



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 08:03 AM UTC

PDB ID : 9KMB / pdb_00009kmb
Title : Crystal structure of human glutaminyl cyclase in complex with N-(2-(1H-imidazol-5-yl)ethyl)-4-methoxybenzenesulfonamide
Authors : Li, G.-B.; Wu, J.-W.; Ning, X.-L.
Deposited on : 2024-11-15
Resolution : 2.28 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

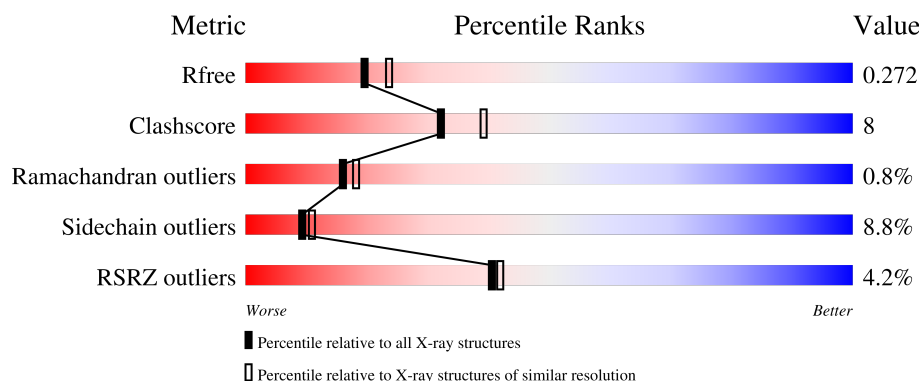
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.28 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	9078 (2.30-2.26)
Clashscore	190562	9802 (2.30-2.26)
Ramachandran outliers	187476	9690 (2.30-2.26)
Sidechain outliers	187428	9691 (2.30-2.26)
RSRZ outliers	180081	9085 (2.30-2.26)

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	329	3% 81% 16% ..
1	B	329	6% 69% 22% 6% .
1	C	329	4% 78% 19% ..

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15560 atoms, of which 7635 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.

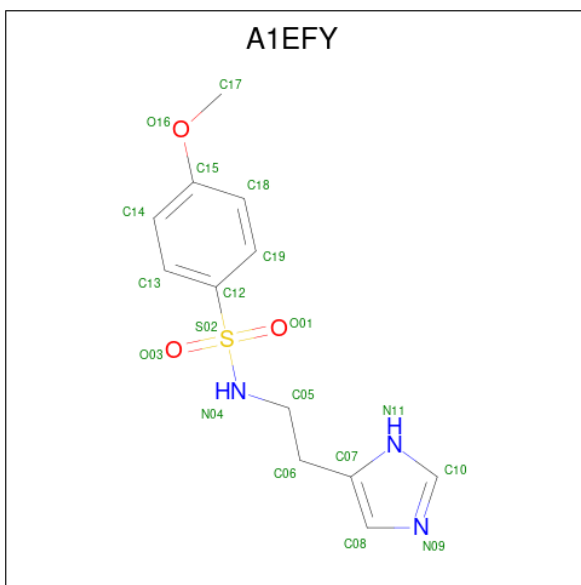
- Molecule 1 is a protein called Glutaminyl-peptide cyclotransferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	323	Total	C	H	N	O	S	0	0	0
			5140	1673	2530	450	478	9			
1	B	323	Total	C	H	N	O	S	0	0	0
			5140	1673	2530	450	478	9			
1	C	323	Total	C	H	N	O	S	0	0	0
			5140	1673	2530	450	478	9			

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

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

- Molecule 3 is {N}-[2-(1 {H}-imidazol-5-yl)ethyl]-4-methoxy-benzenesulfonamide (CCD ID: A1EFY) (formula: C₁₂H₁₅N₃O₃S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total 34	C 12	H 15	N 3	O 3	S 1	0	0
3	B	1	Total 34	C 12	H 15	N 3	O 3	S 1	0	0
3	C	1	Total 34	C 12	H 15	N 3	O 3	S 1	0	0

