



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:16 PM UTC

PDB ID : 8C9D / pdb_00008c9d
Title : Priestia megaterium W130Q mutant of type 2 isoleucyl-tRNA synthetase complexed with an isoleucyl-adenylate analogue
Authors : Brkic, A.; Leibundgut, M.; Jablonska, J.; Zanki, V.; Car, Z.; Petrovic Perokovic, V.; Ban, N.; Gruic-Sovulj, I.
Deposited on : 2023-01-21
Resolution : 2.30 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

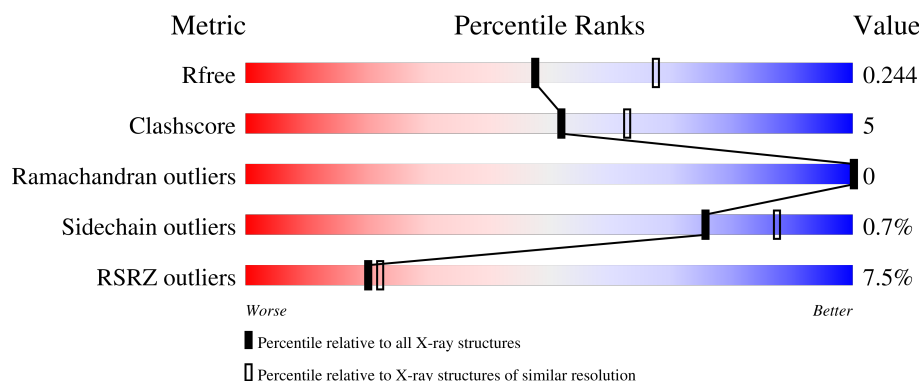
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	1032	

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
4	TAR	A	1105	-	X	-	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 8682 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 Isoleucine-tRNA ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1032	Total	C	N	O	S	0	3	0
			8338	5308	1413	1593	24			

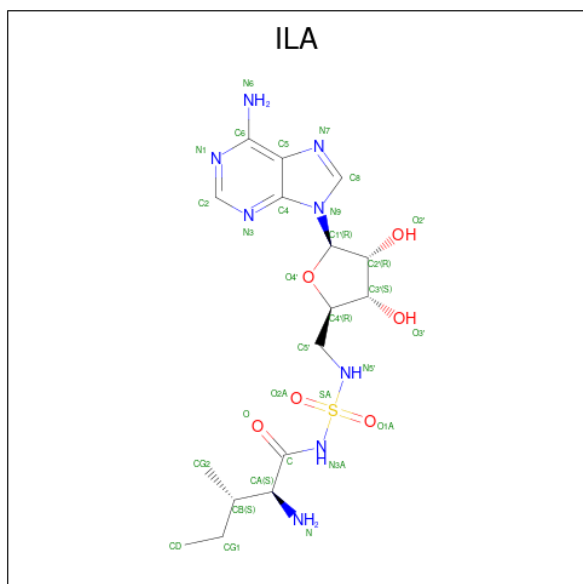
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	130	GLN	TRP	engineered mutation	UNP A0A0B6AVD3

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

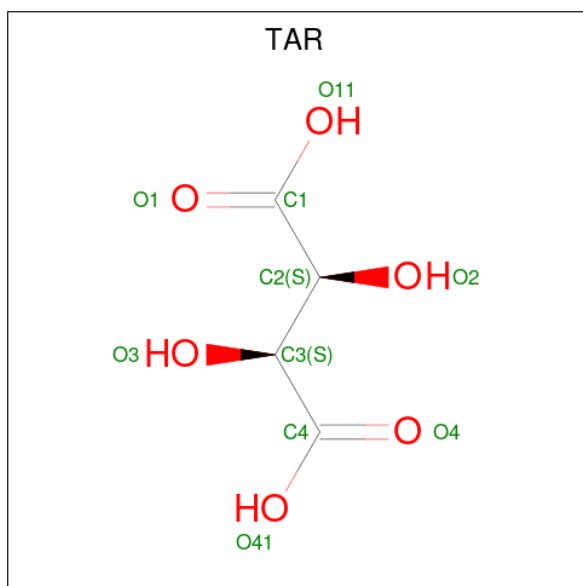
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		

