



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:48 AM UTC

PDB ID : 9CLL / pdb_00009cll
Title : Plasmodium falciparum tyrosyl-tRNA synthetase in complex with ML471-Tyr
Authors : Tai, C.W.; Dogovski, C.; Xie, S.C.; Tilley, L.; Griffin, M.D.W.
Deposited on : 2024-07-11
Resolution : 1.80 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

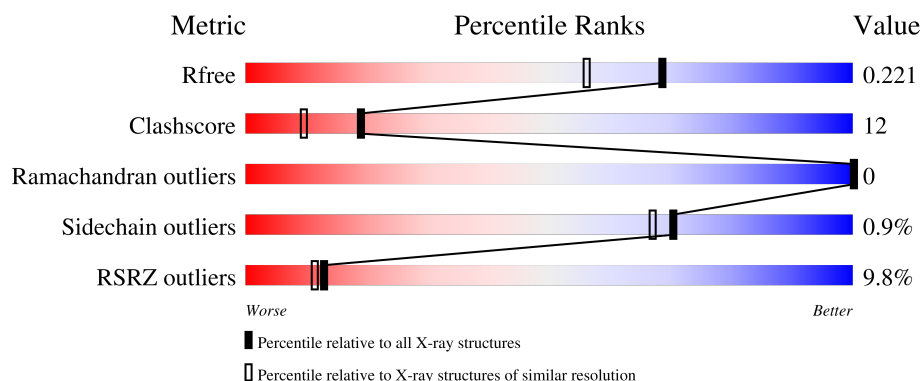
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	373	15% 70% 24% 6%
1	B	373	3% 80% 13% 7%

2 Entry composition [i](#)

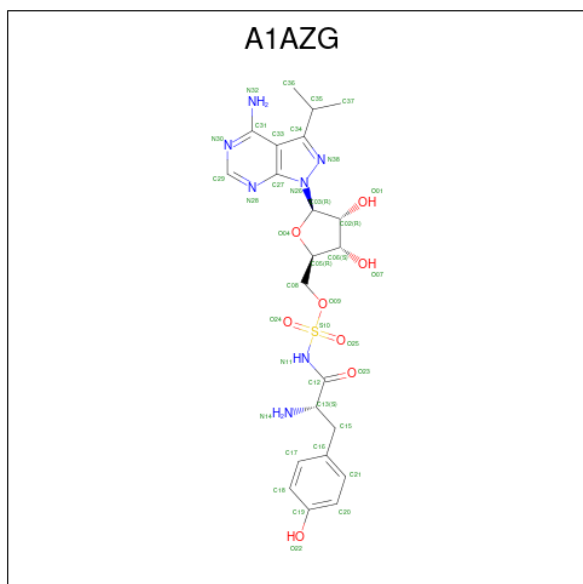
There are 6 unique types of molecules in this entry. The entry contains 6221 atoms, of which 62 are hydrogens and 0 are deuteriums.

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 tyrosine-tRNA ligase.

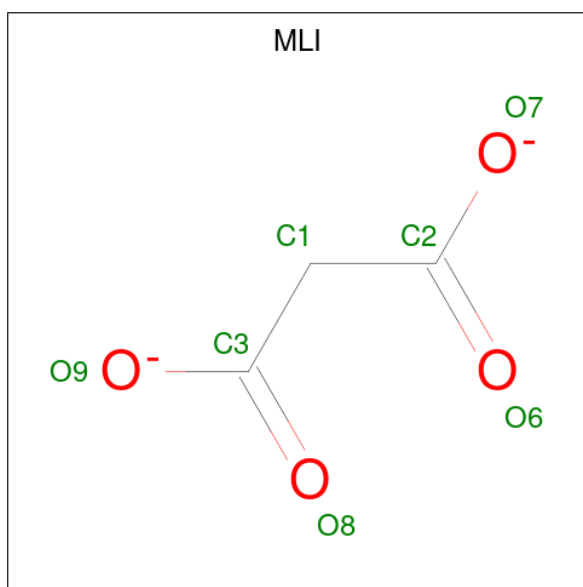
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	349	Total	C	N	O	S	0	0	0
			2843	1819	480	522	22			
1	B	348	Total	C	N	O	S	0	0	0
			2840	1818	479	521	22			

- Molecule 2 is {(2R,3S,4R,5R)-5-[4-amino-3-(propan-2-yl)-1H-pyrazolo[3,4-d]pyrimidin-1-yl]-3,4-dihydroxyoxolan-2-yl}methyl [(2S)-2-amino-3-(4-hydroxyphenyl)propanoyl]sulfamate (CCD ID: A1AZG) (formula: C₂₂H₂₉N₇O₈S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	0	0
			67	22	29	7	8		
2	B	1	Total	C	H	N	O	0	0
			67	22	29	7	8		

- Molecule 3 is MALONATE ION (CCD ID: MLI) (formula: C₃H₂O₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			9	3	2	4		
3	B	1	Total	C	H	O	0	0
			9	3	2	4		

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cl	0	0
			1	1		
4	B	1	Total	Cl	0	0
			1	1		

- Molecule 5 is SODIUM ION (CCD ID: NA) (formula: Na).

