



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:02 AM UTC

PDB ID : 9C83 / pdb_00009c83
Title : X-ray crystal structure of AmpC beta-lactamase with inhibitor
Authors : Liu, F.; Shoichet, B.K.
Deposited on : 2024-06-11
Resolution : 2.90 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

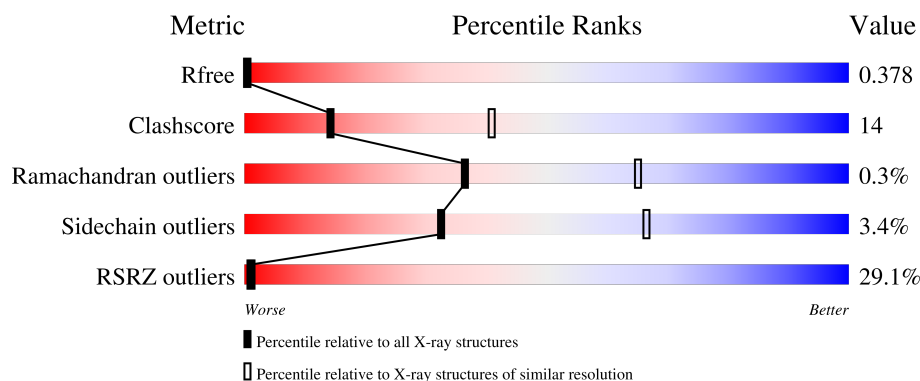
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	377	23% 63% 30% • 6%
1	B	377	32% 64% 29% • 5%

2 Entry composition [i](#)

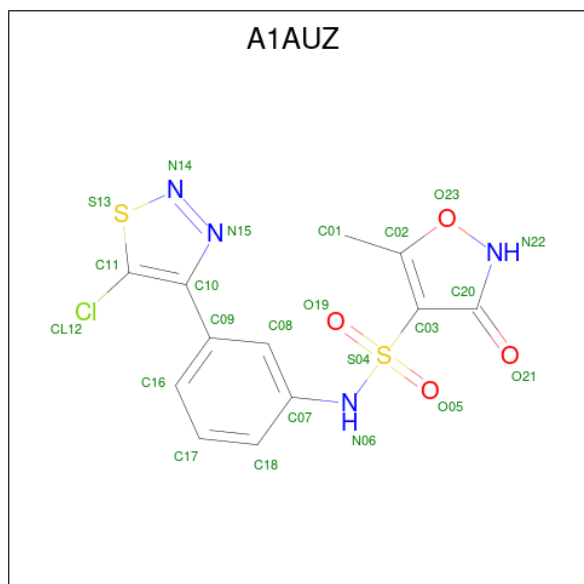
There are 2 unique types of molecules in this entry. The entry contains 5531 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 AmpC Beta-lactamase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	354	Total	C	N	O	S	0	0	0
			2729	1758	462	503	6			
1	B	358	Total	C	N	O	S	0	0	0
			2756	1777	466	507	6			

- Molecule 2 is N-[(3M)-3-(5-chloro-1,2,3-thiadiazol-4-yl)phenyl]-5-methyl-3-oxo-2,3-dihydro-1,2-oxazole-4-sulfonamide (CCD ID: A1AUZ) (formula: $C_{12}H_9ClN_4O_4S_2$) (labeled as "Ligand of Interest" by depositor).

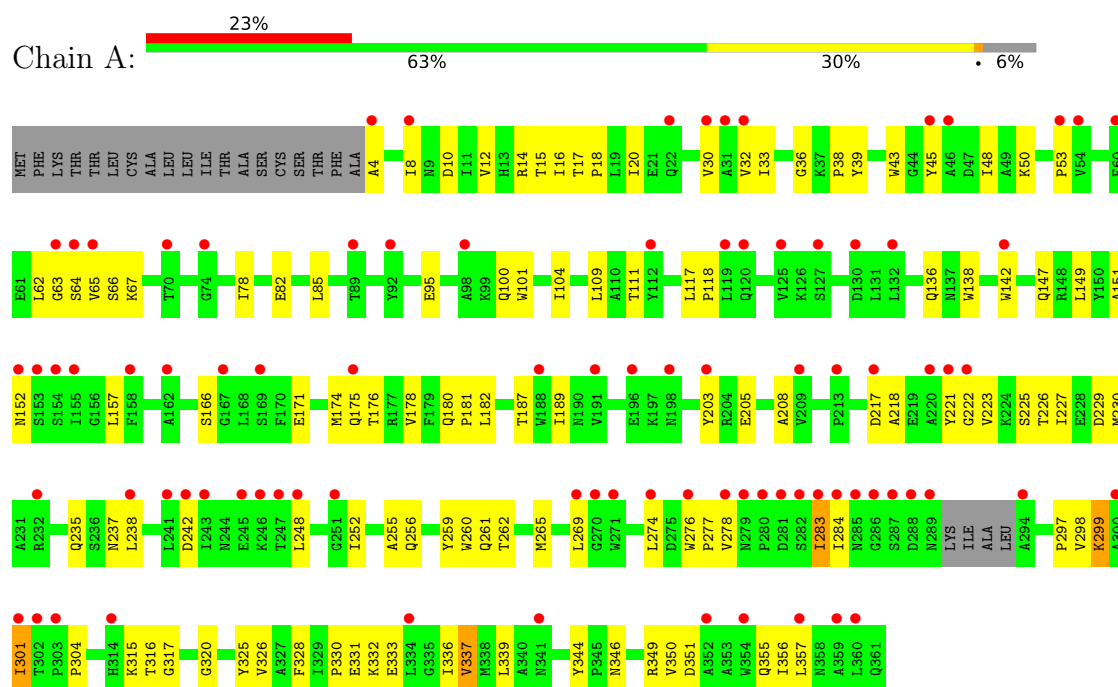


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	O	S	0	0
			23	12	1	4	4	2		
2	B	1	Total	C	Cl	N	O	S	0	0
			23	12	1	4	4	2		