- Molecule 3 is N-[ISOLEUCINYL]-N'-[ADENOSYL]-DIAMINOSUFONE (CCD ID: ILA) (formula: C₁₆H₂₆N₈O₆S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			31	16	8	6	1		

- Molecule 4 is D(-)-TARTARIC ACID (CCD ID: TAR) (formula: $C_4H_6O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			10	4	6		
4	A	1	Total	C	O	0	0
			10	4	6		
4	A	1	Total	C	O	0	0
			10	4	6		
4	A	1	Total	C	O	0	0
			10	4	6		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	271	Total	O	0	0
			271	271		

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Isoleucine-tRNA ligase



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	108.22Å 108.22Å 240.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.34 – 2.30 49.34 – 2.30	Depositor EDS
% Data completeness (in resolution range)	93.3 (49.34-2.30) 93.3 (49.34-2.30)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.26 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.201 , 0.241 0.205 , 0.244	Depositor DCC
R_{free} test set	3018 reflections (4.70%)	wwPDB-VP
Wilson B-factor (Å ²)	43.6	Xtriage
Anisotropy	0.025	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 34.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8682	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.58% 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: TAR, ZN, ILA

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	0.16	0/8533	0.36	0/11565

There are no bond length outliers.

There are no bond angle outliers.

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	8338	0	8160	84	0
2	A	2	0	0	0	0
3	A	31	0	26	1	0
4	A	40	0	16	1	0
5	A	271	0	0	6	0
All	All	8682	0	8202	85	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 5.