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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	123	Total	O	0	0
			123	123		

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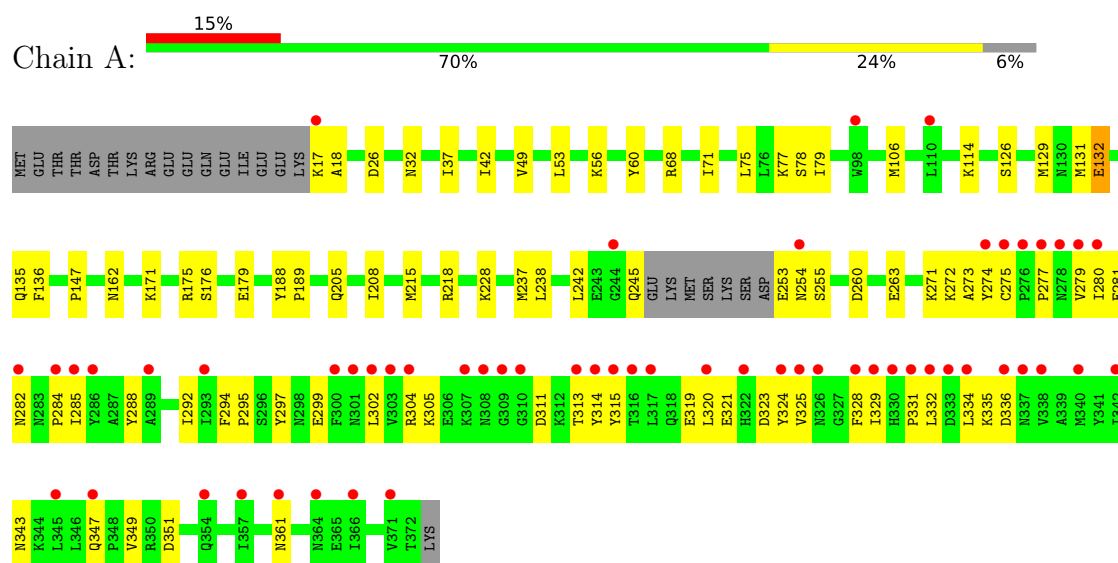
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	257	Total 257	O 257	0	0

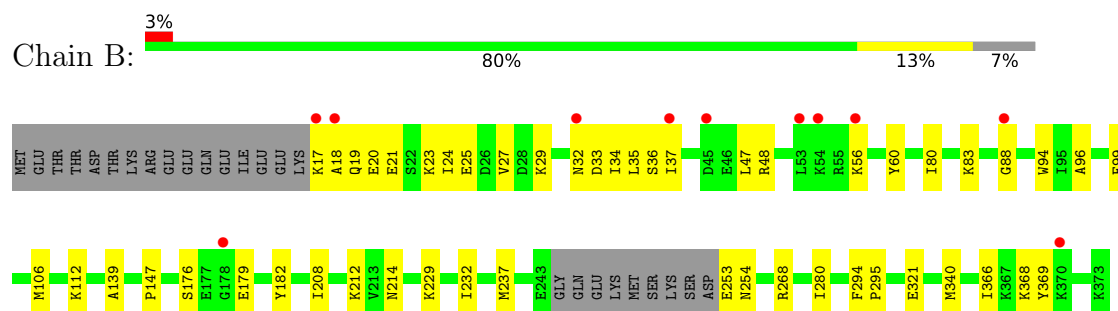
3 Residue-property plots [i](#)

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: tyrosine-tRNA ligase



• Molecule 1: tyrosine-tRNA ligase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	138.21Å 47.27Å 140.51Å 90.00° 94.63° 90.00°	Depositor
Resolution (Å)	46.68 – 1.80 46.68 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.9 (46.68-1.80) 99.9 (46.68-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.58 (at 1.79Å)	Xtriage
Refinement program	PHENIX 1.21.1.5286	Depositor
R, R_{free}	0.183 , 0.220 0.184 , 0.221	Depositor DCC
R_{free} test set	4178 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	32.9	Xtriage
Anisotropy	0.581	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 46.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	6221	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.87% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MLI, A1AZG, NA, CL

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	0.61	0/2898	0.79	1/3897 (0.0%)
1	B	0.79	0/2895	0.89	0/3891
All	All	0.70	0/5793	0.84	1/7788 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	132	GLU	CA-CB-CG	-5.60	102.91	114.10

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	2843	0	2874	85	2
1	B	2840	0	2876	53	1
2	A	38	29	0	0	0
2	B	38	29	0	0	0
3	A	7	2	2	0	0
3	B	7	2	2	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	1	0	0	0	0
5	B	3	0	0	0	0
6	A	123	0	0	7	0
6	B	257	0	0	5	1
All	All	6159	62	5754	136	3

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 12.

