



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 08:13 PM UTC

PDB ID : 8WND / pdb_00008wnd
Title : Crystal structure of *Saccharomyces cerevisiae* isoleucyl-tRNA synthetase in complex with tRNA(Ile) and isoleucine
Authors : Chen, B.; Yi, F.; Zhou, H.
Deposited on : 2023-10-05
Resolution : 2.80 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

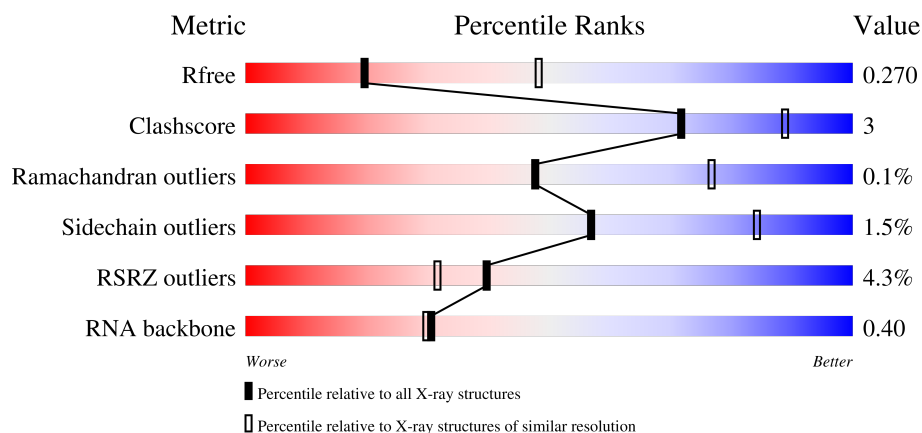
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)
RNA backbone	3983	1114 (3.00-2.60)

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	1080	3% 88% 9% .
1	B	1080	5% 80% 7% 13%
2	R	77	% 56% 27% 6% . 9%
2	T	77	% 66% 32% .

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 18444 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	1061	Total	C	N	O	S	0	0	0
			8192	5265	1354	1547	26			
1	B	936	Total	C	N	O	S	0	0	0
			6875	4393	1152	1306	24			

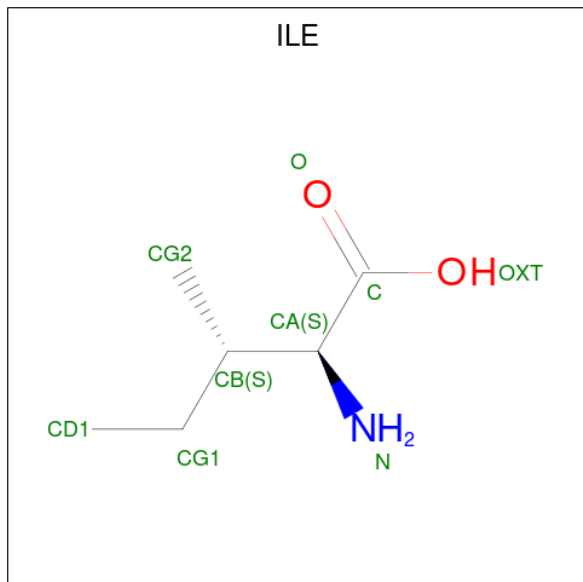
There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1073	LEU	-	expression tag	UNP A0A6A5Q0L4
A	1074	GLU	-	expression tag	UNP A0A6A5Q0L4
A	1075	HIS	-	expression tag	UNP A0A6A5Q0L4
A	1076	HIS	-	expression tag	UNP A0A6A5Q0L4
A	1077	HIS	-	expression tag	UNP A0A6A5Q0L4
A	1078	HIS	-	expression tag	UNP A0A6A5Q0L4
A	1079	HIS	-	expression tag	UNP A0A6A5Q0L4
A	1080	HIS	-	expression tag	UNP A0A6A5Q0L4
B	1073	LEU	-	expression tag	UNP A0A6A5Q0L4
B	1074	GLU	-	expression tag	UNP A0A6A5Q0L4
B	1075	HIS	-	expression tag	UNP A0A6A5Q0L4
B	1076	HIS	-	expression tag	UNP A0A6A5Q0L4
B	1077	HIS	-	expression tag	UNP A0A6A5Q0L4
B	1078	HIS	-	expression tag	UNP A0A6A5Q0L4
B	1079	HIS	-	expression tag	UNP A0A6A5Q0L4
B	1080	HIS	-	expression tag	UNP A0A6A5Q0L4

- Molecule 2 is a RNA chain called tRNA(Ile).

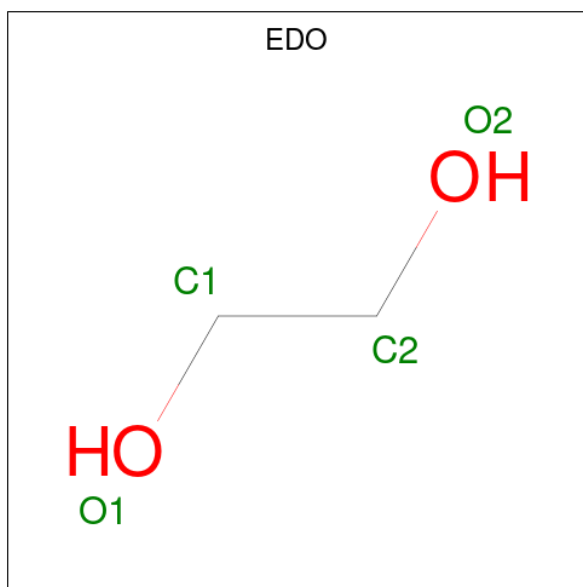
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	T	77	Total	C	N	O	P	0	0	0
			1621	721	288	535	77			
2	R	70	Total	C	N	O	P	0	0	0
			1481	659	264	488	70			

