



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:05 PM UTC

PDB ID : 5AH5 / pdb_00005ah5
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

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	:	2022.3.0, CSD as543be (2022)
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	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

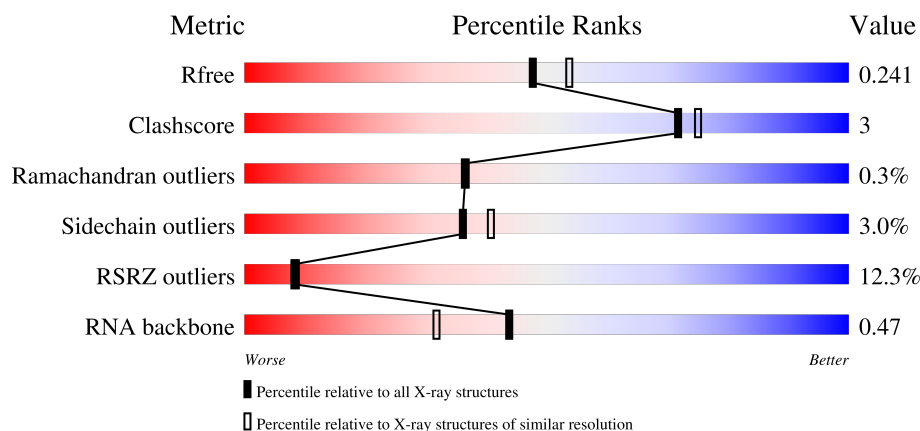
1 Overall quality at a glance

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}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)
RNA backbone	3983	1006 (2.42-1.78)

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	A	822	14% 85% 10% • •
1	B	822	11% 80% 12% • 6%
2	C	84	2% 68% 18% 10% 5%

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Mol	Chain	Length	Quality of chain
2	D	84	2% 68% 21% 7%

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

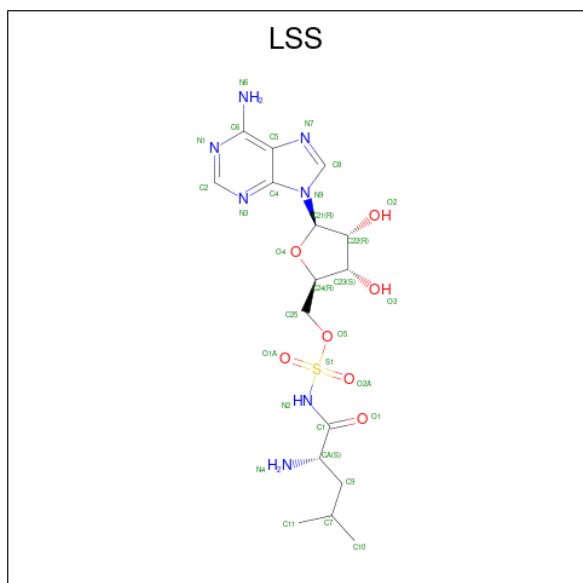
- Molecule 2 is a RNA chain called TRNA-LEU TAA ISOACCEPTOR.

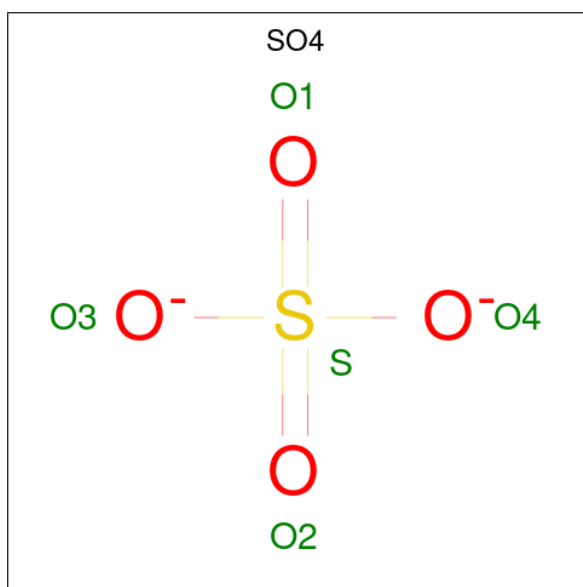
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	80	Total	C	N	O	P	0	0	0
			1702	759	304	559	80			
2	D	81	Total	C	N	O	P	0	0	0
			1721	768	305	567	81			

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 4 is 5'-O-(L-leucylsulfamoyl)adenosine (CCD ID: LSS) (formula: C₁₆H₂₅N₇O₇S).





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 (CCD ID: MN) (formula: Mn).