All (136) 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:324:TYR:HD1	1:A:329:ILE:HB	1.19	1.06
1:B:253:GLU:HG2	1:B:254:ASN:H	1.30	0.95
1:A:171:LYS:NZ	6:A:502:HOH:O	2.07	0.87
1:B:254:ASN:OD1	1:B:268:ARG:NH1	2.06	0.87
1:A:253:GLU:HG2	1:A:254:ASN:H	1.39	0.87
1:A:347:GLN:NE2	1:A:351:ASP:OD2	2.07	0.86
1:B:253:GLU:N	1:B:253:GLU:OE1	2.10	0.85
1:A:280:ILE:HD12	1:A:325:VAL:HG23	1.61	0.81
1:B:17:LYS:HG2	1:B:19:GLN:HG2	1.60	0.81
1:B:106:MET:HE1	1:B:369:TYR:HB3	1.64	0.79
1:A:26:ASP:OD1	6:A:501:HOH:O	2.00	0.78
1:A:242:LEU:O	1:A:245:GLN:HG3	1.85	0.77
1:A:106:MET:HA	1:A:106:MET:HE2	1.66	0.77
1:A:253:GLU:N	1:A:253:GLU:OE1	2.19	0.76
1:A:324:TYR:CD1	1:A:329:ILE:HB	2.12	0.75
1:B:35:LEU:O	6:B:501:HOH:O	2.05	0.74
1:A:302:LEU:HD21	1:A:329:ILE:HG23	1.71	0.73
1:A:68:ARG:HD2	1:A:260:ASP:OD1	1.90	0.72
1:B:106:MET:HE2	1:B:112:LYS:HB3	1.72	0.72
1:A:77:LYS:HA	1:A:77:LYS:HE2	1.70	0.71
1:B:17:LYS:CG	1:B:19:GLN:HG2	2.19	0.71
1:B:368:LYS:HB2	6:B:514:HOH:O	1.90	0.71
1:A:280:ILE:CG1	1:A:324:TYR:HD2	2.04	0.70
1:A:114:LYS:HE2	6:A:517:HOH:O	1.91	0.70
1:A:280:ILE:HG13	1:A:324:TYR:HD2	1.57	0.70
1:B:17:LYS:HD3	1:B:18:ALA:H	1.55	0.69
1:B:253:GLU:HG2	1:B:254:ASN:N	2.07	0.69
1:B:32:ASN:O	6:B:502:HOH:O	2.11	0.68
1:A:314:TYR:CD2	1:A:319:GLU:HG2	2.27	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:ILE:HD11	1:A:324:TYR:HB3	1.75	0.67
1:B:56:LYS:HD3	6:B:549:HOH:O	1.93	0.67
1:B:106:MET:HE1	1:B:369:TYR:CB	2.27	0.64
1:B:56:LYS:CD	1:B:88:GLY:O	2.47	0.63
1:A:79:ILE:HG21	1:A:295:PRO:HB2	1.80	0.63
1:A:314:TYR:HD2	1:A:319:GLU:HG2	1.63	0.62
1:B:37:ILE:HD13	1:B:80:ILE:HG23	1.81	0.62
1:B:176:SER:O	1:B:179:GLU:HG2	1.99	0.61
1:A:304:ARG:NH1	1:A:328:PHE:O	2.34	0.61
1:A:324:TYR:HB2	1:A:329:ILE:HD12	1.83	0.60
1:A:332:LEU:C	1:A:332:LEU:HD23	2.26	0.60
1:A:17:LYS:HD3	1:A:18:ALA:H	1.67	0.59
1:A:215:MET:HE2	1:A:215:MET:HA	1.86	0.58
1:B:33:ASP:O	1:B:36:SER:OG	2.19	0.58
1:A:314:TYR:CD2	1:A:320:LEU:HA	2.39	0.58
1:A:253:GLU:HG2	1:A:254:ASN:N	2.12	0.58
1:A:135:GLN:HG3	6:A:570:HOH:O	2.04	0.57
1:B:56:LYS:HD3	1:B:88:GLY:O	2.04	0.57
1:A:56:LYS:NZ	6:A:503:HOH:O	2.17	0.56
1:A:32:ASN:HB3	6:A:613:HOH:O	2.07	0.55
1:B:17:LYS:CD	1:B:18:ALA:H	2.18	0.55
1:A:242:LEU:HD22	1:A:272:LYS:HE3	1.86	0.55
1:B:106:MET:HE1	1:B:369:TYR:CD2	2.42	0.54
1:A:281:GLU:HA	1:A:281:GLU:OE1	2.05	0.54
1:B:37:ILE:CD1	1:B:80:ILE:HG23	2.37	0.54
1:B:48:ARG:HH11	1:B:48:ARG:HG2	1.72	0.54
1:A:238:LEU:HD21	1:A:288:TYR:CE2	2.44	0.53
1:A:245:GLN:OE1	1:A:255:SER:HB2	2.08	0.53
1:A:280:ILE:HG13	1:A:324:TYR:CD2	2.40	0.53
1:A:274:TYR:O	1:A:284:PRO:HD2	2.08	0.53
1:B:56:LYS:HZ3	1:B:88:GLY:C	2.18	0.52
1:A:114:LYS:HB2	6:A:611:HOH:O	2.09	0.52
1:A:132:GLU:O	1:A:132:GLU:HG2	2.09	0.52
1:A:242:LEU:CD2	1:A:272:LYS:HE3	2.40	0.51
1:A:37:ILE:HD12	1:A:37:ILE:C	2.35	0.51
1:B:17:LYS:HD3	1:B:17:LYS:N	2.26	0.51
1:A:77:LYS:NZ	1:A:205:GLN:OE1	2.44	0.51
1:B:17:LYS:O	1:B:18:ALA:HB3	2.11	0.51
1:B:34:ILE:HG21	1:B:47:LEU:HD21	1.93	0.51
1:A:280:ILE:HG12	1:A:324:TYR:HD2	1.76	0.50