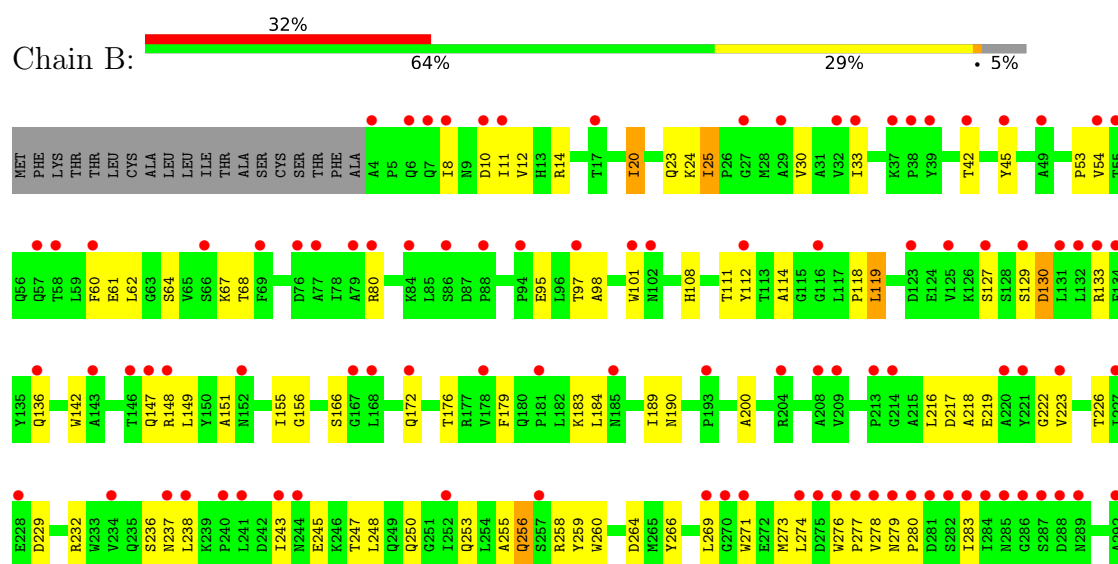
3 Residue-property plots

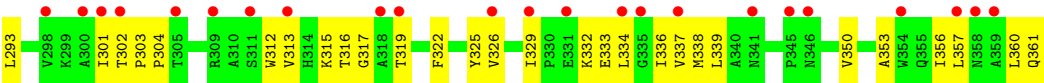
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



• Molecule 1: AmpC Beta-lactamase





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	119.77Å 77.03Å 100.08Å 90.00° 115.47° 90.00°	Depositor
Resolution (Å)	58.87 – 2.90 58.87 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.6 (58.87-2.90) 98.5 (58.87-2.90)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.07 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.307 , 0.377 0.307 , 0.378	Depositor DCC
R_{free} test set	1827 reflections (9.87%)	wwPDB-VP
Wilson B-factor (Å ²)	30.4	Xtriage
Anisotropy	0.806	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 51.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.71	EDS
Total number of atoms	5531	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.52% 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: A1AUZ

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	0.50	0/2808	0.72	0/3844
1	B	0.52	1/2835 (0.0%)	0.77	2/3881 (0.1%)
All	All	0.51	1/5643 (0.0%)	0.74	2/7725 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	147	GLN	CA-CB	-6.22	1.43	1.53

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	147	GLN	N-CA-C	7.13	120.11	108.55
1	B	147	GLN	CB-CG-CD	-5.81	102.72	112.60

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	2729	0	2655	79	0
1	B	2756	0	2694	75	0
2	A	23	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	23	0	0	0	0
All	All	5531	0	5349	154	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 14.