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

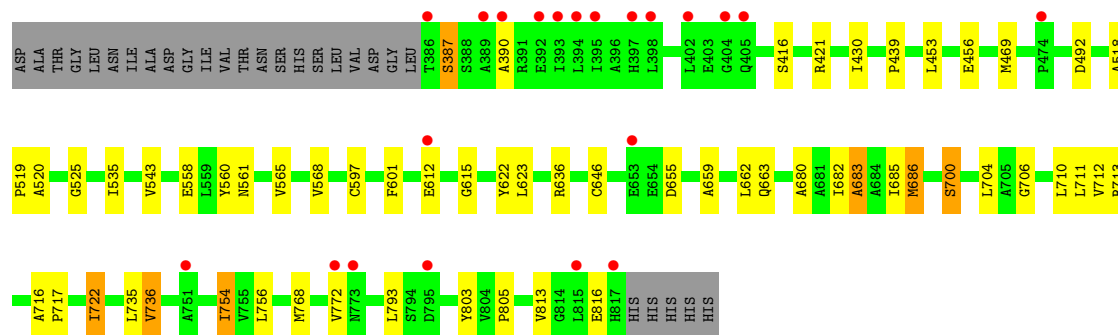
- Molecule 7 is water.

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

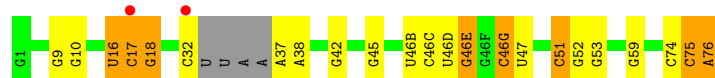
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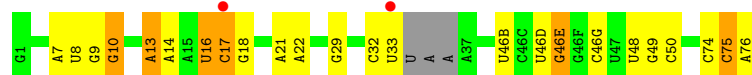
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	C	89	Total	O	0	0
			89	89		
7	D	76	Total	O	0	0
			76	76		



• 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, α , β , γ	169.91Å 50.32Å 170.52Å 90.00° 93.48° 90.00°	Depositor
Resolution (Å)	48.58 – 2.10 48.58 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.5 (48.58-2.10) 99.5 (48.58-2.10)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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 ²)	37.7	Xtriage
Anisotropy	0.085	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 39.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	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 ²)	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.*

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: LSS, SO4, ZN, MN

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	1.14	6/6447 (0.1%)	1.08	12/8760 (0.1%)
1	B	1.22	18/6299 (0.3%)	1.08	8/8559 (0.1%)
2	C	0.59	0/1899	1.07	9/2953 (0.3%)
2	D	0.62	0/1920	1.07	14/2985 (0.5%)
All	All	1.07	24/16565 (0.1%)	1.08	43/23257 (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 (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	615	GLY	C-O	-7.54	1.17	1.24
1	A	73	HIS	CA-C	7.01	1.59	1.52
1	A	716	ALA	C-O	-6.44	1.18	1.24
1	B	680	ALA	N-CA	6.33	1.54	1.46
1	B	421	ARG	CD-NE	-6.29	1.37	1.46
1	B	91	PHE	CA-C	6.17	1.61	1.52
1	A	133	ALA	CA-C	-5.63	1.45	1.52
1	B	88	ALA	C-O	-5.55	1.17	1.24
1	A	40	PRO	CA-C	5.50	1.59	1.52
1	B	683	ALA	N-CA	5.33	1.52	1.46
1	B	686	MET	CA-C	5.33	1.59	1.52
1	B	73	HIS	C-O	-5.30	1.19	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	597	CYS	N-CA	5.25	1.52	1.46
1	B	816	GLU	CA-CB	5.23	1.62	1.53
1	B	565	VAL	C-O	5.22	1.29	1.24
1	B	216	ASN	C-O	-5.19	1.18	1.24
1	B	94	HIS	CA-C	5.18	1.58	1.53
1	A	92	GLY	N-CA	5.15	1.52	1.45
1	B	430	ILE	C-O	-5.12	1.18	1.24
1	B	51	VAL	N-CA	-5.08	1.40	1.46
1	B	816	GLU	N-CA	5.08	1.52	1.46
1	B	71	VAL	CA-C	5.06	1.58	1.52
1	A	579	ASN	N-CA	5.04	1.52	1.46
1	B	520	ALA	C-O	-5.01	1.17	1.23