1:A:17:LYS:CD	1:A:18:ALA:H	2.24	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:VAL:O	1:A:53:LEU:HD13	2.10	0.50
1:A:208:ILE:HG22	1:A:237:MET:HG2	1.94	0.49
1:B:56:LYS:HD2	1:B:88:GLY:O	2.12	0.49
1:A:332:LEU:HD23	1:A:336:ASP:OD2	2.13	0.49
1:B:56:LYS:HZ3	1:B:88:GLY:HA2	1.78	0.49
1:A:297:TYR:O	1:A:299:GLU:HG2	2.12	0.49
1:A:253:GLU:CG	1:A:254:ASN:H	2.13	0.48
1:A:313:THR:HG21	1:A:315:TYR:CE1	2.47	0.48
1:A:302:LEU:O	1:A:311:ASP:HA	2.13	0.48
1:B:229:LYS:NZ	6:B:508:HOH:O	2.47	0.48
1:A:275:CYS:CB	1:A:335:LYS:HE3	2.44	0.48
1:B:106:MET:HE1	1:B:369:TYR:CG	2.49	0.48
1:A:280:ILE:CD1	1:A:321:GLU:HA	2.44	0.47
1:B:34:ILE:CG2	1:B:47:LEU:HD21	2.44	0.47
1:B:17:LYS:HD3	1:B:18:ALA:N	2.28	0.47
1:A:126:SER:OG	1:A:349:VAL:HG22	2.13	0.47
1:A:263:GLU:HA	1:A:343:ASN:OD1	2.15	0.47
1:A:282:ASN:O	1:A:284:PRO:HD3	2.14	0.47
1:A:147:PRO:HG3	1:B:147:PRO:HG3	1.97	0.46
1:B:17:LYS:HG2	1:B:19:GLN:H	1.80	0.46
1:A:314:TYR:OH	1:A:323:ASP:OD2	2.26	0.46
1:B:214:ASN:HB3	1:B:232:ILE:HD12	1.96	0.46
1:A:242:LEU:HB2	1:A:245:GLN:NE2	2.31	0.46
1:B:280:ILE:CD1	1:B:321:GLU:HG3	2.46	0.46
1:B:340:MET:HE3	1:B:340:MET:HB2	1.69	0.46
1:A:79:ILE:CD1	1:A:292:ILE:HA	2.46	0.46
1:A:277:PRO:O	1:A:279:VAL:HG23	2.16	0.46
1:A:71:ILE:HD11	1:A:75:LEU:HD12	1.97	0.45
1:A:324:TYR:OH	1:A:331:PRO:HB3	2.16	0.45
1:A:131:MET:HE1	1:A:136:PHE:CZ	2.53	0.44
1:A:188:TYR:HB3	1:A:189:PRO:CD	2.48	0.44
1:A:279:VAL:O	1:A:324:TYR:HE2	1.99	0.44
1:B:37:ILE:HD12	1:B:37:ILE:C	2.43	0.44
1:B:106:MET:CE	1:B:369:TYR:CD2	3.01	0.44
1:A:280:ILE:CG1	1:A:324:TYR:CD2	2.94	0.43
1:A:131:MET:HE1	1:A:136:PHE:CE2	2.53	0.43
1:B:280:ILE:HD12	1:B:321:GLU:HG3	1.99	0.43
1:A:272:LYS:O	1:A:272:LYS:HG3	2.19	0.43
1:B:208:ILE:HG22	1:B:237:MET:HG2	2.00	0.43
1:A:272:LYS:O	1:A:272:LYS:CG	2.66	0.43
1:A:175:ARG:HD3	1:A:179:GLU:OE2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:LEU:CD2	1:A:336:ASP:OD2	2.67	0.42
1:A:280:ILE:CD1	1:A:324:TYR:HB3	2.47	0.42
1:B:20:GLU:O	1:B:24:ILE:HG13	2.19	0.42
1:B:21:GLU:O	1:B:25:GLU:HG3	2.19	0.42
1:B:48:ARG:HH11	1:B:48:ARG:CG	2.32	0.42
1:A:79:ILE:CG2	1:A:295:PRO:HB2	2.47	0.42
1:B:56:LYS:HZ3	1:B:88:GLY:CA	2.32	0.42
1:A:176:SER:O	1:A:179:GLU:HG2	2.18	0.42
1:A:42:ILE:HG21	1:A:215:MET:HE1	2.01	0.42
1:A:273:ALA:HB3	1:A:285:ILE:HD11	2.00	0.42
1:A:162:ASN:HA	1:B:182:TYR:HA	2.02	0.42
1:B:253:GLU:CG	1:B:254:ASN:N	2.76	0.42
1:B:212:LYS:HD3	1:B:212:LYS:HA	1.83	0.42
1:A:275:CYS:HB2	1:A:335:LYS:HE3	2.01	0.42
1:B:94:TRP:CH2	1:B:139:ALA:HA	2.55	0.42
1:A:332:LEU:HD23	1:A:332:LEU:O	2.19	0.42
1:B:23:LYS:O	1:B:27:VAL:HG23	2.19	0.42
1:B:96:ALA:HB1	1:B:99:PHE:HB2	2.01	0.41
1:A:215:MET:CE	1:A:218:ARG:HD3	2.50	0.41
1:A:78:SER:HB2	1:A:129:MET:HG3	2.03	0.41
1:A:294:PHE:HB3	1:A:295:PRO:HD3	2.02	0.41
1:A:328:PHE:N	1:A:328:PHE:CD1	2.88	0.41
1:B:294:PHE:HB3	1:B:295:PRO:HD3	2.03	0.41
1:A:271:LYS:O	1:A:335:LYS:NZ	2.48	0.40
1:A:285:ILE:HG22	1:A:334:LEU:HG	2.03	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:361:ASN:OD1	1:A:361:ASN:OD1[2_555]	1.99	0.21
6:B:530:HOH:O	6:B:547:HOH:O[4_546]	2.06	0.14
1:A:228:LYS:NZ	1:B:20:GLU:OE1[3_455]	2.16	0.04