All (85) 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:480:HIS:HE1	1:A:497:GLN:H	1.24	0.84
1:A:803[A]:ARG:NH2	1:A:841:GLU:OE2	2.14	0.79
1:A:238:HIS:HB3	1:A:241:MET:HB2	1.70	0.74
1:A:136:GLN:HE22	1:A:606:HIS:CE1	2.08	0.72
1:A:136:GLN:HE22	1:A:606:HIS:HE1	1.37	0.70
1:A:723:ARG:HD3	1:A:732:GLU:HG2	1.74	0.69
1:A:346:THR:HG23	1:A:348:GLU:H	1.58	0.68
1:A:97:LYS:NZ	5:A:1202:HOH:O	2.26	0.68
1:A:294:GLU:N	1:A:294:GLU:OE2	2.26	0.68
1:A:994:THR:O	1:A:998:GLU:HG3	1.94	0.67
1:A:803[A]:ARG:NH2	5:A:1206:HOH:O	2.30	0.65
1:A:19:GLN:HG3	1:A:23:LYS:HE3	1.81	0.61
1:A:974:ARG:HG2	1:A:1001:LEU:HG	1.82	0.60
1:A:894:PHE:HD1	1:A:900:LEU:HB2	1.66	0.60
1:A:42:PHE:HZ	1:A:64:LYS:HD2	1.70	0.56
1:A:929:VAL:HG22	1:A:938:VAL:HG22	1.87	0.56
1:A:799:VAL:O	1:A:803[A]:ARG:HG3	2.06	0.55
1:A:452:THR:HB	1:A:514:ILE:HG12	1.89	0.55
1:A:974:ARG:HH21	1:A:1003:HIS:HA	1.73	0.54
1:A:93:LEU:O	1:A:97:LYS:HE2	2.09	0.53
1:A:820:LEU:HD11	1:A:937:ALA:HB1	1.91	0.53
1:A:523:MET:HG3	1:A:524:PRO:HD3	1.92	0.52
1:A:498:LEU:HB2	1:A:507:MET:HB2	1.91	0.52
1:A:883:LEU:O	1:A:886:LEU:HD12	2.10	0.51
1:A:198:LYS:HE3	1:A:391:ASP:OD1	2.11	0.51
1:A:822:LEU:HG	1:A:824:VAL:HG13	1.92	0.51
1:A:7:ARG:NE	5:A:1217:HOH:O	2.43	0.51
1:A:385:PRO:HB2	1:A:394:LEU:HD12	1.93	0.51
1:A:87:HIS:CG	1:A:451:GLY:HA2	2.46	0.50
1:A:872:PHE:HD1	1:A:910:LEU:HD13	1.75	0.50
1:A:978:GLU:OE2	1:A:1029:LEU:HD11	2.12	0.49
1:A:413:PHE:CG	1:A:439:MET:HE1	2.49	0.48
1:A:410:LYS:O	1:A:413:PHE:HB2	2.13	0.48
1:A:856:LEU:C	1:A:924:LYS:HG3	2.39	0.47
1:A:2:LYS:HD3	1:A:652:TYR:CE2	2.50	0.47
1:A:236:ALA:HB2	1:A:316:LEU:HD11	1.96	0.47
1:A:240:GLU:O	1:A:240:GLU:HG3	2.14	0.47
1:A:822:LEU:HD11	1:A:935:TYR:HB3	1.96	0.46
1:A:995:LEU:HA	1:A:998:GLU:OE2	2.16	0.46
1:A:328:VAL:HG13	1:A:333:PHE:HB2	1.98	0.46
1:A:159:TRP:CE2	1:A:455:ASN:HB3	2.50	0.45
1:A:583:VAL:HG22	1:A:627:LYS:HD2	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:872:PHE:HB2	1:A:876:VAL:HG12	1.97	0.45
1:A:191:HIS:HB2	1:A:555:ARG:O	2.16	0.45
1:A:380:HIS:CE1	1:A:382:HIS:HB3	2.51	0.45
1:A:371:GLN:HB2	1:A:373:VAL:HG22	1.96	0.45
1:A:341:GLU:H	1:A:341:GLU:CD	2.24	0.45
3:A:1103:ILA:H2'	3:A:1103:ILA:HN5	1.82	0.44
1:A:151:GLU:OE1	5:A:1201:HOH:O	2.20	0.44
1:A:238:HIS:O	1:A:276:GLY:HA3	2.18	0.44
1:A:13:ARG:HD2	5:A:1229:HOH:O	2.18	0.44
1:A:125:VAL:HG11	4:A:1106:TAR:H3	1.99	0.44
1:A:592:SER:HB3	1:A:595:LYS:HG2	1.99	0.44
1:A:480:HIS:CE1	1:A:497:GLN:H	2.16	0.43
1:A:863:LEU:HD21	1:A:868:ALA:HB3	2.00	0.43
1:A:632:ARG:O	1:A:636:GLU:HG3	2.18	0.43
1:A:324:ASP:OD1	1:A:324:ASP:N	2.50	0.43
1:A:83:GLY:HA2	1:A:147:TYR:O	2.18	0.43
1:A:333:PHE:N	1:A:333:PHE:CD1	2.87	0.43
1:A:129:GLN:NE2	5:A:1215:HOH:O	2.42	0.43
1:A:399:ASN:HD21	1:A:447:LYS:HE3	1.83	0.43
1:A:616:ALA:HB1	1:A:633:VAL:HG12	2.00	0.42
1:A:233:VAL:O	1:A:297:HIS:N	2.49	0.42
1:A:982:ASP:O	1:A:986:GLN:HG3	2.18	0.42
1:A:280:LYS:HE2	1:A:280:LYS:HB2	1.82	0.42
1:A:853:ASP:O	1:A:857:VAL:HG22	2.20	0.42
1:A:259:LEU:O	1:A:263:VAL:HG23	2.19	0.42
1:A:204:THR:HG23	1:A:380:HIS:HB2	2.01	0.41
1:A:347:SER:HA	1:A:353:GLN:NE2	2.35	0.41
1:A:722:ASP:N	1:A:722:ASP:OD1	2.53	0.41
1:A:885:ASN:HD22	1:A:885:ASN:HA	1.68	0.41
1:A:2:LYS:H	1:A:2:LYS:HG3	1.73	0.41
1:A:231:SER:O	1:A:231:SER:OG	2.37	0.41
1:A:248:GLN:HG3	1:A:267:GLU:O	2.20	0.41
1:A:763:HIS:HB3	1:A:771:VAL:HB	2.01	0.41
1:A:333:PHE:N	1:A:333:PHE:HD1	2.19	0.41
1:A:457:TRP:CE2	1:A:509:ARG:HB2	2.56	0.41
1:A:863:LEU:HB2	1:A:883:LEU:HD12	2.03	0.41
1:A:894:PHE:CD1	1:A:900:LEU:HB2	2.51	0.41
1:A:899:LYS:HA	1:A:899:LYS:HD2	1.87	0.41
1:A:265:LYS:HE3	1:A:265:LYS:HB3	1.79	0.40
1:A:294:GLU:OE2	1:A:334:SER:OG	2.34	0.40
1:A:466:VAL:HG23	1:A:507:MET:HE1	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:GLN:O	1:A:23:LYS:HG3	2.22	0.40
1:A:148:ILE:HG22	1:A:150:LEU:HG	2.03	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	1033/1032 (100%)	1022 (99%)	11 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	A	916/913 (100%)	910 (99%)	6 (1%)	76	87