- Molecule 3 is ISOLEUCINE (CCD ID: ILE) (formula: $C_6H_{13}NO_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			9	6	1	2		
3	B	1	Total	C	N	O	0	0
			9	6	1	2		

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

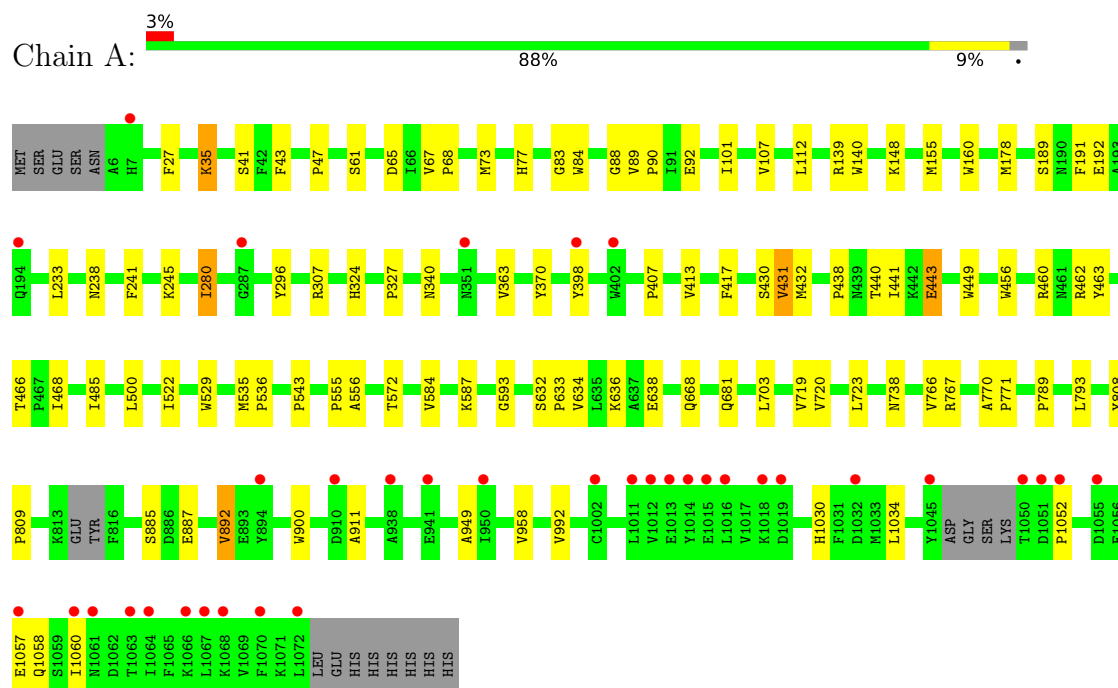
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	112	Total 112	O 112	0	0
6	T	48	Total 48	O 48	0	0
6	B	46	Total 46	O 46	0	0
6	R	2	Total 2	O 2	0	0

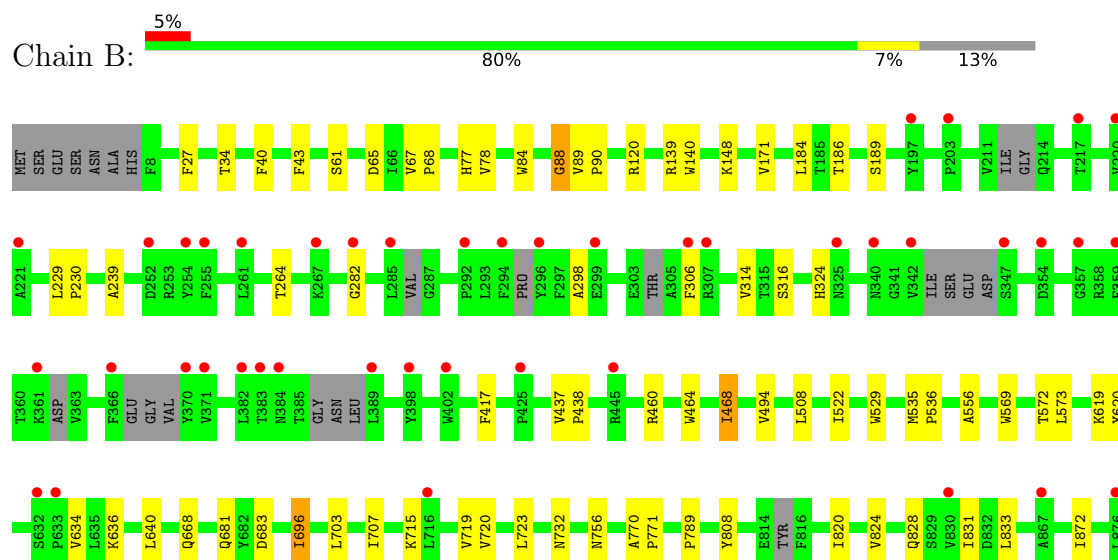
3 Residue-property plots

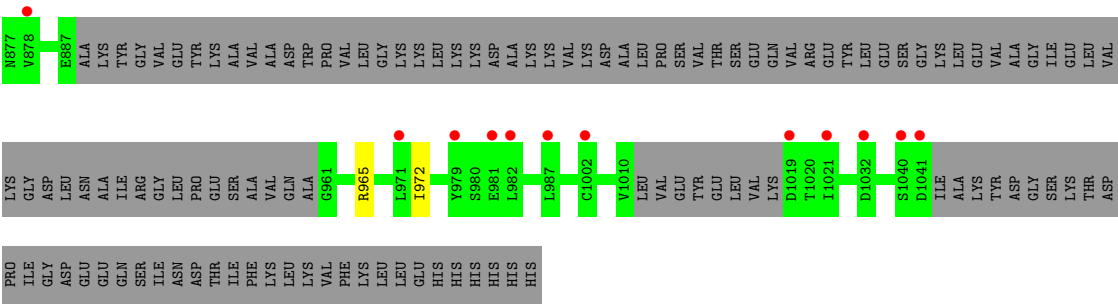
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