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	345/373 (92%)	340 (99%)	5 (1%)	0	100	100
1	B	344/373 (92%)	339 (98%)	5 (2%)	0	100	100
All	All	689/746 (92%)	679 (98%)	10 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	320/344 (93%)	318 (99%)	2 (1%)	78	77
1	B	320/344 (93%)	316 (99%)	4 (1%)	61	54
All	All	640/688 (93%)	634 (99%)	6 (1%)	70	67

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

Mol	Chain	Res	Type
1	A	60	TYR
1	A	305	LYS
1	B	29	LYS
1	B	60	TYR
1	B	83	LYS
1	B	366	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	181	ASN
1	B	19	GLN
1	B	32	ASN

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Mol	Chain	Res	Type
1	B	70	HIS
1	B	82	ASN
1	B	87	ASN
1	B	133	ASN
1	B	181	ASN
1	B	214	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 10 ligands modelled in this entry, 6 are monoatomic - leaving 4 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	$\# Z > 2$
3	MLI	A	402	-	6,6,6	1.99	1 (16%)	7,7,7	1.25	1 (14%)
3	MLI	B	402	-	6,6,6	1.85	1 (16%)	7,7,7	1.12	1 (14%)
2	A1AZG	B	401	5	41,41,41	2.03	9 (21%)	56,61,61	1.68	11 (19%)
2	A1AZG	A	401	5	41,41,41	2.14	13 (31%)	56,61,61	1.57	8 (14%)

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	MLI	A	402	-	-	0/4/4/4	-
3	MLI	B	402	-	-	0/4/4/4	-
2	A1AZG	B	401	5	-	5/26/55/55	0/4/4/4
2	A1AZG	A	401	5	-	2/26/55/55	0/4/4/4

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	A1AZG	O09-S10	6.27	1.72	1.60
2	B	401	A1AZG	O09-S10	5.94	1.72	1.60
2	B	401	A1AZG	C34-N38	5.64	1.37	1.29
2	A	401	A1AZG	C34-N38	5.15	1.37	1.29
2	A	401	A1AZG	C37-C35	4.10	1.67	1.51
2	A	401	A1AZG	C06-C05	4.10	1.63	1.53
2	B	401	A1AZG	O09-C08	-3.99	1.31	1.46
2	B	401	A1AZG	C37-C35	3.71	1.65	1.51
3	A	402	MLI	C1-C3	3.48	1.56	1.51
2	B	401	A1AZG	C27-N26	3.42	1.40	1.36
3	B	402	MLI	C1-C3	3.04	1.55	1.51
2	B	401	A1AZG	C13-N14	-3.03	1.33	1.48
2	A	401	A1AZG	C02-C03	2.88	1.62	1.53
2	A	401	A1AZG	O09-C08	-2.81	1.36	1.46
2	A	401	A1AZG	C15-C16	-2.77	1.44	1.51
2	B	401	A1AZG	C06-C05	2.58	1.59	1.53
2	B	401	A1AZG	C33-C31	-2.58	1.39	1.42
2	A	401	A1AZG	C29-N30	2.51	1.38	1.33
2	A	401	A1AZG	C27-N26	2.42	1.38	1.36
2	A	401	A1AZG	C21-C20	2.39	1.42	1.38
2	A	401	A1AZG	O22-C19	-2.36	1.31	1.37
2	B	401	A1AZG	C29-N30	2.36	1.38	1.33
2	A	401	A1AZG	C35-C34	2.27	1.54	1.51
2	A	401	A1AZG	O24-S10	2.11	1.44	1.42