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	SER
1	A	324	ASP
1	A	504	SER
1	A	765	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	797	GLN
1	A	1021	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	22	GLN
1	A	98	GLN
1	A	185	GLN
1	A	195	GLN
1	A	331	ASN
1	A	353	GLN
1	A	380	HIS
1	A	399	ASN
1	A	412	GLN
1	A	480	HIS
1	A	606	HIS
1	A	665	GLN
1	A	797	GLN
1	A	846	ASN
1	A	851	GLN
1	A	885	ASN
1	A	999	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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 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	TAR	A	1104	-	9,9,9	0.15	0	12,12,12	0.14	0
3	ILA	A	1103	-	33,33,33	0.79	1 (3%)	44,49,49	0.79	2 (4%)
4	TAR	A	1105	-	9,9,9	1.96	4 (44%)	12,12,12	1.84	4 (33%)
4	TAR	A	1107	-	9,9,9	1.40	2 (22%)	12,12,12	1.35	2 (16%)
4	TAR	A	1106	-	9,9,9	0.19	0	12,12,12	0.14	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	TAR	A	1104	-	-	6/12/12/12	-
3	ILA	A	1103	-	-	1/25/41/41	0/3/3/3
4	TAR	A	1105	-	-	6/12/12/12	-
4	TAR	A	1107	-	-	8/12/12/12	-
4	TAR	A	1106	-	-	10/12/12/12	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1105	TAR	O4-C4	3.11	1.31	1.22
4	A	1107	TAR	O4-C4	3.11	1.31	1.22
4	A	1105	TAR	O1-C1	3.09	1.31	1.22
3	A	1103	ILA	SA-N3A	2.94	1.69	1.63
4	A	1105	TAR	O41-C4	-2.78	1.21	1.30
4	A	1107	TAR	O41-C4	-2.77	1.21	1.30
4	A	1105	TAR	O11-C1	-2.76	1.21	1.30

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1107	TAR	O41-C4-C3	3.34	122.60	113.31
4	A	1105	TAR	O11-C1-C2	3.23	122.28	113.31
4	A	1105	TAR	O41-C4-C3	3.22	122.26	113.31
4	A	1107	TAR	O4-C4-C3	-3.22	113.05	121.62
4	A	1105	TAR	O1-C1-C2	-3.16	113.19	121.62
4	A	1105	TAR	O4-C4-C3	-3.12	113.31	121.62
3	A	1103	ILA	C-CA-N	-2.52	106.62	110.31
3	A	1103	ILA	O-C-CA	2.28	122.47	120.66