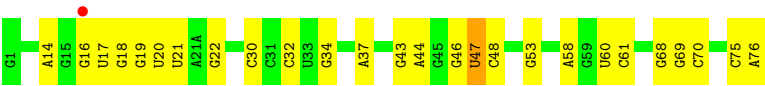


• Molecule 1: isoleucine-tRNA ligase

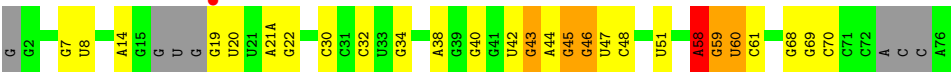




● Molecule 2: tRNA(Ile)



● Molecule 2: tRNA(Ile)



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	53.43Å 173.52Å 171.80Å 90.00° 91.16° 90.00°	Depositor
Resolution (Å)	48.73 – 2.80 48.73 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.2 (48.73-2.80) 98.2 (48.73-2.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.44 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.230 , 0.268 0.234 , 0.270	Depositor DCC
R_{free} test set	3604 reflections (4.69%)	wwPDB-VP
Wilson B-factor (Å ²)	63.3	Xtriage
Anisotropy	0.045	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 59.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.009 for -h,-l,-k 0.000 for -h,l,k 0.031 for h,-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	18444	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.87% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, SO4

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	0.98	0/8391	1.37	6/11430 (0.1%)
1	B	1.02	0/7043	1.42	4/9627 (0.0%)
2	R	0.52	0/1653	0.74	2/2571 (0.1%)
2	T	0.53	0/1811	0.79	0/2822
All	All	0.93	0/18898	1.29	12/26450 (0.0%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	88	GLY	CA-C-N	11.06	127.21	120.24
1	B	88	GLY	C-N-CA	11.06	127.21	120.24
1	A	88	GLY	CA-C-N	9.17	126.01	120.24
1	A	88	GLY	C-N-CA	9.17	126.01	120.24
2	R	60	U	C4'-C3'-O3'	5.64	117.86	109.40
1	B	719	VAL	CA-C-N	5.58	123.75	120.24
1	B	719	VAL	C-N-CA	5.58	123.75	120.24
1	A	719	VAL	CA-C-N	5.32	123.59	120.24
1	A	719	VAL	C-N-CA	5.32	123.59	120.24
1	A	885	SER	N-CA-C	-5.20	106.96	113.72
1	A	1060	ILE	CA-C-O	-5.16	118.14	122.63
2	R	58	A	C4'-C3'-O3'	5.15	117.13	109.40

There are no chirality outliers.

There are no planarity outliers.