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	75	C	C2'-C3'-O3'	8.96	122.95	109.50
2	D	75	C	C2'-C3'-O3'	8.22	121.83	109.50
1	B	736	VAL	CB-CA-C	-8.13	99.56	112.16
2	C	46(E)	G	C1'-C2'-O2'	8.12	120.58	108.40
1	A	532	LEU	N-CA-C	7.79	121.34	108.48
2	C	75	C	C4'-C3'-O3'	7.75	121.03	109.40
2	C	45	G	C1'-C2'-O2'	7.67	119.90	108.40
2	D	46(E)	G	C4'-C3'-O3'	-7.29	102.07	113.00
2	D	22	A	C2'-C3'-O3'	-6.85	103.42	113.70
2	D	46(E)	G	C2'-C3'-O3'	6.69	123.73	113.70
1	A	736	VAL	CB-CA-C	-6.62	103.20	112.14
1	B	387	SER	N-CA-C	6.58	122.12	114.62
1	A	568	VAL	CB-CA-C	-6.36	102.30	112.16
1	B	336	GLY	N-CA-C	6.20	121.06	112.37
1	A	736	VAL	N-CA-CB	6.12	118.86	110.54
2	C	51	C	C3'-C2'-O2'	6.09	119.84	110.70
2	C	76	A	C1'-C2'-O2'	6.08	117.52	108.40
2	D	46(E)	G	C1'-C2'-O2'	6.06	117.50	108.40
2	D	21	A	C4'-C3'-O3'	-6.00	104.00	113.00
1	B	416	SER	CB-CA-C	-5.96	101.31	110.26
2	D	10	G	C1'-C2'-O2'	5.87	117.21	108.40
2	D	17	C	C3'-C2'-O2'	5.77	119.36	110.70
1	A	39	PHE	CA-C-N	5.69	126.17	120.14
1	A	39	PHE	C-N-CA	5.69	126.17	120.14
1	B	469	MET	N-CA-C	5.56	118.27	111.82
1	B	256	PHE	N-CA-C	5.55	115.87	108.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	59	G	C4'-C3'-O3'	-5.52	104.73	113.00
2	C	42	G	C3'-C2'-O2'	5.50	118.94	110.70
1	A	309	VAL	N-CA-C	5.48	115.20	106.88
1	A	449	LEU	CA-C-N	-5.46	114.33	119.85
1	A	449	LEU	C-N-CA	-5.46	114.33	119.85
2	C	16	U	C2'-C3'-O3'	5.46	117.68	109.50
1	A	194	ARG	CG-CD-NE	-5.45	100.02	112.00
1	A	535	ILE	CB-CA-C	-5.32	105.07	112.04
2	D	16	U	C2'-C3'-O3'	5.31	117.47	109.50
2	D	46(G)	C	C2'-C3'-O3'	5.24	121.56	113.70
1	B	309	VAL	N-CA-C	5.18	116.04	108.53
2	D	50	C	C3'-C2'-O2'	5.13	118.40	110.70
2	D	13	A	O5'-C5'-C4'	-5.10	103.85	111.50
1	A	696	GLY	N-CA-C	-5.07	104.64	111.54
2	D	29	G	C3'-C2'-O2'	5.05	118.28	110.70
1	B	535	ILE	CB-CA-C	-5.03	105.45	112.04
2	D	46(G)	C	C5'-C4'-C3'	-5.02	108.47	116.00

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 [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	6288	0	6179	41	0
1	B	6146	0	6030	50	0
2	C	1702	0	868	6	0
2	D	1721	0	876	3	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	7	0
7	C	89	0	0	1	0
7	D	76	0	0	0	0
All	All	16819	0	14003	100	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 (100) 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:B:601:PHE:CZ	1:B:686:MET:HE1	2.06	0.89
1:B:601:PHE:CE1	1:B:686:MET:HE1	2.19	0.77
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:H5''	2:C:46(G):C:H6	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:682:ILE:HG22	1:B:686:MET:HE2	1.85	0.56
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:53:ASN:C	1:B:53:ASN:HD22	2.17	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:37:GLU:OE2	1:B:57:GLY:HA3	2.11	0.50
1:B:47[A]:HIS:HB2	7:B:2065:HOH:O	2.11	0.50
2:C:46(G):C:H6	2:C:46(G):C:C5'	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:601:PHE:CE1	1:B:686:MET:CE	2.94	0.49
1:B:803:TYR:CZ	1:B:805:PRO:HA	2.48	0.48
1:B:683:ALA:HA	1:B:686:MET:HE3	1.95	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: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:A:45:HIS:CE1	7:A:2042:HOH:O	2.68	0.47
1:B:256:PHE:HA	1:B:317:VAL:HG12	1.96	0.47
1:B:622:TYR:CE1	1:B:686:MET:HG2	2.50	0.46
1:A:567:ASP:C	1:A:567:ASP:OD1	2.58	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:518:ALA:HA	1:B:519:PRO:C	2.43	0.43
1:A:518:ALA:HA	1:A:519:PRO:C	2.43	0.43
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
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:282:TYR:O	1:A:285:SER:OG	2.34	0.42
1:B:456:GLU:N	1:B:456:GLU:CD	2.78	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:53:ASN:ND2	4:A:1818:LSS:O3	2.53	0.41
1:A:201:LEU:HD11	1:A:219:ARG:CG	2.50	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
1:B:97[A]:LYS:NZ	7:B:2097:HOH:O	2.37	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

There are no symmetry-related clashes.