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	A1AZG	O09-C08-C05	4.86	116.24	107.57
2	B	401	A1AZG	C02-C03-N26	-4.66	106.46	113.43
2	B	401	A1AZG	O09-C08-C05	4.39	115.39	107.57
2	A	401	A1AZG	C35-C34-N38	4.33	125.34	120.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	A1AZG	O23-C12-N11	-4.30	115.17	122.98
2	B	401	A1AZG	O25-S10-O24	-4.21	114.55	120.85
2	A	401	A1AZG	C16-C15-C13	-3.02	107.95	114.13
2	B	401	A1AZG	O23-C12-N11	-2.75	117.98	122.98
2	B	401	A1AZG	C37-C35-C34	-2.74	106.24	111.40
2	B	401	A1AZG	C33-C34-N38	-2.65	107.54	110.21
2	B	401	A1AZG	C20-C21-C16	2.60	124.41	121.00
2	A	401	A1AZG	C36-C35-C34	2.51	116.13	111.40
2	B	401	A1AZG	C12-N11-S10	2.47	133.12	124.07
2	B	401	A1AZG	C35-C34-N38	2.35	122.98	120.19
2	B	401	A1AZG	C21-C16-C17	-2.33	114.78	118.23
2	B	401	A1AZG	C16-C15-C13	-2.24	109.55	114.13
2	A	401	A1AZG	C33-C34-N38	-2.23	107.97	110.21
2	A	401	A1AZG	O09-S10-N11	-2.19	100.03	105.69
3	A	402	MLI	O6-C2-C1	-2.05	116.29	122.11
2	A	401	A1AZG	C02-C06-C05	-2.04	98.67	102.61
3	B	402	MLI	C3-C1-C2	2.03	120.11	112.95

There are no chirality outliers.

All (7) torsion outliers are listed below:

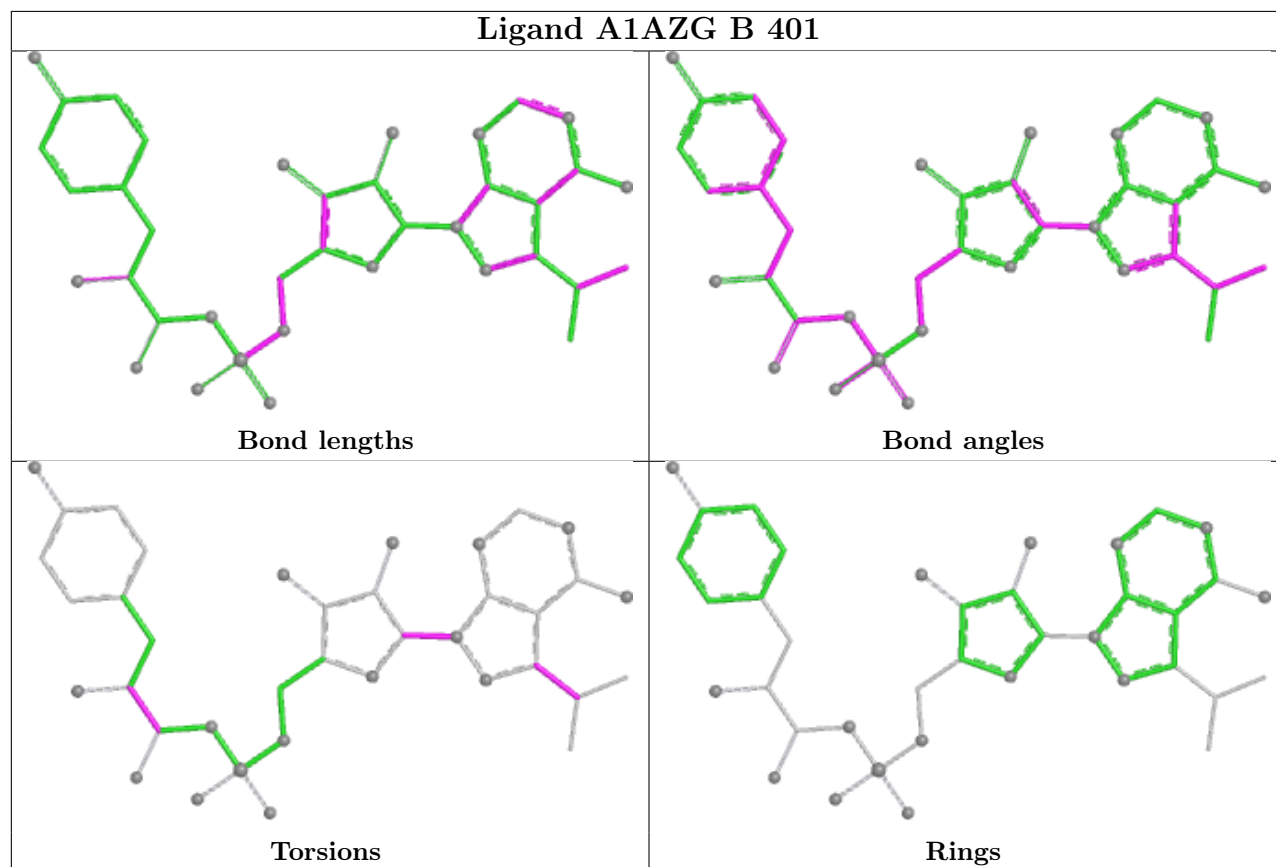
Mol	Chain	Res	Type	Atoms
2	A	401	A1AZG	N11-C12-C13-C15
2	A	401	A1AZG	O23-C12-C13-C15
2	B	401	A1AZG	N11-C12-C13-C15
2	B	401	A1AZG	O23-C12-C13-C15
2	B	401	A1AZG	O04-C03-N26-N38
2	B	401	A1AZG	C33-C34-C35-C36
2	B	401	A1AZG	O04-C03-N26-C27