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	8192	0	7653	59	0
1	B	6875	0	5889	44	0
2	R	1481	0	749	7	0
2	T	1621	0	819	3	0
3	A	9	0	10	0	0
3	B	9	0	10	0	0
4	A	4	0	6	0	0
5	A	25	0	0	0	0
5	B	20	0	0	0	0
6	A	112	0	0	3	0
6	B	46	0	0	0	0
6	R	2	0	0	0	0
6	T	48	0	0	0	0
All	All	18444	0	15136	111	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 (111) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:45:G:H5''	2:R:46:G:OP2	1.39	1.23
1:B:239:ALA:HA	1:B:282:GLY:HA3	1.48	0.92
2:R:45:G:C5'	2:R:46:G:OP2	2.24	0.84
1:B:634:VAL:HG11	1:B:640:LEU:HB3	1.73	0.69
1:A:703:LEU:HD21	1:A:723:LEU:HD23	1.74	0.68
2:R:58:A:H4'	2:R:59:G:OP1	1.94	0.68
1:B:703:LEU:HD21	1:B:723:LEU:HD23	1.77	0.66
1:A:432:MET:HE1	1:A:443:GLU:HG3	1.76	0.65
1:A:431:VAL:HG23	1:A:584:VAL:HG11	1.80	0.62
1:A:529:TRP:HB3	1:A:572:THR:HG21	1.80	0.62
1:B:89:VAL:N	1:B:90:PRO:CD	2.63	0.62
1:A:468:ILE:HB	1:A:522:ILE:HD11	1.80	0.62
1:B:239:ALA:HA	1:B:282:GLY:CA	2.28	0.61
2:R:43:G:H2'	2:R:44:A:C8	2.36	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:89:VAL:N	1:B:90:PRO:HD2	2.16	0.60
1:B:634:VAL:HG13	1:B:640:LEU:HB2	1.85	0.59
1:B:529:TRP:HB3	1:B:572:THR:HG21	1.84	0.59
1:A:101:ILE:HG21	1:A:107:VAL:HG23	1.84	0.59
1:B:634:VAL:HG11	1:B:640:LEU:CB	2.32	0.59
1:A:958:VAL:HA	6:A:1203:HOH:O	2.03	0.58
1:B:88:GLY:C	1:B:90:PRO:HD2	2.29	0.58
1:A:67:VAL:HB	1:A:68:PRO:HD3	1.86	0.58
1:B:634:VAL:CG1	1:B:640:LEU:HB2	2.35	0.57
1:B:634:VAL:CG1	1:B:640:LEU:CB	2.82	0.56
1:A:35:LYS:HA	1:A:77:HIS:CD2	2.41	0.55
1:A:307:ARG:NH2	1:A:340:ASN:O	2.38	0.54
1:A:41:SER:HB3	1:A:556:ALA:HA	1.90	0.53
1:B:770:ALA:HB3	1:B:771:PRO:HD3	1.92	0.53
1:A:178:MET:HE3	1:A:413:VAL:HG23	1.91	0.51
1:A:632:SER:OG	1:A:634:VAL:HG22	2.11	0.51
1:B:824:VAL:O	1:B:828:GLN:HG3	2.11	0.51
1:B:833:LEU:HD22	1:B:965:ARG:HB3	1.94	0.50
1:B:468:ILE:HB	1:B:522:ILE:HD11	1.93	0.50
1:B:535:MET:HG3	1:B:536:PRO:HD3	1.93	0.50
1:A:438:PRO:HG2	1:A:441:ILE:HG12	1.93	0.50
1:A:238:ASN:HB3	1:A:241:PHE:CD2	2.47	0.50
1:A:555:PRO:HG2	1:A:587:LYS:HD2	1.94	0.50
1:B:184:LEU:HB3	1:B:186:THR:HG22	1.93	0.50
1:A:296:TYR:CE2	1:A:363:VAL:HG13	2.47	0.49
1:A:245:LYS:HB2	1:A:280:ILE:HD11	1.93	0.49
1:A:992:VAL:HG23	1:A:1034:LEU:HD23	1.94	0.49
1:A:47:PRO:HD2	1:A:83:GLY:O	2.12	0.49
1:A:191:PHE:HB3	1:A:449:TRP:HZ2	1.78	0.49
1:A:1057:GLU:C	1:A:1058:GLN:HG3	2.38	0.49
1:B:619:LYS:HD2	1:B:620:TYR:CZ	2.48	0.49
1:A:535:MET:HG3	1:A:536:PRO:HD3	1.94	0.48
1:A:233:LEU:HD12	1:A:327:PRO:HG3	1.95	0.48
1:B:84:TRP:HB2	1:B:148:LYS:HG2	1.94	0.48
1:B:65:ASP:HB2	1:B:139:ARG:HG3	1.95	0.48
1:B:720:VAL:HA	1:B:723:LEU:HD12	1.95	0.48
1:A:89:VAL:N	1:A:90:PRO:CD	2.76	0.47
1:A:27:PHE:CD1	1:A:140:TRP:HB3	2.49	0.47
1:A:65:ASP:HB2	1:A:139:ARG:HG3	1.95	0.47
1:A:593:GLY:HA3	1:A:638:GLU:O	2.15	0.47
1:A:633:PRO:HB2	1:A:638:GLU:HB2	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:189:SER:HB3	1:B:460:ARG:NH2	2.29	0.47
1:B:171:VAL:HA	1:B:417:PHE:O	2.14	0.46
1:A:681:GLN:HG3	1:A:789:PRO:HG3	1.97	0.46
1:A:887:GLU:HB3	1:A:892:VAL:HG22	1.96	0.46
1:A:900:TRP:HZ3	1:A:911:ALA:HB1	1.81	0.46
1:A:634:VAL:HA	1:A:638:GLU:O	2.15	0.46
1:A:189:SER:HB3	1:A:460:ARG:HH22	1.81	0.46
1:B:634:VAL:CG1	1:B:640:LEU:HB3	2.44	0.46
1:A:720:VAL:HA	1:A:723:LEU:HD12	1.98	0.45
1:A:160:TRP:NE1	1:A:543:PRO:HG3	2.32	0.45
1:A:92:GLU:HB3	1:A:462:ARG:HH21	1.82	0.45
1:A:160:TRP:CD2	1:A:543:PRO:HD3	2.52	0.45
1:B:120:ARG:HG2	1:B:464:TRP:CH2	2.52	0.45
1:B:298:ALA:HB2	1:B:306:PHE:CD1	2.52	0.44
1:A:417:PHE:HA	1:A:456:TRP:O	2.18	0.44
1:A:73:MET:HB3	1:A:808:TYR:HB2	1.99	0.44
2:T:47:U:OP1	2:T:47:U:H2'	2.17	0.44
1:B:683:ASP:O	1:B:756:ASN:ND2	2.45	0.44
1:B:229:LEU:N	1:B:230:PRO:CD	2.80	0.44
1:A:949:ALA:HB3	6:A:1210:HOH:O	2.18	0.44
2:R:45:G:C4'	2:R:46:G:OP2	2.65	0.44
1:A:43:PHE:CE2	1:A:556:ALA:HB2	2.54	0.43
1:A:767:ARG:HB3	1:A:809:PRO:HD3	2.00	0.43
1:A:61:SER:HB3	1:A:139:ARG:HD2	2.00	0.43
1:A:84:TRP:HB2	1:A:148:LYS:HG2	2.00	0.43
1:B:707:ILE:HG21	1:B:808:TYR:OH	2.18	0.43
1:A:178:MET:HE3	1:A:178:MET:HB2	1.92	0.43
1:A:112:LEU:HD11	1:A:463:TYR:HB3	2.00	0.43
1:B:569:TRP:CE2	1:B:573:LEU:HD11	2.53	0.43
1:B:696:ILE:HD12	1:B:696:ILE:HA	1.78	0.43
1:B:732:ASN:OD1	2:R:40:G:H5''	2.19	0.43
1:A:398:TYR:HE1	2:T:75:C:H1'	1.83	0.43
1:A:485:ILE:HG12	1:A:500:LEU:HD21	2.01	0.43
1:A:430:SER:HB3	1:A:584:VAL:HG13	2.01	0.43
1:A:738:ASN:HA	6:A:1247:HOH:O	2.19	0.43
1:B:40:PHE:HB3	1:B:78:VAL:HG22	2.01	0.42
1:A:1030:HIS:O	1:A:1034:LEU:HD12	2.19	0.42
1:A:992:VAL:HG23	1:A:1034:LEU:CD2	2.49	0.42
1:B:67:VAL:HB	1:B:68:PRO:HD3	2.00	0.42
1:B:61:SER:HB3	1:B:139:ARG:HD2	2.01	0.42
1:B:43:PHE:CE2	1:B:556:ALA:HB2	2.53	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:770:ALA:HB3	1:A:771:PRO:HD3	2.00	0.42
1:B:229:LEU:N	1:B:230:PRO:HD2	2.35	0.42
1:B:437:VAL:HA	1:B:438:PRO:HA	1.78	0.42
2:T:43:G:H2'	2:T:44:A:C8	2.55	0.41
1:A:155:MET:HE3	1:A:466:THR:HA	2.01	0.41
1:A:887:GLU:HB3	1:A:892:VAL:CG2	2.50	0.41
1:A:793:LEU:HD23	1:A:793:LEU:HA	1.86	0.41
1:A:189:SER:HB3	1:A:460:ARG:NH2	2.36	0.40
1:B:27:PHE:CD1	1:B:140:TRP:HB3	2.55	0.40
1:B:494:VAL:HG21	1:B:508:LEU:HD22	2.03	0.40
1:B:681:GLN:CG	1:B:789:PRO:HG3	2.51	0.40
1:A:370:TYR:OH	1:A:407:PRO:HG2	2.21	0.40
2:R:42:U:C2'	2:R:43:G:O5'	2.69	0.40
1:B:34:THR:O	1:B:77:HIS:HB2	2.21	0.40
1:B:831:ILE:HD11	1:B:872:ILE:HA	2.04	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	1055/1080 (98%)	1007 (96%)	47 (4%)	1 (0%)	48	77
1	B	912/1080 (84%)	850 (93%)	62 (7%)	0	100	100
All	All	1967/2160 (91%)	1857 (94%)	109 (6%)	1 (0%)	48	77