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	A	786/822 (96%)	751 (96%)	33 (4%)	2 (0%)	36	36
1	B	767/822 (93%)	735 (96%)	30 (4%)	2 (0%)	36	36
All	All	1553/1644 (94%)	1486 (96%)	63 (4%)	4 (0%)	36	36

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%)	664 (97%)	20 (3%)	37	42
1	B	667/707 (94%)	646 (97%)	21 (3%)	35	39
All	All	1351/1414 (96%)	1310 (97%)	41 (3%)	36	41

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	VAL
1	A	39	PHE

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Mol	Chain	Res	Type
1	A	154	VAL
1	A	181	VAL
1	A	191	VAL
1	A	219	ARG
1	A	225	THR
1	A	250	THR
1	A	261	PRO
1	A	317	VAL
1	A	350	LEU
1	A	355	VAL
1	A	379	HIS
1	A	492	ASP
1	A	514	CYS
1	A	568	VAL
1	A	668	LYS
1	A	712	VAL
1	A	736	VAL
1	A	788	GLU
1	B	14	GLN
1	B	35	VAL
1	B	39	PHE
1	B	47[A]	HIS
1	B	47[B]	HIS
1	B	80	PHE
1	B	191	VAL
1	B	226	GLU
1	B	242	ASN
1	B	245	THR
1	B	255	THR
1	B	262	GLU
1	B	288	VAL
1	B	306	LEU
1	B	334	VAL
1	B	453	LEU
1	B	700	SER
1	B	712	VAL
1	B	722	ILE
1	B	736	VAL
1	B	754	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	ASN
1	A	263	HIS
1	B	397	HIS
1	B	409	GLN
1	B	444	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	C	79/84 (94%)	15 (18%)	7 (8%)
2	D	79/84 (94%)	12 (15%)	3 (3%)
All	All	158/168 (94%)	27 (17%)	10 (6%)

All (27) 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(B)	U
2	C	46(C)	C
2	C	46(D)	U
2	C	46(E)	G
2	C	46(G)	C
2	C	47	U
2	C	74	C
2	C	75	C
2	C	76	A
2	D	10	G
2	D	16	U
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

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Mol	Chain	Res	Type
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 oligosaccharides 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	$\# Z > 2$
5	SO4	B	1820	-	4,4,4	0.57	0	6,6,6	0.54	0
5	SO4	D	1078	-	4,4,4	0.52	0	6,6,6	0.32	0
5	SO4	B	1819	-	4,4,4	0.50	0	6,6,6	0.28	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	SO4	C	1078	-	4,4,4	0.54	0	6,6,6	0.42	0
5	SO4	A	1819	-	4,4,4	0.61	0	6,6,6	0.58	0
4	LSS	B	1818	-	32,33,33	1.86	5 (15%)	43,49,49	2.18	13 (30%)
4	LSS	A	1818	-	32,33,33	1.60	6 (18%)	43,49,49	1.86	11 (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	LSS	A	1818	-	-	0/22/39/39	0/3/3/3
4	LSS	B	1818	-	-	0/22/39/39	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	S1-N2	-5.93	1.49	1.59
4	B	1818	LSS	O1A-S1	5.68	1.47	1.42
4	A	1818	LSS	S1-N2	-5.50	1.50	1.59
4	A	1818	LSS	C1-N2	-3.32	1.31	1.37
4	B	1818	LSS	O2A-S1	3.13	1.45	1.42
4	B	1818	LSS	C1-N2	-2.84	1.32	1.37
4	A	1818	LSS	C4-N9	-2.61	1.32	1.37
4	B	1818	LSS	C8-N7	2.54	1.36	1.31
4	A	1818	LSS	O2A-S1	2.46	1.44	1.42
4	A	1818	LSS	C5-N7	-2.38	1.34	1.39
4	A	1818	LSS	O2-C22	-2.21	1.37	1.43

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1818	LSS	O2A-S1-O1A	-7.96	108.94	120.85
4	A	1818	LSS	O2A-S1-O1A	-4.83	113.62	120.85
4	A	1818	LSS	N3-C2-N1	-4.31	122.06	128.58
4	B	1818	LSS	N9-C8-N7	-4.29	107.86	113.94
4	B	1818	LSS	C5-C4-N3	-4.10	121.07	126.72
4	A	1818	LSS	O5-C25-C24	4.10	114.88	107.57
4	B	1818	LSS	N3-C2-N1	-3.69	123.00	128.58
4	B	1818	LSS	O5-C25-C24	3.52	113.85	107.57
4	B	1818	LSS	C4-N9-C8	3.33	109.23	105.74
4	A	1818	LSS	N9-C8-N7	-3.28	109.29	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1818	LSS	C5-C4-N3	-2.92	122.69	126.72
4	B	1818	LSS	C5-N7-C8	2.87	107.97	103.45
4	A	1818	LSS	C4-N9-C8	2.75	108.62	105.74
4	B	1818	LSS	C2-N3-C4	2.68	118.37	111.83
4	B	1818	LSS	N3-C4-N9	2.66	131.69	127.17
4	A	1818	LSS	C2-N1-C6	2.63	123.05	118.73
4	B	1818	LSS	O4-C21-N9	2.53	112.95	108.09
4	A	1818	LSS	C22-C23-C24	-2.52	97.75	102.61
4	A	1818	LSS	O4-C21-C22	-2.48	101.31	106.62
4	B	1818	LSS	C4-C5-N7	-2.46	107.77	110.58
4	A	1818	LSS	N3-C4-N9	2.29	131.06	127.17
4	B	1818	LSS	O4-C24-C25	-2.20	102.29	109.33
4	B	1818	LSS	O4-C24-C23	2.03	109.18	105.15
4	A	1818	LSS	O4-C24-C23	2.00	109.13	105.15

There are no chirality outliers.