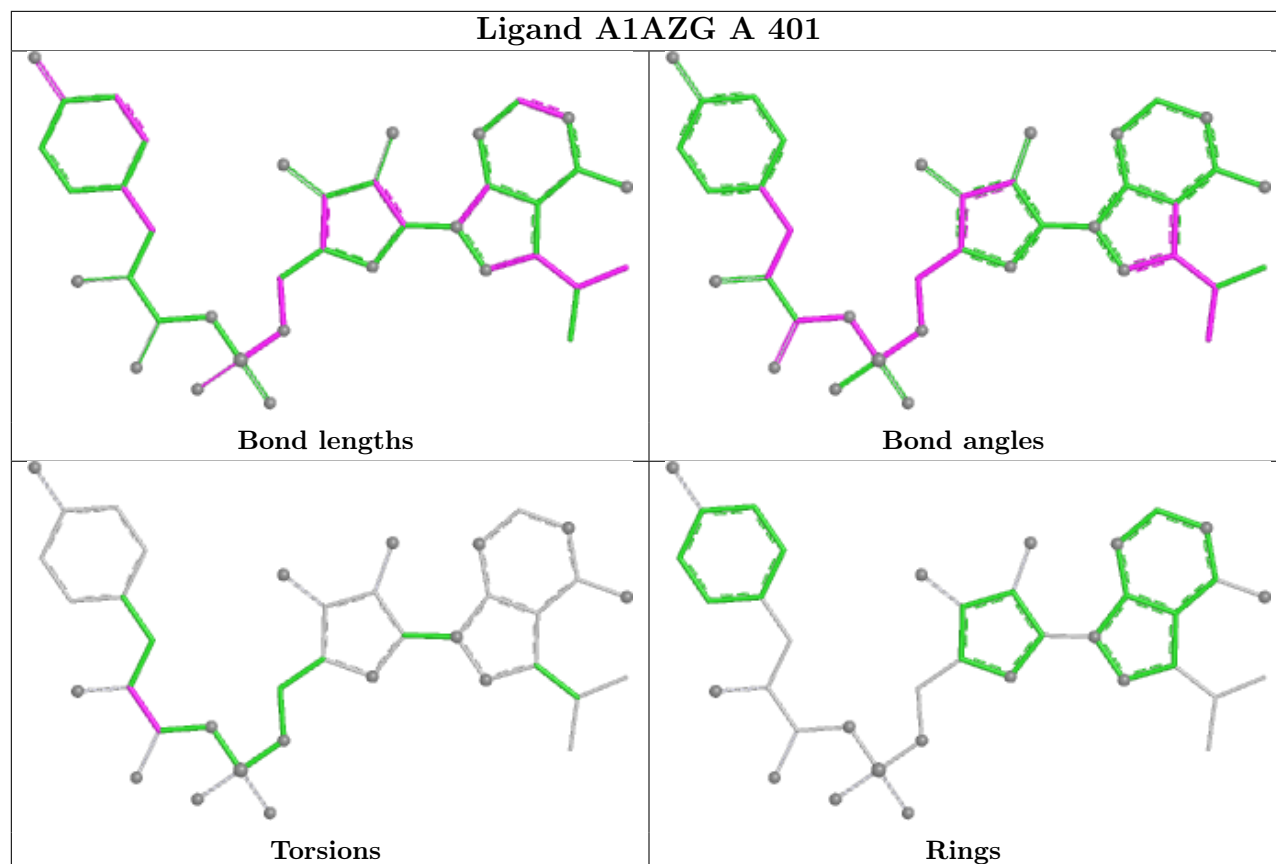
There are no ring outliers.