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1052	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	824/967 (85%)	813 (99%)	11 (1%)	61	86
1	B	611/967 (63%)	600 (98%)	11 (2%)	51	82
All	All	1435/1934 (74%)	1413 (98%)	22 (2%)	57	84

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	LYS
1	A	192	GLU
1	A	280	ILE
1	A	324	HIS
1	A	431	VAL
1	A	440	THR
1	A	443	GLU
1	A	636	LYS
1	A	668	GLN
1	A	766	VAL
1	A	892	VAL
1	B	264	THR
1	B	314	VAL
1	B	316	SER
1	B	324	HIS
1	B	468	ILE
1	B	636	LYS
1	B	668	GLN
1	B	696	ILE
1	B	715	LYS
1	B	820	ILE
1	B	972	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	HIS
1	A	210	ASN
1	A	232	ASN
1	A	439	ASN
1	A	948	ASN
1	A	977	ASN
1	B	57	HIS
1	B	166	HIS
1	B	232	ASN
1	B	334	ASN
1	B	514	GLN
1	B	681	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	R	68/77 (88%)	19 (27%)	6 (8%)
2	T	76/77 (98%)	22 (28%)	3 (3%)
All	All	144/154 (93%)	41 (28%)	9 (6%)

All (41) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	T	14	A
2	T	16	G
2	T	17	U
2	T	18	G
2	T	19	G
2	T	20	U
2	T	21	U
2	T	22	G
2	T	30	C
2	T	32	C
2	T	34	G
2	T	37	A
2	T	46	G
2	T	47	U
2	T	48	C
2	T	53	G
2	T	58	A
2	T	61	C
2	T	68	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	T	69	G
2	T	70	C
2	T	76	A
2	R	8	U
2	R	14	A
2	R	20	U
2	R	21(A)	A
2	R	22	G
2	R	30	C
2	R	32	C
2	R	34	G
2	R	38	A
2	R	43	G
2	R	46	G
2	R	47	U
2	R	48	C
2	R	51	U
2	R	59	G
2	R	61	C
2	R	68	G
2	R	69	G
2	R	70	C

All (9) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	T	18	G
2	T	46	G
2	T	60	U
2	R	7	G
2	R	19	G
2	R	45	G
2	R	48	C
2	R	58	A
2	R	60	U

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](#)

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	$\# Z > 2$
5	SO4	A	1104	-	4,4,4	0.24	0	6,6,6	0.09	0
5	SO4	A	1106	-	4,4,4	0.29	0	6,6,6	0.10	0
5	SO4	B	1105	-	4,4,4	0.23	0	6,6,6	0.10	0
5	SO4	A	1107	-	4,4,4	0.24	0	6,6,6	0.07	0
5	SO4	B	1102	-	4,4,4	0.21	0	6,6,6	0.08	0
5	SO4	A	1105	-	4,4,4	0.24	0	6,6,6	0.10	0
5	SO4	B	1103	-	4,4,4	0.23	0	6,6,6	0.10	0
5	SO4	B	1104	-	4,4,4	0.26	0	6,6,6	0.06	0
3	ILE	B	1101	-	8,8,8	0.48	0	9,10,10	0.40	0
3	ILE	A	1101	-	8,8,8	1.25	2 (25%)	9,10,10	0.95	0
5	SO4	A	1103	-	4,4,4	0.24	0	6,6,6	0.10	0
4	EDO	A	1102	-	3,3,3	0.08	0	2,2,2	0.19	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	ILE	B	1101	-	-	3/10/10/10	-
3	ILE	A	1101	-	-	3/10/10/10	-
4	EDO	A	1102	-	-	0/1/1/1	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1101	ILE	OXT-C	-2.51	1.22	1.30
3	A	1101	ILE	O-C	2.29	1.28	1.22

There are no bond angle outliers.

There are no chirality outliers.