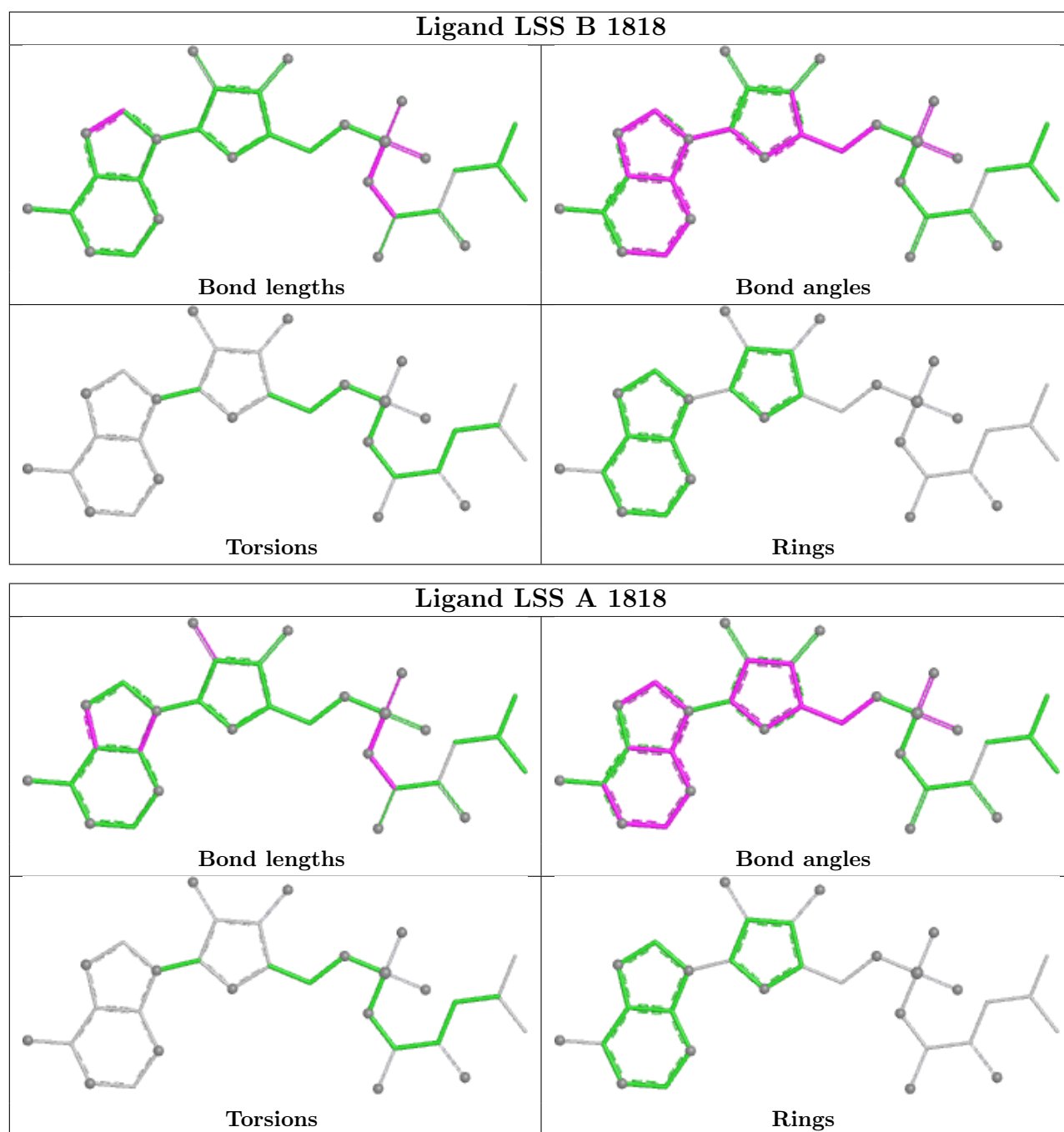
There are no torsion outliers.

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, 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	A	789/822 (95%)	0.68	115 (14%) 6 6	15, 41, 115, 147	5 (0%)
1	B	771/822 (93%)	0.49	93 (12%) 8 9	15, 38, 119, 146	4 (0%)
2	C	80/84 (95%)	0.11	2 (2%) 58 61	31, 52, 106, 141	0
2	D	81/84 (96%)	-0.10	2 (2%) 58 61	29, 48, 82, 136	0
All	All	1721/1812 (94%)	0.53	212 (12%) 8 8	15, 41, 115, 147	9 (0%)