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	349/373 (93%)	0.88	57 (16%) 4 3	30, 54, 96, 123	0
1	B	348/373 (93%)	0.11	11 (3%) 50 50	28, 37, 65, 110	0
All	All	697/746 (93%)	0.50	68 (9%) 13 11	28, 44, 88, 123	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	18	ALA	5.3
1	A	329	ILE	5.0
1	A	357	ILE	4.8
1	A	277	PRO	4.8
1	A	303	VAL	4.6
1	A	280	ILE	4.6
1	A	320	LEU	4.6
1	A	331	PRO	4.0
1	A	286	TYR	3.9
1	A	325	VAL	3.8
1	A	317	LEU	3.7
1	B	53	LEU	3.7
1	A	328	PHE	3.7
1	A	279	VAL	3.6
1	A	309	GLY	3.6
1	A	300	PHE	3.4
1	A	326	ASN	3.2
1	A	330	HIS	3.2
1	A	334	LEU	3.2
1	A	302	LEU	3.1
1	A	17	LYS	3.1
1	A	371	VAL	3.1
1	A	310	GLY	3.1
1	A	332	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	324	TYR	3.0
1	B	56	LYS	3.0
1	A	314	TYR	2.9
1	A	301	ASN	2.9
1	A	307	LYS	2.9
1	B	37	ILE	2.9
1	A	338	VAL	2.9
1	A	274	TYR	2.9
1	A	361	ASN	2.9
1	A	333	ASP	2.7
1	A	315	TYR	2.6
1	A	284	PRO	2.6
1	A	304	ARG	2.6
1	A	337	ASN	2.6
1	A	289	ALA	2.5
1	A	340	MET	2.5
1	A	110	LEU	2.4
1	B	17	LYS	2.4
1	A	354	GLN	2.4
1	A	347	GLN	2.4
1	A	278	ASN	2.4
1	B	32	ASN	2.4
1	A	244	GLY	2.4
1	B	370	LYS	2.4
1	A	293	ILE	2.3
1	A	342	ILE	2.3
1	A	364	ASN	2.3
1	A	276	PRO	2.3
1	B	88	GLY	2.3
1	A	336	ASP	2.2
1	A	275	CYS	2.2
1	A	345	LEU	2.2
1	A	366	ILE	2.2
1	A	254	ASN	2.2
1	A	285	ILE	2.2
1	A	322	HIS	2.1
1	A	313	THR	2.1
1	A	308	ASN	2.1
1	A	98	TRP	2.1
1	B	54	LYS	2.1
1	A	282	ASN	2.1
1	A	316	THR	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	45	ASP	2.0
1	B	178	GLY	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](#)

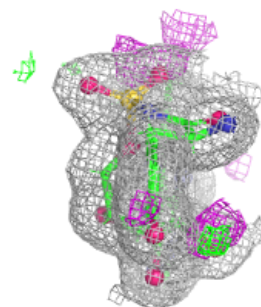
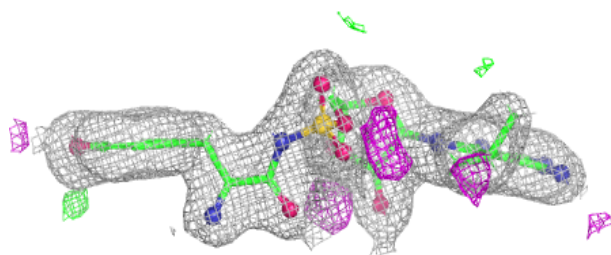
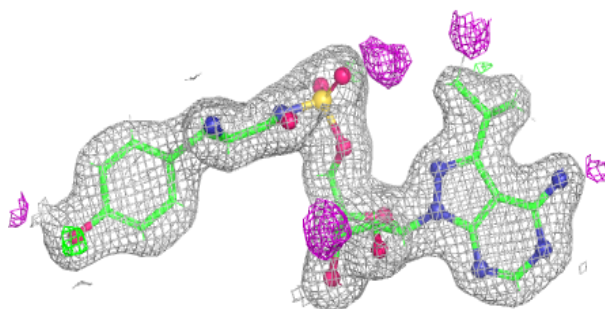
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MLI	A	402	7/7	0.87	0.12	53,58,67,67	0
3	MLI	B	402	7/7	0.88	0.11	51,58,69,70	0
4	CL	B	403	1/1	0.90	0.16	49,49,49,49	0
4	CL	A	403	1/1	0.91	0.12	58,58,58,58	0
5	NA	B	405	1/1	0.96	0.16	48,48,48,48	0
2	A1AZG	B	401	38/38	0.98	0.05	24,33,47,53	0
5	NA	A	404	1/1	0.98	0.11	40,40,40,40	0
5	NA	B	404	1/1	0.98	0.05	37,37,37,37	0
2	A1AZG	A	401	38/38	0.98	0.06	30,41,65,69	0
5	NA	B	406	1/1	0.99	0.05	34,34,34,34	0

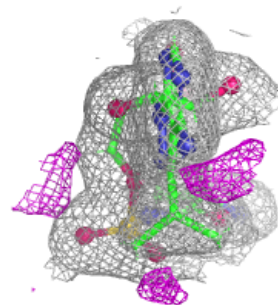
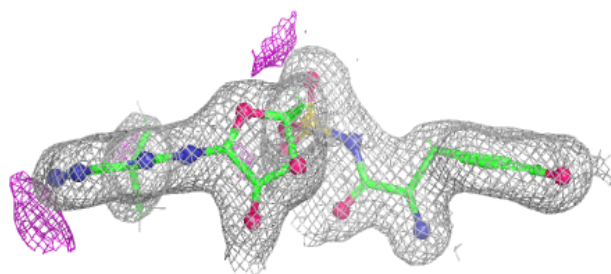
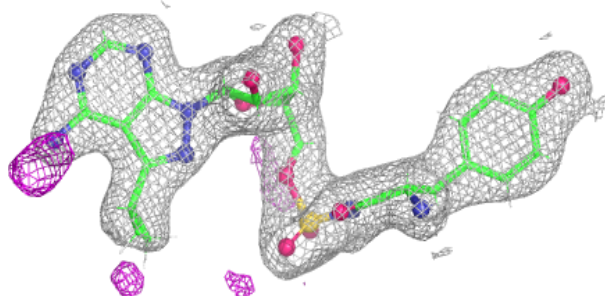
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around A1AZG B 401:

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

**Electron density around A1AZG A 401:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.