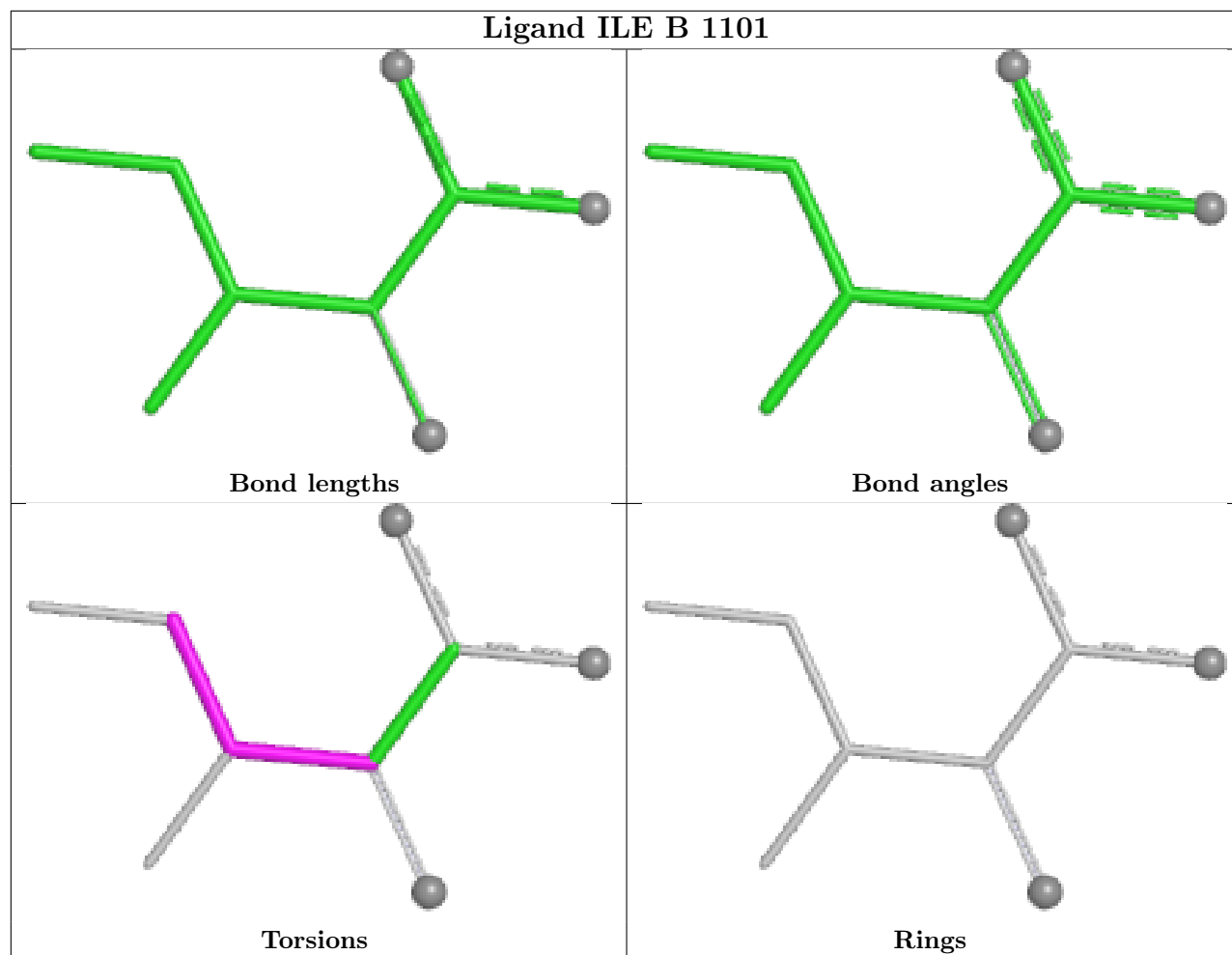
All (6) torsion outliers are listed below:

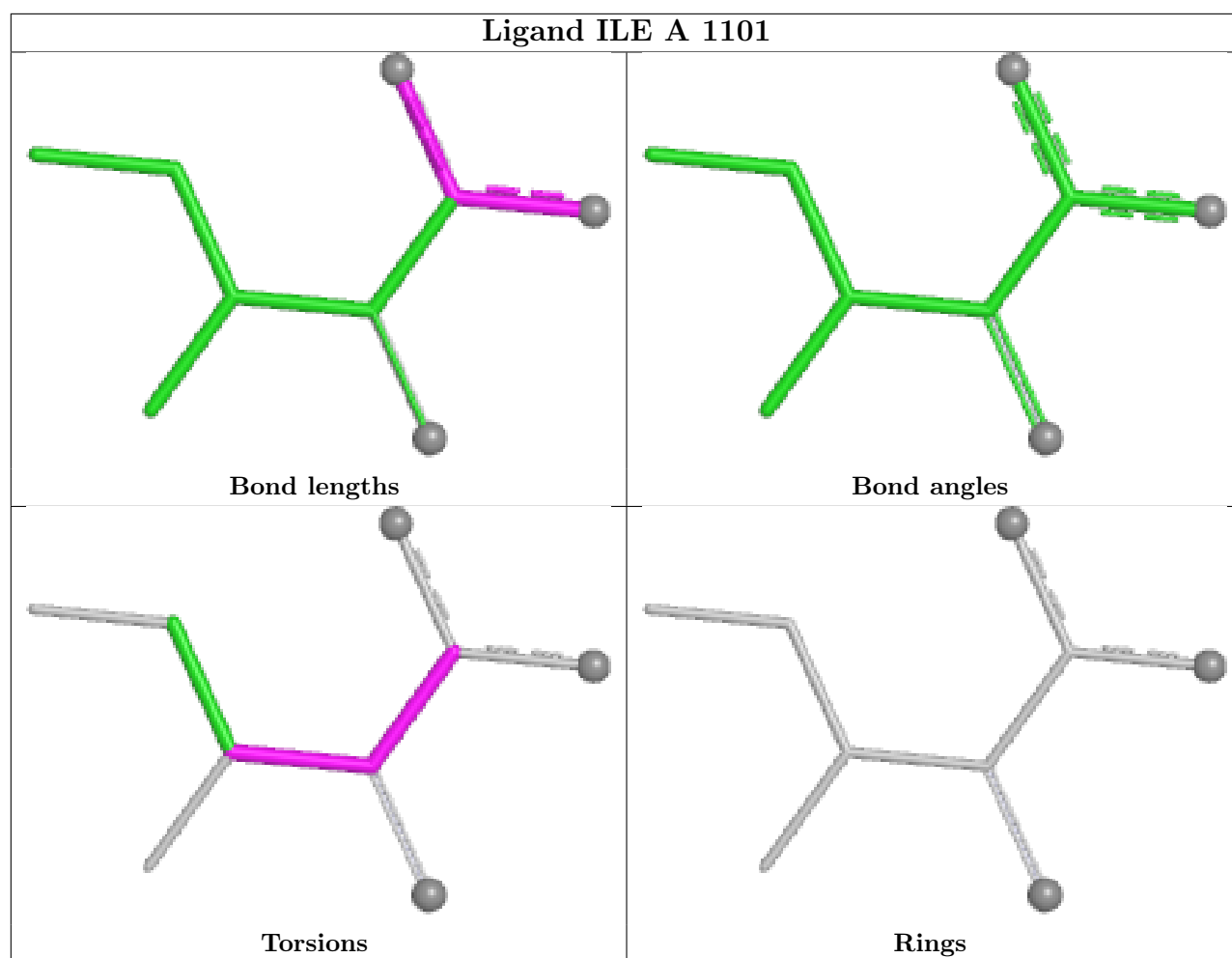
Mol	Chain	Res	Type	Atoms
3	B	1101	ILE	C-CA-CB-CG1
3	A	1101	ILE	C-CA-CB-CG1
3	B	1101	ILE	CA-CB-CG1-CD1
3	B	1101	ILE	CG2-CB-CG1-CD1
3	A	1101	ILE	OXT-C-CA-N
3	A	1101	ILE	O-C-CA-N