All (154) 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:331:GLU:HG2	1:A:332:LYS:HD3	1.57	0.85
1:A:64:SER:HB2	1:A:317:GLY:HA2	1.66	0.77
1:B:183:LYS:HD2	1:B:232:ARG:HH21	1.56	0.70
1:B:245:GLU:N	1:B:245:GLU:OE2	2.25	0.69
1:B:326:VAL:HG13	1:B:337:VAL:HG12	1.74	0.69
1:A:111:THR:OG1	1:A:260:TRP:NE1	2.26	0.68
1:A:326:VAL:HG13	1:A:337:VAL:HG12	1.77	0.66
1:A:50:LYS:O	1:A:50:LYS:HG3	1.97	0.65
1:A:230:MET:HG3	1:A:339:LEU:HD11	1.78	0.65
1:A:62:LEU:HD11	1:A:230:MET:SD	2.38	0.63
1:B:273:MET:HG3	1:B:313:VAL:HG22	1.81	0.62
1:B:276:TRP:CD2	1:B:277:PRO:HA	2.35	0.62
1:B:237:ASN:OD1	1:B:256:GLN:NE2	2.32	0.61
1:A:101:TRP:HA	1:A:104:ILE:HD12	1.82	0.61
1:A:20:ILE:HD12	1:A:20:ILE:H	1.66	0.61
1:B:64:SER:HB2	1:B:317:GLY:HA2	1.84	0.60
1:A:16:ILE:O	1:A:20:ILE:HD12	2.03	0.59
1:A:109:LEU:CD1	1:A:157:LEU:HD23	2.33	0.58
1:A:261:GLN:HB2	1:A:301:ILE:HD11	1.85	0.58
1:B:98:ALA:HB3	1:B:101:TRP:HD1	1.69	0.57
1:A:62:LEU:HB2	1:A:223:VAL:O	2.05	0.56
1:A:262:THR:HB	1:A:298:VAL:HG12	1.87	0.56
1:A:175:GLN:HG3	1:A:176:THR:N	2.19	0.56
1:B:259:TYR:CD1	1:B:304:PRO:HB3	2.41	0.56
1:A:109:LEU:HD11	1:A:157:LEU:HD23	1.87	0.56
1:B:111:THR:OG1	1:B:260:TRP:NE1	2.36	0.55
1:A:38:PRO:HD3	1:A:235:GLN:HE22	1.71	0.55
1:B:226:THR:HG23	1:B:229:ASP:H	1.72	0.55
1:A:259:TYR:CD1	1:A:304:PRO:HB3	2.42	0.55
1:A:63:GLY:O	1:A:221:TYR:HA	2.07	0.54
1:B:61:GLU:OE1	1:B:319:THR:HG21	2.07	0.54
1:B:62:LEU:HB2	1:B:223:VAL:O	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:95:GLU:H	1:B:95:GLU:CD	2.15	0.54
1:A:15:THR:O	1:A:18:PRO:HD2	2.08	0.54
1:A:100:GLN:NE2	1:A:138:TRP:O	2.41	0.54
1:A:82:GLU:OE1	1:A:166:SER:OG	2.21	0.53
1:A:237:ASN:OD1	1:A:256:GLN:NE2	2.40	0.53
1:B:332:LYS:HZ2	1:B:361:GLN:HG3	1.74	0.53
1:A:346:ASN:HA	1:A:349:ARG:HD2	1.90	0.53
1:A:238:LEU:HD13	1:A:330:PRO:HA	1.89	0.53
1:B:338:MET:HE1	1:B:353:ALA:HB2	1.90	0.53
1:B:255:ALA:HA	1:B:269:LEU:HB2	1.90	0.52
1:A:261:GLN:HG2	1:A:299:LYS:HE2	1.91	0.52
1:A:255:ALA:HA	1:A:269:LEU:HB2	1.92	0.52
1:B:112:TYR:HD2	1:B:148:ARG:HH11	1.58	0.52
1:B:156:GLY:C	1:B:216:LEU:HD23	2.35	0.51
1:A:36:GLY:O	1:A:235:GLN:NE2	2.41	0.51
1:B:112:TYR:HD2	1:B:148:ARG:NH1	2.09	0.51
1:A:276:TRP:CD2	1:A:277:PRO:HA	2.45	0.51
1:B:112:TYR:CD2	1:B:148:ARG:NH1	2.79	0.51
1:A:78:ILE:HD11	1:A:85:LEU:HG	1.92	0.50
1:A:175:GLN:HG3	1:A:176:THR:HG23	1.92	0.50
1:A:95:GLU:H	1:A:95:GLU:CD	2.20	0.50
1:A:203:TYR:HE1	1:A:208:ALA:HB2	1.77	0.50
1:A:45:TYR:HA	1:A:53:PRO:HA	1.94	0.49
1:B:130:ASP:OD1	1:B:130:ASP:N	2.44	0.49
1:B:325:TYR:CZ	1:B:350:VAL:HG22	2.47	0.49
1:B:217:ASP:OD1	1:B:218:ALA:N	2.44	0.49
1:A:48:ILE:HG22	1:A:203:TYR:CZ	2.47	0.49
1:A:238:LEU:HD12	1:A:333:GLU:HA	1.95	0.49
1:A:248:LEU:O	1:A:252:ILE:HG13	2.12	0.48
1:A:64:SER:OG	2:A:401:A1AUZ:O21	2.27	0.48
1:A:175:GLN:OE1	1:A:180:GLN:NE2	2.46	0.48
1:A:187:THR:HG23	1:A:225:SER:HB2	1.95	0.48
1:B:142:TRP:HH2	1:B:149:LEU:HD13	1.78	0.48
1:A:33:ILE:HD12	1:A:33:ILE:N	2.29	0.48
1:B:10:ASP:OD1	1:B:14:ARG:HD3	2.12	0.48
1:B:218:ALA:HA	1:B:222:GLY:HA3	1.95	0.48
1:A:8:ILE:O	1:A:12:VAL:HG23	2.13	0.48
1:A:32:VAL:HG12	1:A:39:TYR:HB2	1.95	0.47
1:A:283:ILE:HG13	1:A:284:ILE:N	2.29	0.47
1:B:315:LYS:HE3	1:B:316:THR:O	2.14	0.47
1:B:183:LYS:HD2	1:B:232:ARG:NH2	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:119:LEU:CD2	1:B:293:LEU:HD13	2.45	0.47
1:B:8:ILE:HG12	1:B:360:LEU:HD13	1.97	0.47
1:B:189:ILE:HG22	1:B:190:ASN:OD1	2.15	0.46
1:A:217:ASP:OD1	1:A:218:ALA:N	2.49	0.46
1:B:276:TRP:HE3	1:B:278:VAL:HG13	1.80	0.46