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1104	TAR	C1-C2-C3-O3
4	A	1104	TAR	C1-C2-C3-C4
4	A	1104	TAR	O2-C2-C3-O3
4	A	1104	TAR	O2-C2-C3-C4
4	A	1105	TAR	C1-C2-C3-O3
4	A	1105	TAR	C1-C2-C3-C4
4	A	1105	TAR	O2-C2-C3-O3
4	A	1105	TAR	O2-C2-C3-C4
4	A	1106	TAR	O1-C1-C2-O2
4	A	1106	TAR	O11-C1-C2-O2
4	A	1106	TAR	O3-C3-C4-O4
4	A	1106	TAR	O3-C3-C4-O41
4	A	1107	TAR	O1-C1-C2-O2
4	A	1107	TAR	O11-C1-C2-O2
4	A	1107	TAR	C1-C2-C3-C4
4	A	1107	TAR	O3-C3-C4-O4
4	A	1107	TAR	O3-C3-C4-O41
4	A	1107	TAR	O2-C2-C3-O3
4	A	1106	TAR	C1-C2-C3-O3
4	A	1106	TAR	O2-C2-C3-C4
4	A	1105	TAR	O3-C3-C4-O4
4	A	1105	TAR	O3-C3-C4-O41
4	A	1106	TAR	C2-C3-C4-O4
4	A	1106	TAR	C2-C3-C4-O41
4	A	1107	TAR	C1-C2-C3-O3
4	A	1107	TAR	O2-C2-C3-C4
4	A	1106	TAR	O2-C2-C3-O3
4	A	1106	TAR	C1-C2-C3-C4
4	A	1104	TAR	O1-C1-C2-O2
4	A	1104	TAR	O11-C1-C2-O2

Continued on next page...

Continued from previous page...

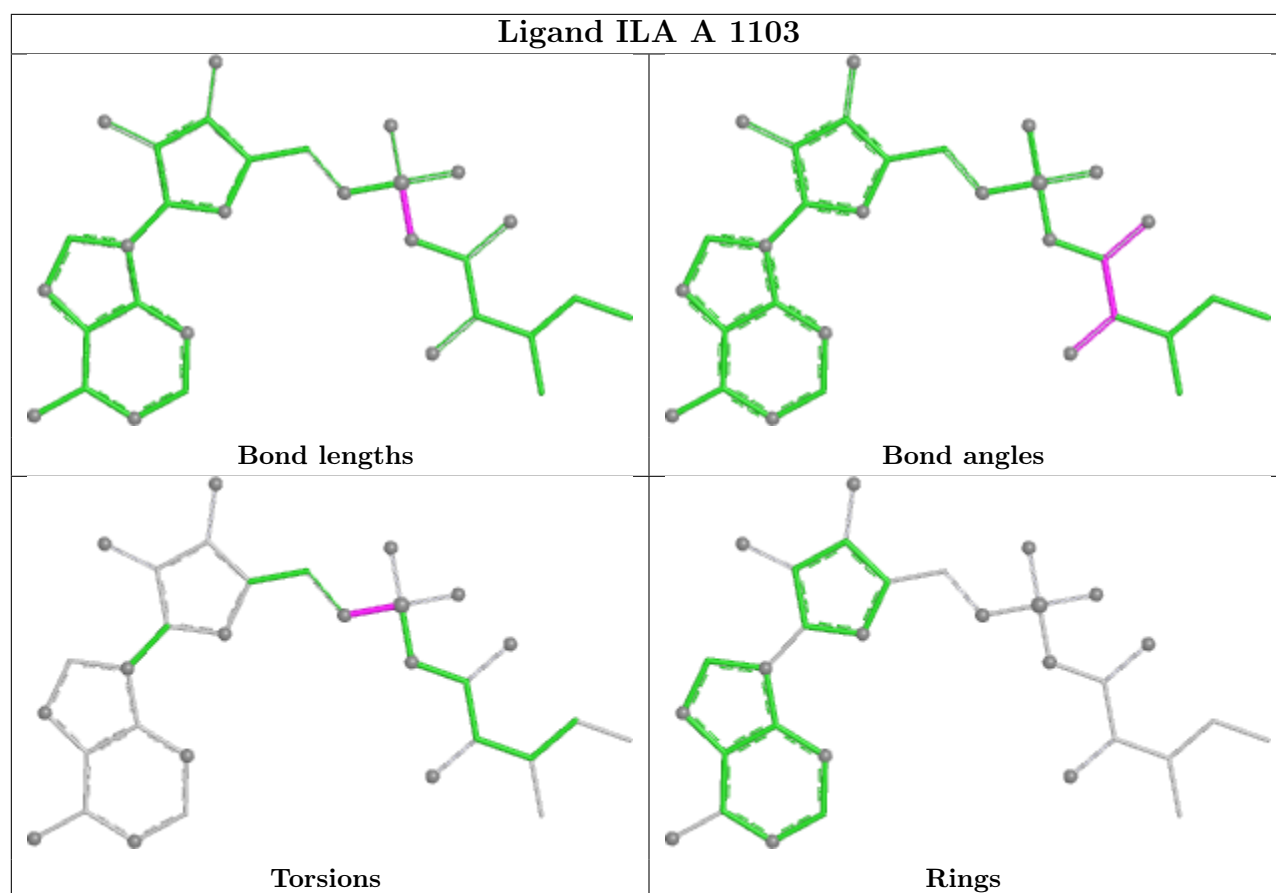
Mol	Chain	Res	Type	Atoms
3	A	1103	ILA	C5'-N5'-SA-O1A