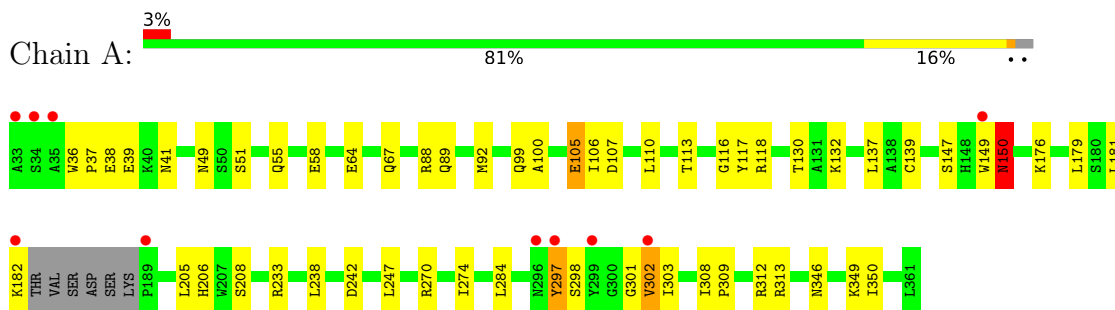
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	22	Total O 22 22	0	0
4	B	4	Total O 4 4	0	0
4	C	9	Total O 9 9	0	0

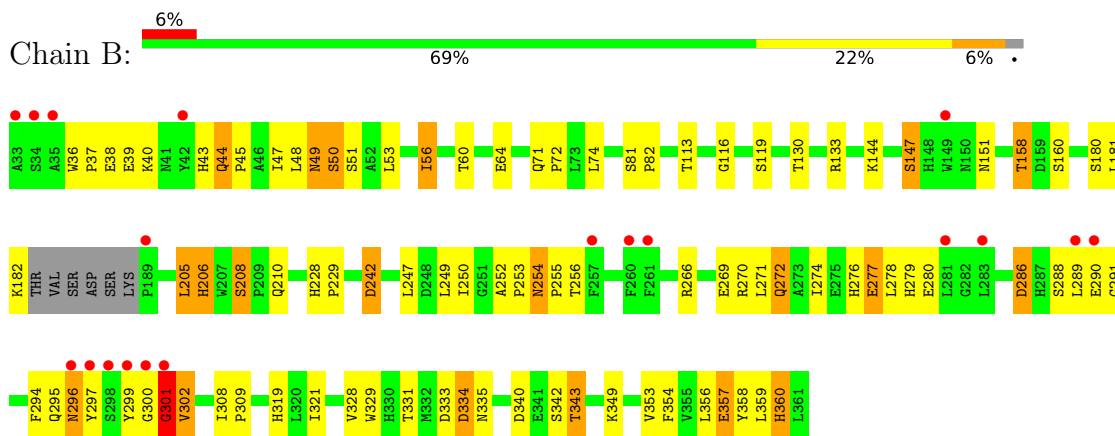
3 Residue-property plots [i](#)

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.

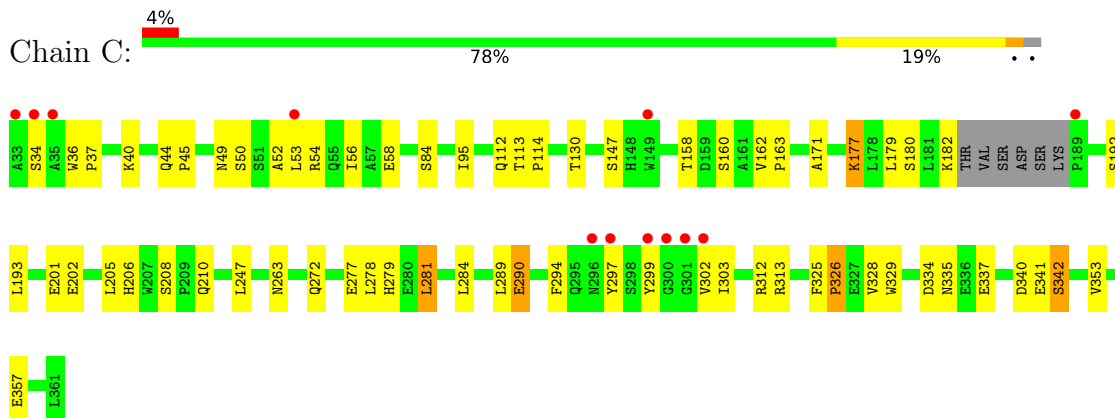
- Molecule 1: Glutaminyl-peptide cyclotransferase