All (212) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	306	LEU	7.1
1	B	312	LEU	7.0
1	A	358	VAL	6.5
1	B	239	LEU	6.1
1	A	308	VAL	6.0
1	B	317	VAL	5.9
1	A	393	ILE	5.8
1	B	393	ILE	5.8
1	B	337	VAL	5.6
1	A	306	LEU	5.5
1	A	389	ALA	5.4
1	A	275	MET	5.4
1	B	335	ILE	5.3
1	A	385	LEU	5.3
1	B	309	VAL	5.2
1	A	357	VAL	5.0
1	B	256	PHE	5.0
1	A	386	THR	4.9
1	B	241	ILE	4.9
1	B	348	GLY	4.8
1	A	381	LEU	4.7

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Mol	Chain	Res	Type	RSRZ
1	A	345	ALA	4.6
1	A	335	ILE	4.6
1	A	337	VAL	4.6
1	A	230	VAL	4.5
1	A	395	ILE	4.5
1	B	316	ARG	4.4
1	A	382	VAL	4.4
1	A	350	LEU	4.4
1	B	336	GLY	4.3
1	A	277	ALA	4.3
1	A	334	VAL	4.3
1	A	384	GLY	4.3
1	B	386	THR	4.3
1	A	402	LEU	4.2
1	B	402	LEU	4.2
1	B	319	LEU	4.2
1	A	305	GLY	4.1
1	A	317	VAL	4.1
1	A	353	LEU	4.1
1	B	279	VAL	4.1
1	A	255	THR	4.1
1	B	236	ALA	4.0
1	B	398	LEU	4.0
1	B	320	TYR	4.0
1	A	253	GLY	4.0
1	B	394	LEU	3.9
1	B	234	VAL	3.9
1	A	392	GLU	3.9
1	A	403	GLU	3.9
1	A	233	LEU	3.9
1	A	379	HIS	3.9
1	B	233	LEU	3.9
1	B	304	THR	3.8
1	A	380	SER	3.8
1	B	390	ALA	3.8
1	B	255	THR	3.8
1	B	305	GLY	3.8
1	A	236	ALA	3.7
1	B	265	ILE	3.7
1	A	249	ASP	3.7
1	A	349	ALA	3.7
1	A	248	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	266	LEU	3.6
1	A	232	PHE	3.6
1	A	241	ILE	3.6
1	B	395	ILE	3.6
1	B	257	ILE	3.6
1	A	309	VAL	3.6
1	B	308	VAL	3.6
1	A	228	ALA	3.5
1	A	307	MET	3.5
1	A	354	PRO	3.4
1	A	256	PHE	3.4
1	A	404	GLY	3.4
1	B	318	PRO	3.4
1	A	276	ARG	3.4
1	A	312	LEU	3.4
1	A	795	ASP	3.4
1	A	817	HIS	3.3
1	B	817	HIS	3.3
1	A	355	VAL	3.3
1	B	230	VAL	3.3
1	A	333	ALA	3.3
1	B	345	ALA	3.3
1	B	347	PHE	3.3
1	A	245	THR	3.3
1	B	334	VAL	3.3
1	B	389	ALA	3.3
1	A	338	PRO	3.2
1	A	234	VAL	3.2
1	A	244	PHE	3.2
1	A	348	GLY	3.2
2	C	17	C	3.2
1	A	390	ALA	3.1
1	A	319	LEU	3.1
1	A	226	GLU	3.1
1	B	333	ALA	3.1
1	A	397	HIS	3.1
1	B	249	ASP	3.1
1	A	279	VAL	3.1
1	B	299	LYS	3.1
1	B	404	GLY	3.0
1	B	350	LEU	3.0
1	A	239	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	247	ARG	3.0
1	A	401	LYS	3.0
1	B	277	ALA	2.9
1	B	303	PHE	2.9
1	B	243	ALA	2.9
1	B	349	ALA	2.9
1	A	254	CYS	2.9
1	B	254	CYS	2.9
1	B	331	THR	2.9
1	B	653	GLU	2.9
1	A	347	PHE	2.9
1	A	650	CYS	2.8
1	B	321	VAL	2.8
1	B	285	SER	2.8
1	A	303	PHE	2.8
1	B	313	ASN	2.8
1	A	336	GLY	2.8
1	A	352	GLY	2.8
1	A	246	THR	2.8
1	A	329	PHE	2.8
1	A	258	ALA	2.8
1	B	258	ALA	2.8
1	A	634	LEU	2.8
1	B	302	ILE	2.8
2	D	33	U	2.7
1	A	747	ARG	2.7
1	A	251	LEU	2.7
1	B	324	TYR	2.7
1	A	387	SER	2.7
1	B	301	GLY	2.7
1	A	343	ARG	2.7
1	A	318	PRO	2.7
1	B	311	PRO	2.7
1	B	392	GLU	2.7
1	A	378	SER	2.7
1	B	322	ALA	2.6
1	A	324	TYR	2.6
1	A	304	THR	2.6
1	A	257	ILE	2.6
1	A	265	ILE	2.6
2	D	17	C	2.6
1	B	342	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	307	MET	2.6
1	A	391	ARG	2.6
1	B	773	ASN	2.6
1	B	338	PRO	2.6
1	B	795	ASP	2.6
1	A	816	GLU	2.5
1	B	286	ILE	2.5
1	A	697	GLY	2.5
1	B	232	PHE	2.5
1	B	612	GLU	2.5
1	B	245	THR	2.5
1	B	251	LEU	2.5
1	B	287	LEU	2.5
1	A	356	ARG	2.5
1	A	636	ARG	2.4
1	A	351	PHE	2.4
1	B	405	GLN	2.4
1	B	296	ALA	2.4
1	B	276	ARG	2.4
1	A	278	SER	2.4
1	A	474	PRO	2.4
1	B	2	GLN	2.3
1	B	244	PHE	2.3
1	A	2	GLN	2.3
1	A	243	ALA	2.3
1	B	252	ALA	2.3
1	A	344	ASP	2.3
1	A	342	GLU	2.3
1	A	654	GLU	2.3
1	B	240	THR	2.3
1	B	310	ASN	2.3
1	B	280	LYS	2.3
1	B	397	HIS	2.3
1	A	346	ASP	2.3
1	A	696	GLY	2.3
1	A	286	ILE	2.2
1	A	229	GLU	2.2
1	A	639	SER	2.2
1	B	17	ASP	2.2
1	A	252	ALA	2.2
1	B	284	GLU	2.2
1	B	153	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	289	LEU	2.2
1	A	396	ALA	2.1
1	B	228	ALA	2.1
1	A	388	SER	2.1
2	C	32	C	2.1
1	B	772	VAL	2.1
1	A	266	LEU	2.1
1	A	310	ASN	2.1
1	A	341	ASP	2.1
1	A	635	ASP	2.1
1	A	288	VAL	2.1
1	A	320	TYR	2.1
1	B	250	THR	2.1
1	B	474	PRO	2.1
1	A	299	LYS	2.1
1	A	268	GLU	2.0
1	A	588	GLN	2.0
1	A	280	LYS	2.0
1	B	751	ALA	2.0
1	A	815	LEU	2.0
1	B	815	LEU	2.0
1	B	283	CYS	2.0
1	A	225	THR	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