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1103	ILA	1	0
4	A	1106	TAR	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	1032/1032 (100%)	0.33	77 (7%)	20 22	21, 53, 101, 123	3 (0%)

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1032	SER	6.1
1	A	6	VAL	6.0
1	A	5	ASN	5.5
1	A	367	TYR	5.2
1	A	369	ALA	5.0
1	A	265	LYS	5.0
1	A	803[A]	ARG	4.9
1	A	2	LYS	4.8
1	A	4	VAL	4.8
1	A	902	VAL	3.9
1	A	374	LEU	3.9
1	A	372	ASP	3.8
1	A	373	VAL	3.8
1	A	352	PHE	3.8
1	A	365	VAL	3.6
1	A	912	LEU	3.6
1	A	900	LEU	3.5
1	A	879	VAL	3.4
1	A	826	GLU	3.3
1	A	3	GLU	3.2
1	A	903	THR	3.2
1	A	290	PHE	3.1
1	A	368	LEU	3.1
1	A	291	VAL	3.0
1	A	360	CYS	3.0
1	A	594	SER	2.9
1	A	375	TYR	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	346	THR	2.8
1	A	371	GLN	2.8
1	A	1001	LEU	2.8
1	A	288	PHE	2.8
1	A	336	VAL	2.8
1	A	266	GLY	2.7
1	A	886	LEU	2.7
1	A	378	GLU	2.7
1	A	905	ALA	2.6
1	A	362	VAL	2.6
1	A	1	MET	2.6
1	A	370	ASN	2.6
1	A	366	ARG	2.6
1	A	593	LYS	2.6
1	A	302	ALA	2.6
1	A	207	VAL	2.6
1	A	825	THR	2.5
1	A	870	PRO	2.5
1	A	301	THR	2.4
1	A	898	GLY	2.4
1	A	349	VAL	2.4
1	A	971	VAL	2.4
1	A	1031	GLN	2.4
1	A	233	VAL	2.4
1	A	715	TRP	2.4
1	A	296	GLY	2.4
1	A	934	MET	2.4
1	A	294	GLU	2.4
1	A	216	ASN	2.3
1	A	363	ASP	2.3
1	A	598	ALA	2.3
1	A	379	LYS	2.3
1	A	218	TYR	2.2
1	A	914	THR	2.2
1	A	883	LEU	2.2
1	A	359	ASP	2.2
1	A	281	GLY	2.2
1	A	203	LEU	2.2
1	A	970	PRO	2.2
1	A	234	ALA	2.2
1	A	364	ILE	2.1
1	A	289	ASN	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	345	TYR	2.1
1	A	596	GLY	2.1
1	A	351	PRO	2.1
1	A	1028	VAL	2.1
1	A	333	PHE	2.1
1	A	666	THR	2.1
1	A	911	THR	2.1
1	A	308	GLN	2.1