- Molecule 1: Glutaminyl-peptide cyclotransferase



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4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	106.58Å 147.17Å 160.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.56 – 2.28 44.56 – 2.28	Depositor EDS
% Data completeness (in resolution range)	99.8 (44.56-2.28) 99.7 (44.56-2.28)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.47 (at 2.29Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.216 , 0.266 0.220 , 0.272	Depositor DCC
R_{free} test set	2000 reflections (3.47%)	wwPDB-VP
Wilson B-factor (Å ²)	47.2	Xtriage
Anisotropy	0.302	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 46.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	15560	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.27% 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: ZN, A1EFY

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	0.89	2/2687 (0.1%)	0.81	0/3656
1	B	0.74	0/2687	0.72	2/3656 (0.1%)
1	C	0.75	0/2687	0.72	0/3656
All	All	0.79	2/8061 (0.0%)	0.75	2/10968 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	139	CYS	CB-SG	-5.77	1.62	1.81
1	A	150	ASN	CG-OD1	5.06	1.33	1.23

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	301	GLY	CA-C-N	5.32	131.28	121.70
1	B	301	GLY	C-N-CA	5.32	131.28	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	301	GLY	Peptide

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	2610	2530	2529	28	0
1	B	2610	2530	2529	71	1
1	C	2610	2530	2529	32	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	19	15	0	0	0
3	B	19	15	0	0	0
3	C	19	15	0	0	0
4	A	22	0	0	3	0
4	B	4	0	0	1	0
4	C	9	0	0	3	0
All	All	7925	7635	7587	123	1

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 8.