1:B:274:LEU:HB2	1:B:278:VAL:HG11	1.97	0.46
1:A:344:TYR:O	1:A:349:ARG:NH2	2.48	0.46
1:B:127:SER:OG	1:B:130:ASP:OD1	2.34	0.46
1:A:142:TRP:HH2	1:A:149:LEU:HD13	1.80	0.46
1:B:97:THR:H	1:B:136:GLN:HE22	1.63	0.46
1:A:226:THR:HG23	1:A:229:ASP:H	1.80	0.45
1:A:218:ALA:HA	1:A:222:GLY:HA3	1.98	0.45
1:A:325:TYR:CZ	1:A:350:VAL:HG22	2.50	0.45
1:B:179:PHE:HD1	1:B:184:LEU:HD12	1.81	0.45
1:B:243:ILE:HD13	1:B:248:LEU:HD22	1.97	0.45
1:B:278:VAL:HG11	1:B:312:TRP:HB3	1.99	0.45
1:B:68:THR:HB	1:B:271:TRP:NE1	2.31	0.45
1:A:238:LEU:HD21	1:A:328:PHE:HB2	1.98	0.45
1:A:48:ILE:HG22	1:A:203:TYR:OH	2.17	0.44
1:A:351:ASP:O	1:A:355:GLN:HG2	2.16	0.44
1:B:42:THR:OG1	1:B:54:VAL:HB	2.17	0.44
1:A:10:ASP:O	1:A:14:ARG:HG3	2.18	0.44
1:B:129:SER:O	1:B:133:ARG:HG3	2.18	0.44
1:B:302:THR:HA	1:B:303:PRO:HA	1.78	0.44
1:B:332:LYS:NZ	1:B:361:GLN:HG3	2.32	0.44
1:A:315:LYS:HE3	1:A:316:THR:O	2.18	0.44
1:A:182:LEU:HD11	1:A:248:LEU:HD21	1.99	0.44
1:B:95:GLU:CD	1:B:95:GLU:N	2.76	0.44
1:B:279:ASN:O	1:B:283:ILE:HG23	2.17	0.44
1:A:259:TYR:HE2	1:A:269:LEU:HG	1.83	0.44
1:B:33:ILE:HD12	1:B:33:ILE:N	2.32	0.44
1:A:4:ALA:HA	1:A:39:TYR:CE2	2.53	0.43
1:B:30:VAL:HG22	1:B:338:MET:HG2	2.01	0.43
1:B:67:LYS:HB3	1:B:155:ILE:HD13	2.01	0.43
1:B:264:ASP:OD1	1:B:264:ASP:N	2.40	0.43
1:A:336:ILE:HD12	1:A:356:ILE:HG21	1.99	0.43
1:B:60:PHE:HB2	1:B:339:LEU:CD2	2.48	0.43
1:B:80:ARG:HG2	1:B:247:THR:HG21	2.01	0.43
1:A:171:GLU:HA	1:A:189:ILE:HD12	2.00	0.43
1:B:108:HIS:HB3	1:B:114:ALA:HA	2.01	0.43
1:B:200:ALA:O	1:B:322:PHE:HZ	2.02	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:357:LEU:HA	1:B:357:LEU:HD23	1.68	0.43
1:A:65:VAL:O	1:A:65:VAL:HG12	2.19	0.43
1:A:95:GLU:CD	1:A:95:GLU:N	2.77	0.42
1:A:265:MET:HA	1:A:274:LEU:HD23	2.00	0.42
1:B:11:ILE:HA	1:B:11:ILE:HD12	1.69	0.42
1:A:67:LYS:NZ	1:A:152:ASN:OD1	2.40	0.42
1:A:357:LEU:HD23	1:A:357:LEU:HA	1.84	0.42
1:A:30:VAL:HB	1:A:43:TRP:HZ3	1.84	0.42
1:A:242:ASP:OD2	1:A:242:ASP:N	2.52	0.42
1:A:16:ILE:HG21	1:A:43:TRP:CH2	2.55	0.42
1:A:38:PRO:HD3	1:A:235:GLN:NE2	2.34	0.42
1:B:97:THR:H	1:B:136:GLN:NE2	2.18	0.42
1:A:147:GLN:HA	1:A:297:PRO:HA	2.01	0.42
1:B:98:ALA:N	1:B:136:GLN:HE22	2.18	0.42
1:B:274:LEU:HD12	1:B:312:TRP:CD1	2.55	0.42
1:B:329:ILE:HG21	1:B:332:LYS:HG2	2.02	0.42
1:A:178:VAL:C	1:A:181:PRO:HD2	2.44	0.42
1:B:60:PHE:HB2	1:B:339:LEU:HD23	2.02	0.42
1:B:119:LEU:HD21	1:B:293:LEU:HD13	2.02	0.42
1:A:62:LEU:HD21	1:A:230:MET:SD	2.60	0.41
1:A:117:LEU:HD23	1:A:118:PRO:HD2	2.02	0.41
1:A:118:PRO:O	1:A:151:ALA:HB1	2.19	0.41
1:A:227:ILE:HD12	1:A:227:ILE:HA	1.91	0.41
1:A:299:LYS:H	1:A:299:LYS:HG2	1.72	0.41
1:B:172:GLN:O	1:B:176:THR:HG23	2.20	0.41
1:A:64:SER:C	1:A:66:SER:N	2.76	0.41
1:B:23:GLN:O	1:B:24:LYS:C	2.62	0.41
1:B:219:GLU:OE1	1:B:219:GLU:N	2.43	0.41
1:B:258:ARG:HB3	1:B:266:TYR:HB3	2.03	0.41
1:B:45:TYR:HA	1:B:53:PRO:HA	2.03	0.41
1:B:334:LEU:HD21	1:B:361:GLN:HA	2.03	0.41
1:B:336:ILE:HD12	1:B:356:ILE:HG21	2.02	0.41
1:B:329:ILE:CG2	1:B:332:LYS:HG2	2.51	0.41
1:A:16:ILE:HG22	1:A:20:ILE:HD11	2.04	0.40
1:B:20:ILE:HG23	1:B:25:ILE:HB	2.02	0.40
1:B:118:PRO:O	1:B:151:ALA:HB1	2.21	0.40
1:B:238:LEU:HD12	1:B:333:GLU:HA	2.03	0.40
1:B:61:GLU:CD	1:B:322:PHE:CE1	2.99	0.40
1:B:325:TYR:OH	1:B:350:VAL:HG22	2.21	0.40
1:A:174:MET:HE3	1:A:178:VAL:HB	2.02	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	350/377 (93%)	335 (96%)	14 (4%)	1 (0%)	36	65
1	B	356/377 (94%)	346 (97%)	9 (2%)	1 (0%)	36	65
All	All	706/754 (94%)	681 (96%)	23 (3%)	2 (0%)	36	65