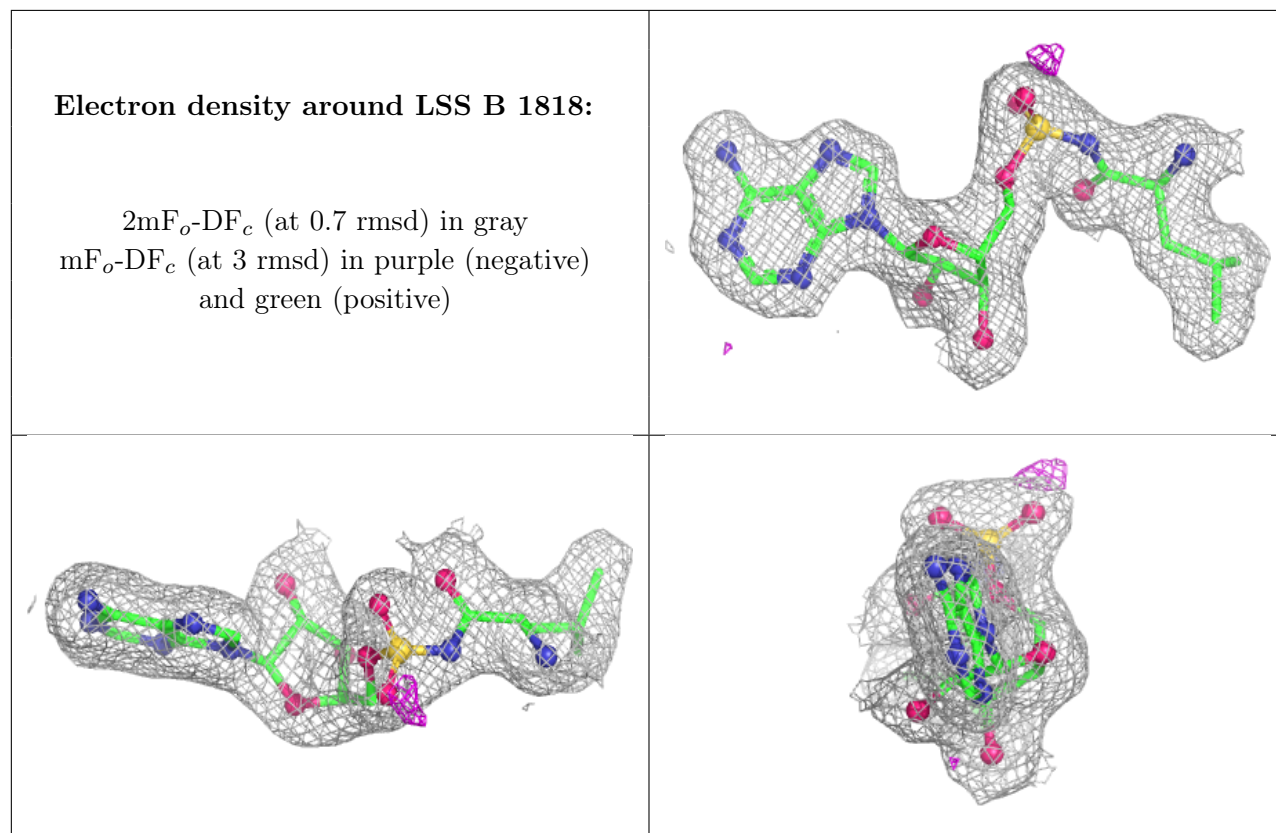
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

