ASP	2.6
1	B	338	PRO	2.6
1	A	386	THR	2.6
1	A	406	LYS	2.5
1	A	241	ILE	2.5
1	A	636	ARG	2.5
1	A	311	PRO	2.5
1	A	240	THR	2.5
2	C	37	A	2.5
1	B	315	GLU	2.5
1	A	317	VAL	2.4
1	A	474	PRO	2.4
1	A	342	GLU	2.4
1	B	398	LEU	2.4
1	B	331	THR	2.4
1	A	382	VAL	2.4
1	B	248	LEU	2.4
1	B	324	TYR	2.4
1	B	284	GLU	2.3
1	B	266	LEU	2.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	347	PHE	2.3
1	B	342	GLU	2.3
1	A	351	PHE	2.3
1	A	434	GLU	2.2
1	A	246	THR	2.2
1	A	795	ASP	2.2
1	B	402	LEU	2.2
1	B	333	ALA	2.2
1	A	349	ALA	2.2
1	A	265	ILE	2.2
1	A	635	ASP	2.2
1	B	279	VAL	2.1
1	A	235	GLU	2.1
1	B	310	ASN	2.1
1	A	231	ARG	2.1
1	B	307	MET	2.1
1	B	475	GLN	2.1
1	B	343	ARG	2.1
1	B	280	LYS	2.1
1	B	653	GLU	2.0
1	B	265	ILE	2.0
1	A	697	GLY	2.0
1	A	479	ASP	2.0
1	B	391	ARG	2.0
1	B	313	ASN	2.0