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

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

6.3 Carbohydrates ⓘ

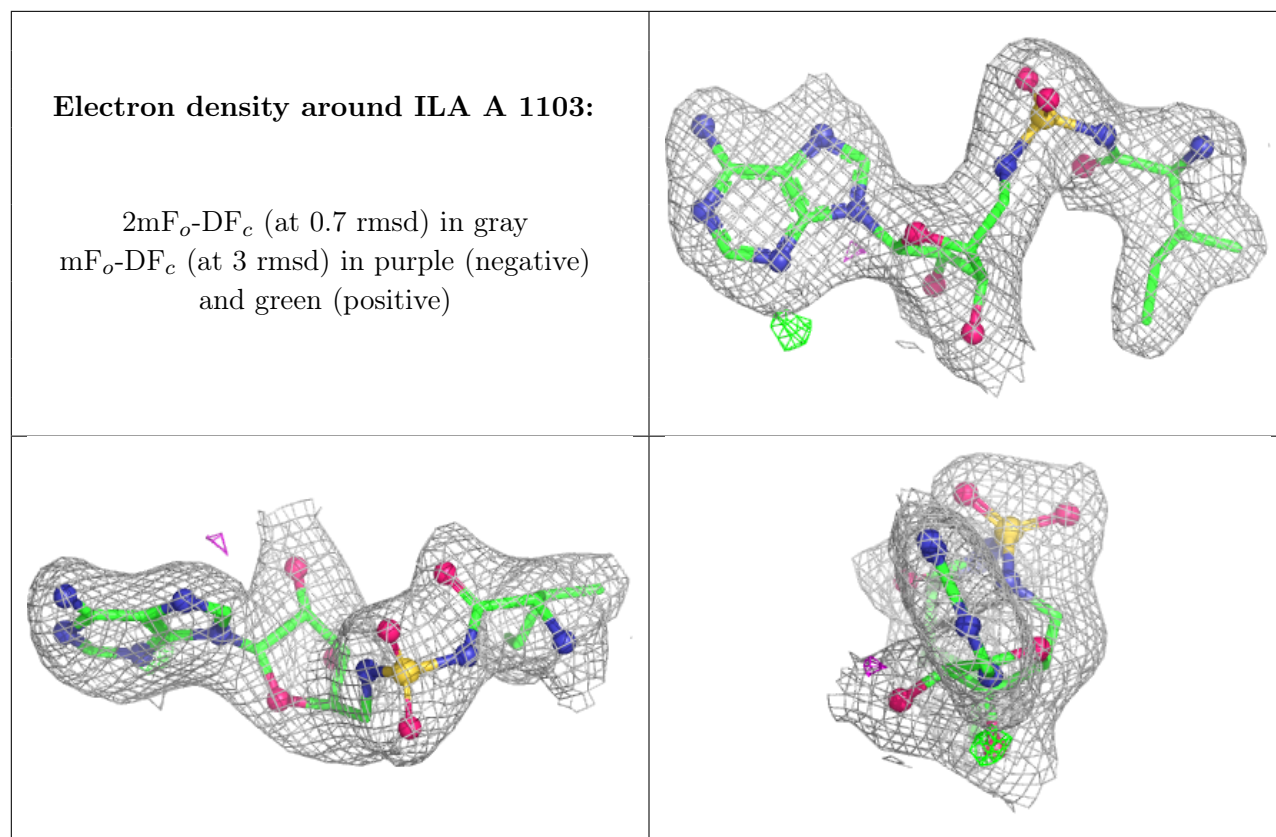
There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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
4	TAR	A	1105	10/10	0.71	0.12	79,83,87,89	0
4	TAR	A	1104	10/10	0.76	0.12	70,82,90,91	0
4	TAR	A	1106	10/10	0.76	0.12	68,72,89,93	0
4	TAR	A	1107	10/10	0.82	0.10	57,59,73,75	0
3	ILA	A	1103	31/31	0.97	0.06	27,35,41,42	0
2	ZN	A	1101	1/1	0.99	0.04	49,49,49,49	0
2	ZN	A	1102	1/1	1.00	0.02	44,44,44,44	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.