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	320	GLY
1	B	280	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	279/308 (91%)	271 (97%)	8 (3%)	37	71
1	B	281/308 (91%)	270 (96%)	11 (4%)	28	63
All	All	560/616 (91%)	541 (97%)	19 (3%)	32	66

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	THR
1	A	136	GLN
1	A	205	GLU
1	A	278	VAL

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Mol	Chain	Res	Type
1	A	283	ILE
1	A	299	LYS
1	A	301	ILE
1	A	337	VAL
1	B	12	VAL
1	B	20	ILE
1	B	25	ILE
1	B	119	LEU
1	B	130	ASP
1	B	166	SER
1	B	236	SER
1	B	250	GLN
1	B	253	GLN
1	B	256	GLN
1	B	301	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	136	GLN
1	A	175	GLN
1	A	180	GLN
1	A	210	HIS
1	A	235	GLN
1	A	244	ASN
1	B	13	HIS
1	B	56	GLN
1	B	136	GLN
1	B	175	GLN
1	B	237	ASN
1	B	256	GLN
1	B	261	GLN
1	B	289	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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](#)

2 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
2	A1AUZ	A	401	-	21,25,25	5.88	13 (61%)	24,37,37	3.71	8 (33%)
2	A1AUZ	B	401	-	21,25,25	5.72	13 (61%)	24,37,37	3.61	7 (29%)

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
2	A1AUZ	A	401	-	-	10/13/15/15	0/3/3/3
2	A1AUZ	B	401	-	-	10/13/15/15	0/3/3/3

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	A1AUZ	C11-S13	-20.75	1.61	1.70
2	B	401	A1AUZ	C11-S13	-19.13	1.61	1.70
2	B	401	A1AUZ	O21-C20	8.91	1.40	1.23
2	A	401	A1AUZ	O21-C20	8.69	1.40	1.23
2	B	401	A1AUZ	N15-N14	7.67	1.42	1.30
2	A	401	A1AUZ	N15-N14	7.52	1.42	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	A1AUZ	C10-N15	6.44	1.48	1.37
2	A	401	A1AUZ	S04-N06	5.90	1.72	1.62
2	B	401	A1AUZ	S04-N06	5.88	1.72	1.62
2	A	401	A1AUZ	C10-N15	5.78	1.47	1.37
2	B	401	A1AUZ	C11-CL12	4.56	1.79	1.71
2	B	401	A1AUZ	C11-C10	4.53	1.44	1.37
2	A	401	A1AUZ	C11-CL12	4.38	1.79	1.71
2	A	401	A1AUZ	C11-C10	4.04	1.43	1.37
2	B	401	A1AUZ	C09-C10	4.03	1.54	1.48
2	B	401	A1AUZ	C20-C03	-3.89	1.39	1.48
2	A	401	A1AUZ	S13-N14	-3.74	1.58	1.68
2	B	401	A1AUZ	S13-N14	-3.38	1.59	1.68
2	A	401	A1AUZ	O05-S04	3.21	1.48	1.43
2	B	401	A1AUZ	O19-S04	3.09	1.47	1.43
2	A	401	A1AUZ	C20-C03	-3.09	1.41	1.48
2	A	401	A1AUZ	C09-C10	2.96	1.52	1.48
2	A	401	A1AUZ	O19-S04	2.75	1.47	1.43
2	A	401	A1AUZ	C07-N06	2.45	1.47	1.43
2	B	401	A1AUZ	O05-S04	2.29	1.46	1.43
2	B	401	A1AUZ	C01-C02	2.03	1.53	1.49

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	A1AUZ	O19-S04-O05	-11.08	99.51	119.82
2	A	401	A1AUZ	C11-S13-N14	10.30	100.79	92.76
2	B	401	A1AUZ	O19-S04-O05	-9.86	101.73	119.82
2	B	401	A1AUZ	C11-S13-N14	9.48	100.15	92.76
2	B	401	A1AUZ	O23-C02-C01	8.58	124.29	115.36
2	A	401	A1AUZ	O23-C02-C01	6.20	121.81	115.36
2	A	401	A1AUZ	C10-N15-N14	-4.64	109.98	114.29
2	B	401	A1AUZ	C10-N15-N14	-4.14	110.45	114.29
2	B	401	A1AUZ	O21-C20-C03	-2.96	124.20	128.89
2	B	401	A1AUZ	C09-C10-N15	2.63	124.26	120.07
2	A	401	A1AUZ	CL12-C11-S13	2.35	125.20	122.36
2	A	401	A1AUZ	O19-S04-N06	2.31	111.22	107.35
2	A	401	A1AUZ	C09-C10-N15	2.22	123.61	120.07
2	A	401	A1AUZ	O21-C20-N22	-2.21	123.63	126.11
2	B	401	A1AUZ	CL12-C11-S13	2.00	124.78	122.36

There are no chirality outliers.