1	A	338	PRO	2.0
2	D	17	C	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.

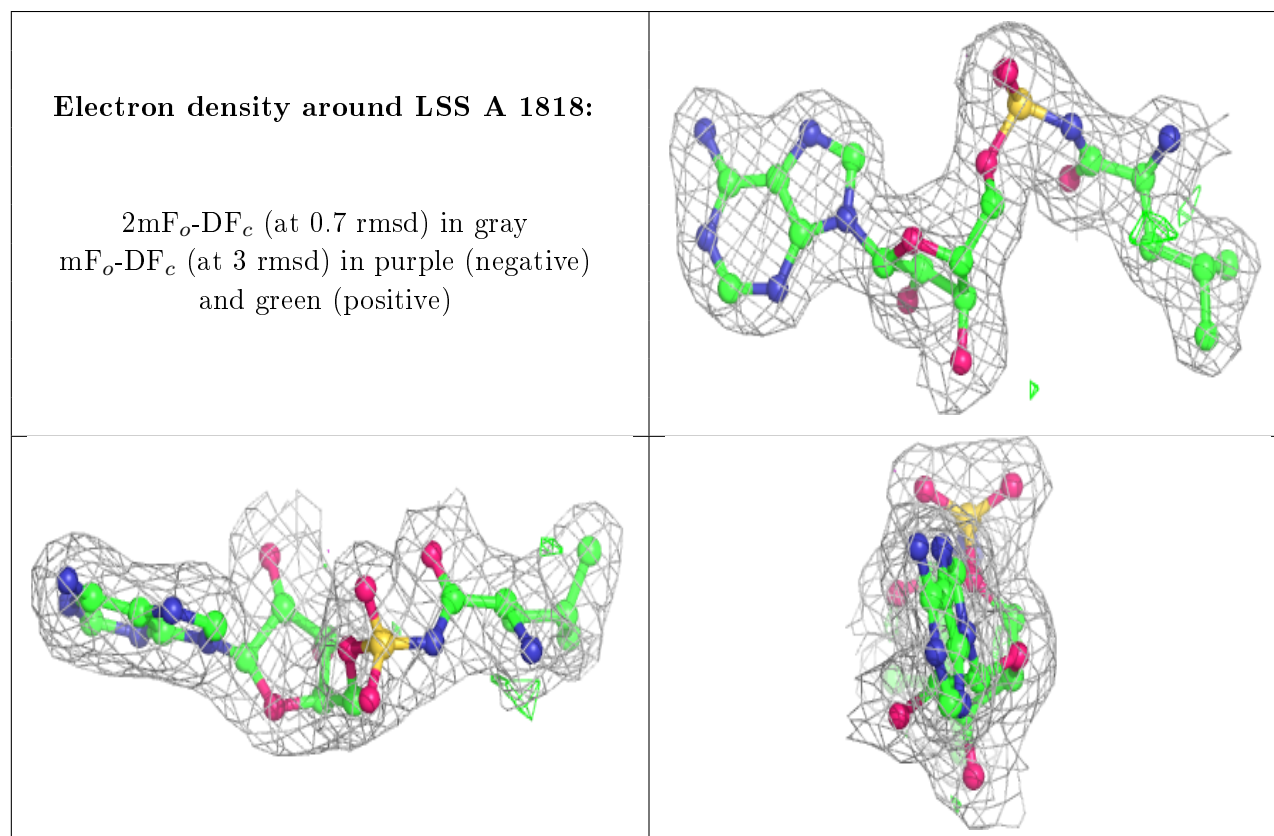
## 6.4 Ligands [i](#)

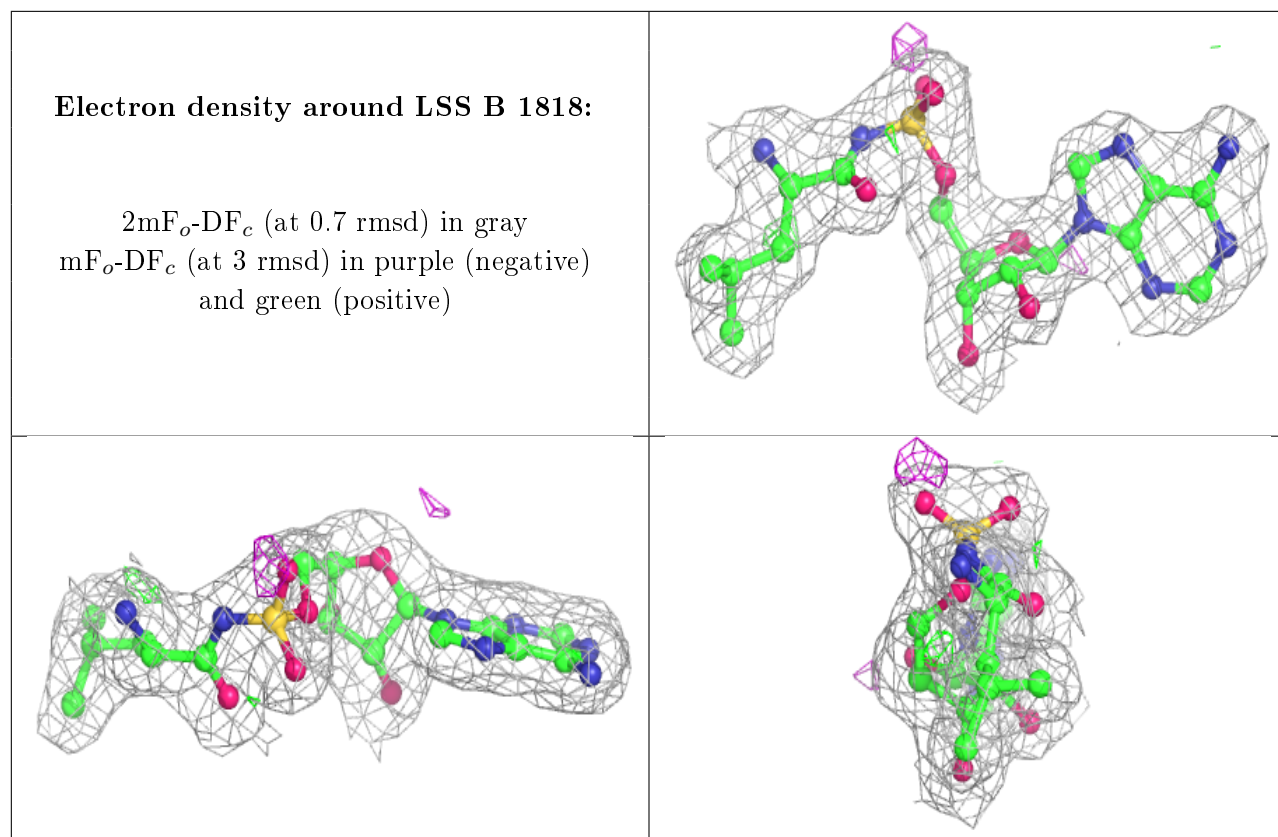
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
5	SO4	A	1819	5/5	0.84	0.17	69,70,91,94	0
6	MN	D	1077	1/1	0.86	0.06	91,91,91,91	0
5	SO4	B	1819	5/5	0.88	0.15	105,113,114,115	0
5	SO4	B	1820	5/5	0.92	0.19	61,61,79,93	0
5	SO4	D	1078	5/5	0.92	0.21	80,80,83,92	0
5	SO4	C	1078	5/5	0.95	0.17	74,76,83,84	0
6	MN	C	1077	1/1	0.96	0.08	84,84,84,84	0
3	ZN	A	900	1/1	0.98	0.03	73,73,73,73	0
3	ZN	B	900	1/1	0.98	0.04	63,63,63,63	0
4	LSS	A	1818	31/31	0.98	0.12	22,27,32,34	0
4	LSS	B	1818	31/31	0.98	0.13	20,26,30,32	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.