There are no ring outliers.

No monomer is involved in short contacts.

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	1061/1080 (98%)	0.21	36 (3%) 48 39	32, 53, 97, 136	0
1	B	936/1080 (86%)	0.69	55 (5%) 28 21	43, 74, 109, 130	0
2	R	70/77 (90%)	0.64	1 (1%) 73 64	70, 130, 181, 196	0
2	T	77/77 (100%)	-0.15	1 (1%) 75 66	33, 66, 101, 133	0
All	All	2144/2314 (92%)	0.42	93 (4%) 40 31	32, 63, 111, 196	0

All (93) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1068	LYS	3.6
1	A	1061	ASN	3.5
1	A	1060	ILE	3.4
1	A	1050	THR	3.3
1	A	1013	GLU	3.3
1	A	1072	LEU	3.3
1	A	1051	ASP	3.3
1	B	632	SER	3.3
1	B	292	PRO	3.2
1	A	7	HIS	3.1
1	B	325	ASN	3.1
1	B	384	ASN	3.1
1	B	306	PHE	3.0
1	B	366	PHE	3.0
1	B	370	TYR	3.0
1	A	1064	ILE	3.0
1	B	307	ARG	3.0
1	B	203	PRO	2.9
1	B	1002	CYS	2.9
1	B	299	GLU	2.9
1	A	894	TYR	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	294	PHE	2.9
1	B	347	SER	2.8
1	A	194	GLN	2.8
1	A	398	TYR	2.8
1	B	445	ARG	2.7
1	A	1067	LEU	2.7
1	B	1019	ASP	2.7
1	B	633	PRO	2.7
1	A	1015	GLU	2.6
1	B	402	TRP	2.6
1	B	254	TYR	2.6
1	B	383	THR	2.6
1	A	1002	CYS	2.6
1	A	1055	ASP	2.6
1	B	221	ALA	2.6
1	B	1032	ASP	2.6
1	B	389	LEU	2.6
1	A	351	ASN	2.6
1	A	1016	LEU	2.5
1	A	941	GLU	2.5
1	A	938	ALA	2.5
1	A	950	ILE	2.5
2	T	16	G	2.5
1	A	1057	GLU	2.5
1	B	382	LEU	2.5
1	A	1052	PRO	2.5
1	B	425	PRO	2.5
1	B	342	VAL	2.4
1	B	296	TYR	2.4
1	B	357	GLY	2.4
1	A	1045	TYR	2.4
1	B	867	ALA	2.4
1	A	1014	TYR	2.4
1	B	197	TYR	2.4
1	B	878	VAL	2.4
1	B	359	PHE	2.4
1	B	398	TYR	2.3
1	B	371	VAL	2.3
1	A	1032	ASP	2.3
1	A	910	ASP	2.3
1	B	971	LEU	2.3
1	B	982	LEU	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	987	LEU	2.3
1	A	402	TRP	2.3
1	B	340	ASN	2.2
1	B	981	GLU	2.2
1	B	1021	ILE	2.2
1	B	1041	ASP	2.2
1	A	1012	VAL	2.2
1	B	285	LEU	2.2
1	B	979	TYR	2.2
1	B	361	LYS	2.2
1	B	261	LEU	2.2
1	B	830	VAL	2.1
2	R	19	G	2.1
1	B	716	LEU	2.1
1	B	220	VAL	2.1
1	A	1066	LYS	2.1
1	A	1019	ASP	2.1
1	B	354	ASP	2.1
1	A	1070	PHE	2.1
1	B	255	PHE	2.1
1	B	876	LEU	2.1
1	A	287	GLY	2.1
1	A	1011	LEU	2.1
1	B	282	GLY	2.1
1	B	267	LYS	2.1
1	A	1063	THR	2.1
1	B	252	ASP	2.1
1	A	1018	LYS	2.0
1	B	217	THR	2.0
1	B	1040	SER	2.0