All (20) torsion outliers are listed below:

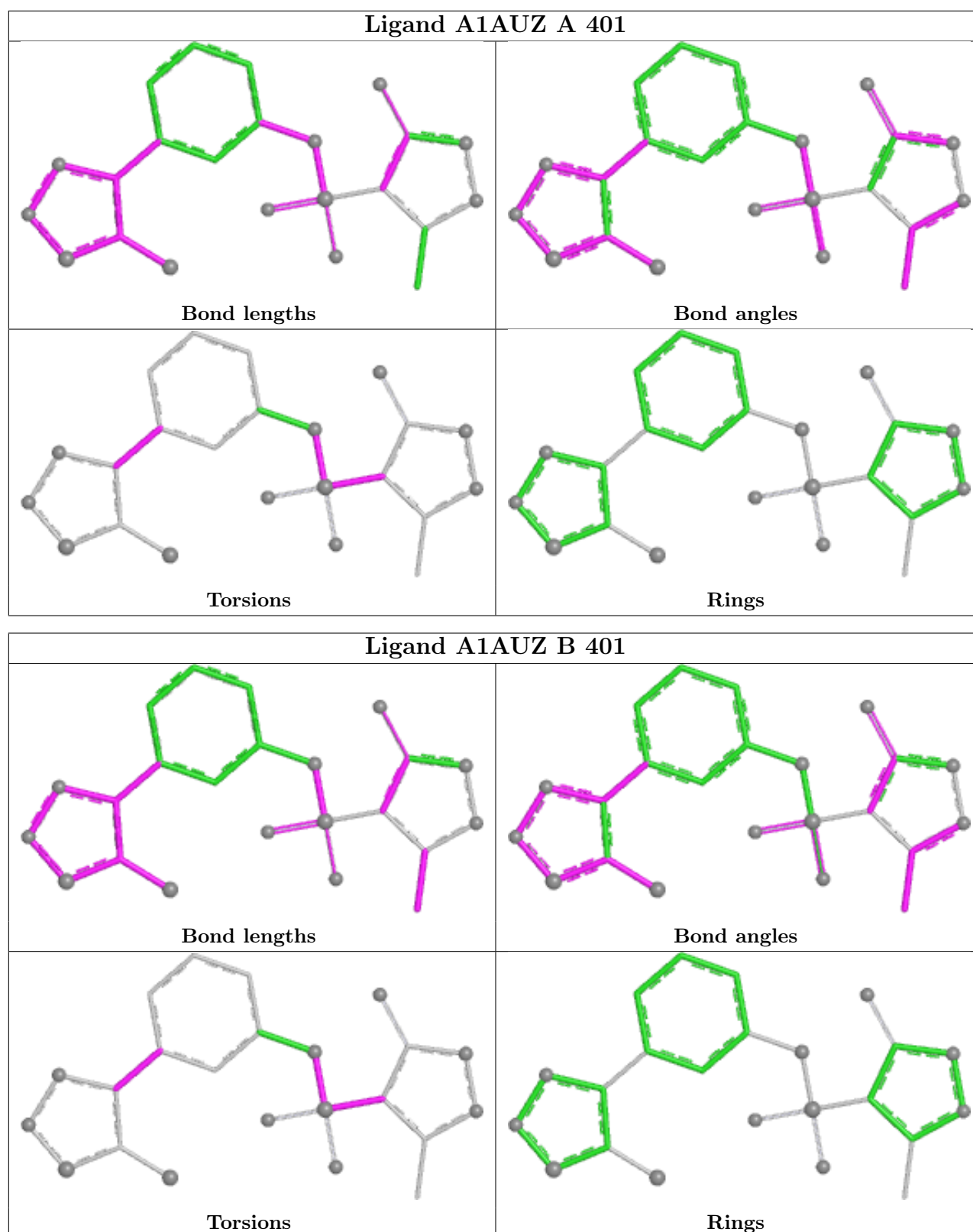
Mol	Chain	Res	Type	Atoms
2	A	401	A1AUZ	C02-C03-S04-O05
2	A	401	A1AUZ	C02-C03-S04-O19
2	A	401	A1AUZ	C20-C03-S04-O05
2	A	401	A1AUZ	C07-N06-S04-C03
2	A	401	A1AUZ	C07-N06-S04-O19
2	B	401	A1AUZ	C02-C03-S04-O05
2	B	401	A1AUZ	C20-C03-S04-O05
2	B	401	A1AUZ	C07-N06-S04-C03
2	B	401	A1AUZ	C07-N06-S04-O05
2	B	401	A1AUZ	C07-N06-S04-O19
2	A	401	A1AUZ	C08-C09-C10-C11
2	A	401	A1AUZ	C16-C09-C10-C11
2	B	401	A1AUZ	C08-C09-C10-C11
2	B	401	A1AUZ	C16-C09-C10-C11
2	B	401	A1AUZ	C02-C03-S04-O19
2	A	401	A1AUZ	C07-N06-S04-O05
2	B	401	A1AUZ	C16-C09-C10-N15
2	B	401	A1AUZ	C08-C09-C10-N15
2	A	401	A1AUZ	C16-C09-C10-N15
2	A	401	A1AUZ	C08-C09-C10-N15

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	A1AUZ	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	354/377 (93%)	1.56	87 (24%) 2 1	9, 20, 38, 54	0
1	B	358/377 (94%)	1.75	120 (33%) 1 1	10, 24, 39, 55	0
All	All	712/754 (94%)	1.65	207 (29%) 1 1	9, 22, 39, 55	0