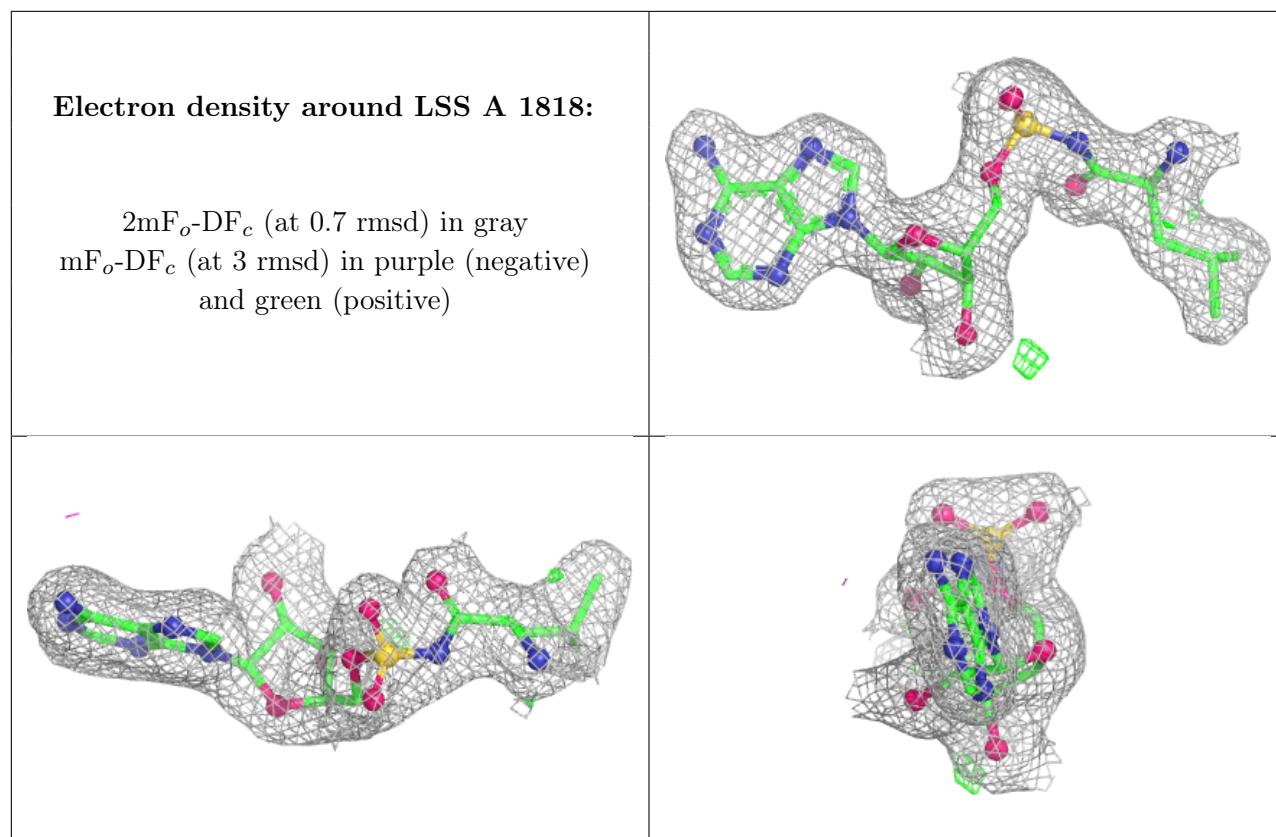
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	SO4	A	1819	5/5	0.73	0.14	69,70,91,94	0
5	SO4	D	1078	5/5	0.81	0.15	80,80,83,92	0
5	SO4	B	1819	5/5	0.85	0.14	105,113,114,115	0
5	SO4	C	1078	5/5	0.88	0.12	74,76,83,84	0
5	SO4	B	1820	5/5	0.89	0.09	61,61,79,93	0
6	MN	D	1077	1/1	0.91	0.13	91,91,91,91	0
6	MN	C	1077	1/1	0.97	0.13	84,84,84,84	0
4	LSS	B	1818	31/31	0.98	0.06	20,26,30,32	0
4	LSS	A	1818	31/31	0.98	0.06	22,27,32,34	0
3	ZN	B	900	1/1	0.99	0.04	63,63,63,63	0
3	ZN	A	900	1/1	0.99	0.03	73,73,73,73	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.