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

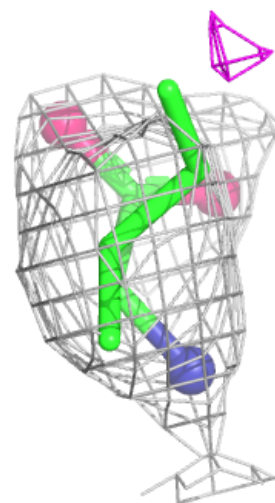
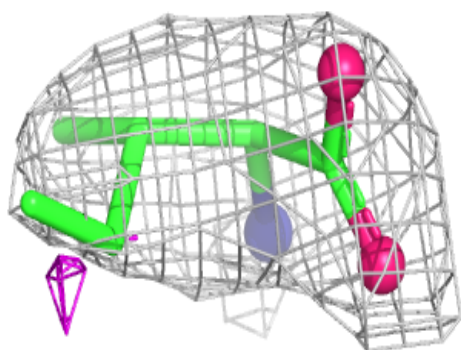
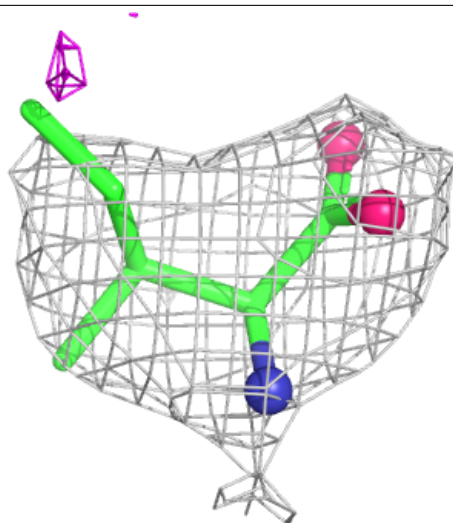
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

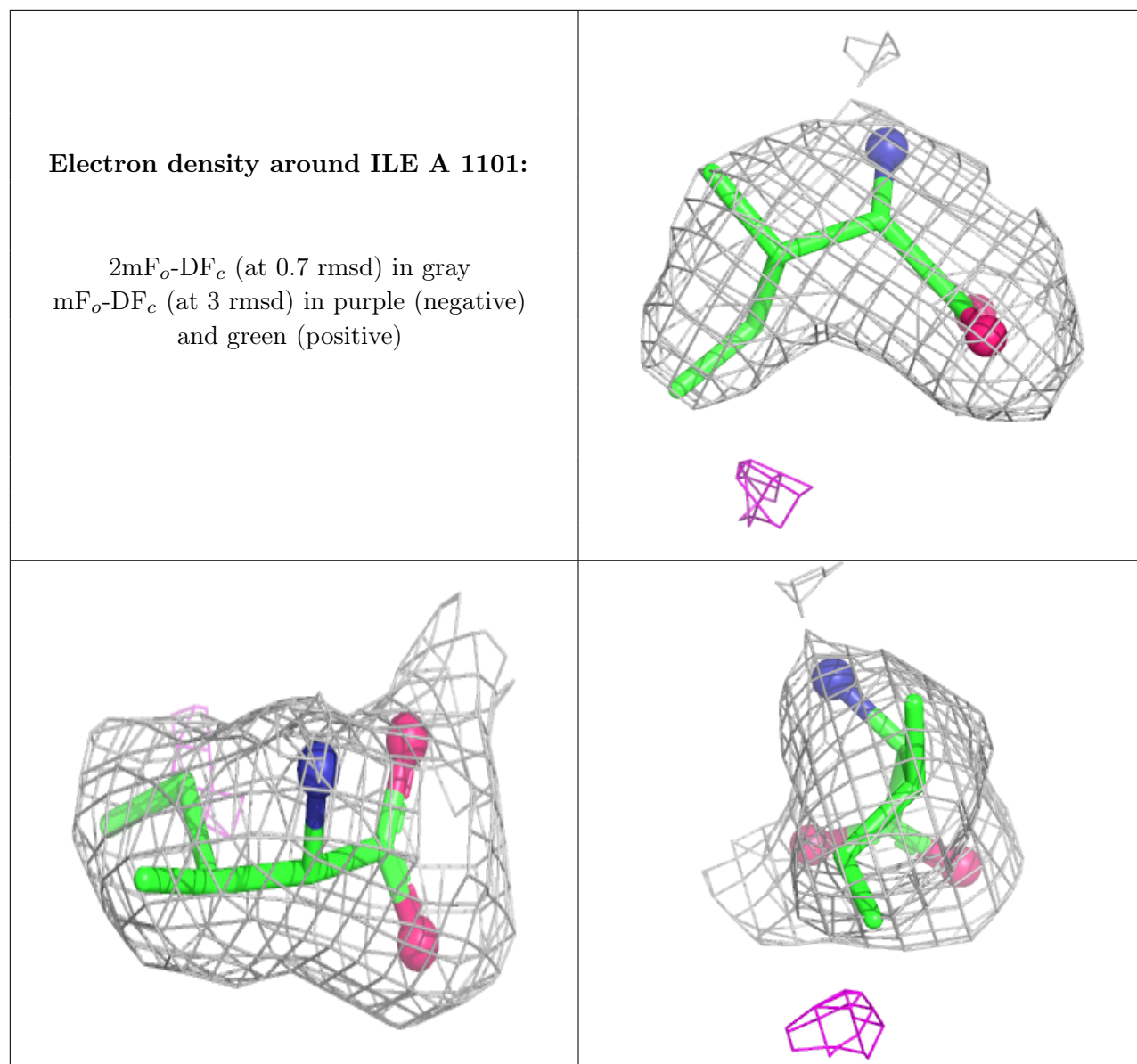
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	EDO	A	1102	4/4	0.77	0.16	45,48,48,50	0
5	SO4	A	1106	5/5	0.81	0.16	68,73,75,79	0
5	SO4	B	1103	5/5	0.86	0.19	64,66,68,71	0
5	SO4	B	1102	5/5	0.90	0.22	68,70,73,80	0
5	SO4	A	1103	5/5	0.90	0.18	63,66,73,76	0
5	SO4	B	1105	5/5	0.90	0.17	60,60,67,68	0
3	ILE	B	1101	9/9	0.92	0.15	56,58,62,63	0
5	SO4	A	1105	5/5	0.92	0.15	58,58,63,64	0
5	SO4	B	1104	5/5	0.93	0.15	55,57,61,63	0
5	SO4	A	1107	5/5	0.93	0.14	62,62,67,68	0
5	SO4	A	1104	5/5	0.95	0.11	62,65,67,71	0
3	ILE	A	1101	9/9	0.96	0.10	42,44,48,49	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 ILE B 1101:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.