All (207) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	282	SER	5.5
1	B	129	SER	5.2
1	A	274	LEU	5.1
1	B	285	ASN	5.0
1	B	27	GLY	4.9
1	B	281	ASP	4.9
1	B	208	ALA	4.7
1	B	39	TYR	4.4
1	A	289	ASN	4.3
1	A	278	VAL	4.2
1	A	300	ALA	4.2
1	B	6	GLN	4.1
1	A	213	PRO	4.1
1	B	276	TRP	4.1
1	B	4	ALA	4.1
1	B	32	VAL	4.0
1	B	143	ALA	4.0
1	A	286	GLY	4.0
1	A	287	SER	3.9
1	B	17	THR	3.9
1	B	237	ASN	3.9
1	A	360	LEU	3.8
1	A	98	ALA	3.8
1	B	335	GLY	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	326	VAL	3.8
1	B	287	SER	3.8
1	A	65	VAL	3.7
1	B	123	ASP	3.7
1	A	285	ASN	3.7
1	A	284	ILE	3.7
1	A	53	PRO	3.6
1	B	69	PHE	3.6
1	B	213	PRO	3.6
1	A	270	GLY	3.5
1	B	37	LYS	3.5
1	B	244	ASN	3.5
1	B	329	ILE	3.5
1	A	241	LEU	3.5
1	B	241	LEU	3.5
1	A	280	PRO	3.5
1	A	279	ASN	3.5
1	A	142	TRP	3.4
1	A	64	SER	3.4
1	A	281	ASP	3.3
1	A	245	GLU	3.3
1	A	130	ASP	3.3
1	A	32	VAL	3.3
1	A	283	ILE	3.3
1	B	152	ASN	3.2
1	A	271	TRP	3.2
1	B	345	PRO	3.2
1	A	31	ALA	3.2
1	B	132	LEU	3.1
1	B	112	TYR	3.1
1	B	337	VAL	3.1
1	B	221	TYR	3.1
1	A	198	ASN	3.1
1	B	131	LEU	3.1
1	A	63	GLY	3.1
1	A	119	LEU	3.1
1	B	319	THR	3.1
1	B	79	ALA	3.0
1	A	242	ASP	3.0
1	B	280	PRO	3.0
1	A	54	VAL	3.0
1	A	89	THR	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	45	TYR	3.0
1	B	11	ILE	3.0
1	A	154	SER	3.0
1	A	288	ASP	3.0
1	B	33	ILE	2.9
1	A	152	ASN	2.9
1	B	277	PRO	2.9
1	B	125	VAL	2.9
1	B	101	TRP	2.9
1	A	45	TYR	2.8
1	B	228	GLU	2.8
1	B	77	ALA	2.8
1	B	223	VAL	2.8
1	A	222	GLY	2.8
1	B	55	THR	2.8
1	B	66	SER	2.8
1	B	146	THR	2.8
1	B	204	ARG	2.8
1	B	178	VAL	2.8
1	B	243	ILE	2.8
1	A	127	SER	2.8
1	B	286	GLY	2.8
1	A	243	ILE	2.7
1	A	294	ALA	2.7
1	B	279	ASN	2.7
1	B	302	THR	2.7
1	B	38	PRO	2.7
1	A	314	HIS	2.7
1	B	278	VAL	2.7
1	A	60	PHE	2.7
1	A	301	ILE	2.7
1	A	334	LEU	2.7
1	A	221	TYR	2.7
1	A	22	GLN	2.6
1	B	76	ASP	2.6
1	B	311	SER	2.6
1	A	112	TYR	2.6
1	B	148	ARG	2.6
1	B	181	PRO	2.6
1	A	357	LEU	2.6
1	B	127	SER	2.6
1	B	42	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	357	LEU	2.6
1	A	167	GLY	2.6
1	A	203	TYR	2.6
1	A	220	ALA	2.6
1	B	288	ASP	2.6
1	B	309	ARG	2.5
1	B	168	LEU	2.5
1	A	191	VAL	2.5
1	B	283	ILE	2.5
1	B	86	SER	2.5
1	A	302	THR	2.5
1	B	305	THR	2.5
1	B	318	ALA	2.5
1	A	132	LEU	2.5
1	A	354	TRP	2.5
1	A	155	ILE	2.5
1	B	252	ILE	2.5
1	B	301	ILE	2.5
1	B	147	GLN	2.5
1	B	300	ALA	2.5
1	B	193	PRO	2.4
1	B	58	THR	2.4
1	A	269	LEU	2.4
1	A	125	VAL	2.4
1	A	153	SER	2.4
1	A	282	SER	2.4
1	B	60	PHE	2.4
1	A	359	ALA	2.4
1	B	29	ALA	2.4
1	B	354	TRP	2.4
1	B	57	GLN	2.4
1	B	172	GLN	2.4
1	A	70	THR	2.4
1	B	334	LEU	2.4
1	B	341	ASN	2.4
1	B	284	ILE	2.4
1	A	251	GLY	2.4
1	A	4	ALA	2.4
1	A	162	ALA	2.4
1	A	8	ILE	2.4
1	A	246	LYS	2.4
1	B	271	TRP	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	136	GLN	2.3
1	A	276	TRP	2.3
1	B	274	LEU	2.3
1	A	232	ARG	2.3
1	A	92	TYR	2.3
1	B	97	THR	2.3
1	A	158	PHE	2.3
1	A	352	ALA	2.3
1	A	46	ALA	2.3
1	B	359	ALA	2.3
1	A	74	GLY	2.3
1	B	292	ALA	2.2
1	B	238	LEU	2.2
1	B	227	ILE	2.2
1	A	30	VAL	2.2
1	B	313	VAL	2.2
1	B	185	ASN	2.2
1	A	217	ASP	2.2
1	B	270	GLY	2.2
1	B	84	LYS	2.2
1	B	8	ILE	2.2
1	A	175	GLN	2.2
1	A	303	PRO	2.2
1	B	214	GLY	2.2
1	B	7	GLN	2.1
1	B	94	PRO	2.1
1	B	209	VAL	2.1
1	A	247	THR	2.1
1	B	133	ARG	2.1
1	B	331	GLU	2.1
1	B	289	ASN	2.1
1	B	167	GLY	2.1
1	A	238	LEU	2.1
1	B	134	PHE	2.1
1	A	188	TRP	2.1
1	A	169	SER	2.1
1	B	257	SER	2.1
1	B	54	VAL	2.1
1	B	234	VAL	2.1
1	B	358	ASN	2.1
1	B	10	ASP	2.1
1	B	80	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	49	ALA	2.1
1	B	220	ALA	2.1
1	A	196	GLU	2.1
1	B	298	VAL	2.1
1	B	88	PRO	2.1
1	B	240	PRO	2.1
1	A	248	LEU	2.1
1	B	346	ASN	2.0
1	B	116	GLY	2.0
1	A	120	GLN	2.0
1	B	269	LEU	2.0
1	A	341	ASN	2.0
1	B	102	ASN	2.0
1	B	275	ASP	2.0
1	A	209	VAL	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](#)

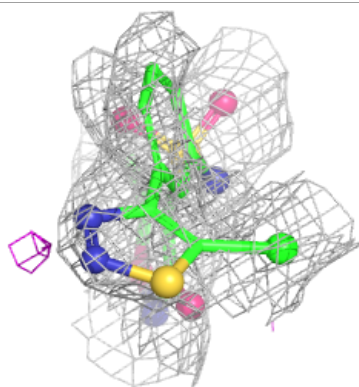
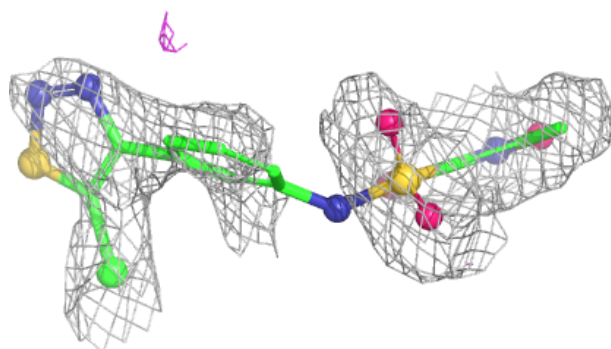
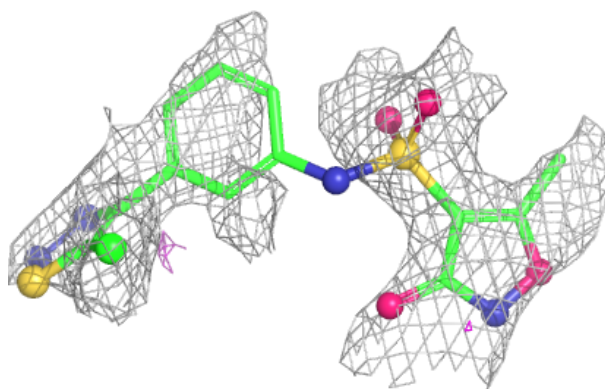
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
2	A1AUZ	A	401	23/23	0.66	0.19	29,47,67,86	0
2	A1AUZ	B	401	23/23	0.68	0.20	31,49,65,87	0

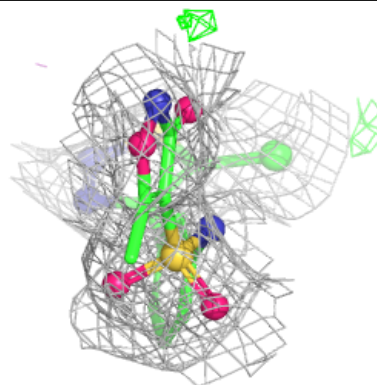
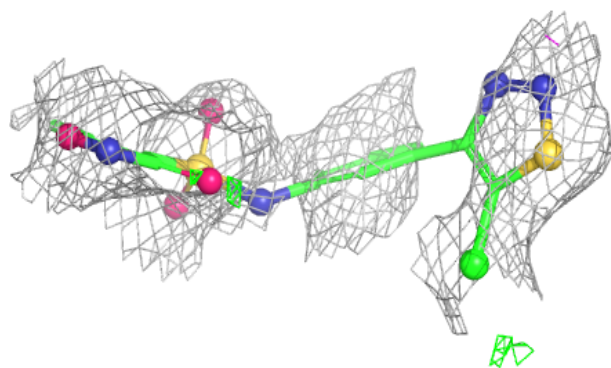
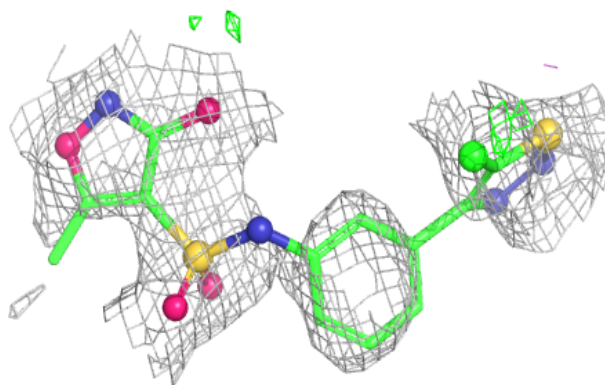
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around A1AUZ 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)

**Electron density around A1AUZ 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.