All (123) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:49:ASN:OD1	1:B:51:SER:N	2.03	0.91
1:B:113:THR:OG1	1:B:116:GLY:O	1.94	0.86
1:B:38:GLU:OE1	1:C:147:SER:OG	1.94	0.83
1:C:130:THR:HG22	4:C:504:HOH:O	1.84	0.77
1:A:113:THR:OG1	1:A:116:GLY:O	2.09	0.69
1:C:171:ALA:O	4:C:501:HOH:O	2.12	0.68
1:B:277:GLU:O	1:B:280:GLU:N	2.26	0.67
1:B:286:ASP:N	1:B:286:ASP:OD1	2.28	0.67
1:A:349:LYS:NZ	4:A:501:HOH:O	1.96	0.65
1:B:43:HIS:O	1:B:266:ARG:NH1	2.24	0.64
1:B:144:LYS:NZ	4:B:501:HOH:O	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:301:GLY:N	1:B:302:VAL:HG21	2.14	0.62
1:B:39:GLU:OE1	1:B:133:ARG:NH1	2.34	0.60
1:A:346:ASN:O	1:A:350:ILE:HG13	2.03	0.59
1:B:44:GLN:HG3	1:B:45:PRO:HD2	1.84	0.58
1:B:279:HIS:NE2	1:B:289:LEU:HD11	2.18	0.58
1:B:254:ASN:N	1:B:255:PRO:CD	2.68	0.57
1:B:333:ASP:O	1:B:335:ASN:N	2.37	0.57
1:B:288:SER:O	1:B:291:GLY:N	2.38	0.56
1:B:301:GLY:HA2	1:B:302:VAL:HG23	1.85	0.56
1:B:71:GLN:HA	1:B:74:LEU:HD12	1.87	0.55
1:A:302:VAL:HG22	1:A:303:ILE:H	1.72	0.55
1:B:38:GLU:CD	1:C:147:SER:HG	2.14	0.54
1:A:38:GLU:OE1	1:B:147:SER:OG	2.25	0.54
1:A:49:ASN:OD1	1:A:49:ASN:C	2.50	0.54
1:B:49:ASN:OD1	1:B:50:SER:N	2.41	0.53
1:B:349:LYS:O	1:B:353:VAL:HG23	2.09	0.52
1:B:301:GLY:HA2	1:B:302:VAL:CG2	2.39	0.52
1:B:301:GLY:CA	1:B:302:VAL:HB	2.39	0.52
1:B:36:TRP:N	1:B:37:PRO:CD	2.72	0.52
1:B:49:ASN:OD1	1:B:49:ASN:C	2.53	0.51
1:B:158:THR:OG1	1:B:334:ASP:OD1	2.28	0.51
1:C:302:VAL:HG12	1:C:303:ILE:N	2.25	0.51
1:B:301:GLY:HA2	1:B:302:VAL:CB	2.40	0.51
1:B:301:GLY:HA2	1:B:302:VAL:HB	1.93	0.51
1:B:359:LEU:O	1:B:360:HIS:HB2	2.10	0.51
1:A:206:HIS:CE1	1:C:313:ARG:HA	2.46	0.51
1:A:117:TYR:O	1:A:118:ARG:HG2	2.11	0.51
1:C:247:LEU:O	4:C:502:HOH:O	2.20	0.50
1:A:302:VAL:HG13	1:A:303:ILE:N	2.25	0.50
1:B:228:HIS:ND1	1:B:229:PRO:HA	2.26	0.50
1:B:242:ASP:OD2	1:B:358:TYR:OH	2.25	0.50
1:A:149:TRP:CD2	1:A:150:ASN:ND2	2.80	0.50
1:B:340:ASP:OD2	1:B:343:THR:OG1	2.30	0.49
1:B:49:ASN:O	1:B:53:LEU:HG	2.13	0.49
1:B:47:ILE:HA	1:B:357:GLU:CG	2.43	0.48
1:B:205:LEU:O	1:B:205:LEU:HD13	2.12	0.48
1:B:276:HIS:O	1:B:279:HIS:HB3	2.12	0.48
1:A:130:THR:HB	4:A:503:HOH:O	2.13	0.48
1:C:53:LEU:O	1:C:54:ARG:C	2.54	0.48
1:A:313:ARG:O	1:B:206:HIS:HD2	1.97	0.48
1:B:329:TRP:O	1:B:331:THR:HG23	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:277:GLU:O	1:B:278:LEU:C	2.57	0.47
1:B:276:HIS:O	1:B:277:GLU:C	2.57	0.47
1:C:335:ASN:OD1	1:C:335:ASN:C	2.57	0.47
1:C:340:ASP:OD1	1:C:342:SER:N	2.48	0.47
1:A:297:TYR:C	1:A:297:TYR:CD1	2.93	0.46
1:C:279:HIS:C	1:C:279:HIS:CD2	2.93	0.46
1:A:297:TYR:CD1	1:A:298:SER:O	2.68	0.46
1:B:181:LEU:O	1:B:182:LYS:CB	2.64	0.46
1:C:328:VAL:O	1:C:329:TRP:C	2.59	0.46
1:B:271:LEU:HD13	1:B:294:PHE:CE2	2.51	0.46
1:A:181:LEU:O	1:A:182:LYS:HG2	2.17	0.45
1:B:247:LEU:HB3	1:B:250:ILE:HD12	1.98	0.45
1:C:290:GLU:O	1:C:290:GLU:CG	2.65	0.45
1:C:325:PHE:O	1:C:326:PRO:C	2.58	0.45
1:B:206:HIS:O	1:B:208:SER:OG	2.31	0.45
1:C:53:LEU:O	1:C:56:ILE:N	2.48	0.45
1:B:249:LEU:HD12	1:B:321:ILE:HD11	1.98	0.45
1:B:302:VAL:O	1:B:302:VAL:CG1	2.65	0.45
1:B:328:VAL:O	1:B:329:TRP:C	2.61	0.44
1:C:277:GLU:O	1:C:281:LEU:HD12	2.17	0.44
1:A:92:MET:SD	1:A:106:ILE:HD11	2.57	0.44
1:B:277:GLU:O	1:B:279:HIS:N	2.50	0.44
1:A:149:TRP:CE3	1:A:150:ASN:ND2	2.85	0.44
1:B:297:TYR:C	1:B:297:TYR:CD1	2.95	0.44
1:C:177:LYS:O	1:C:180:SER:HB3	2.17	0.44
1:B:269:GLU:O	1:B:272:GLN:N	2.47	0.44
1:B:247:LEU:HD12	1:B:247:LEU:N	2.33	0.44
1:C:272:GLN:HG2	1:C:294:PHE:O	2.17	0.43
1:B:48:LEU:HB2	1:B:53:LEU:HD21	2.00	0.43
1:A:38:GLU:CD	1:B:147:SER:OG	2.61	0.43
1:C:36:TRP:N	1:C:37:PRO:CD	2.82	0.43
1:B:81:SER:HB2	1:B:82:PRO:CD	2.48	0.43
1:C:158:THR:OG1	1:C:334:ASP:OD2	2.36	0.43
1:B:299:TYR:CD1	1:B:300:GLY:N	2.87	0.43
1:C:49:ASN:OD1	1:C:49:ASN:C	2.61	0.43
1:B:354:PHE:C	1:B:354:PHE:CD1	2.96	0.42
1:C:113:THR:HB	1:C:114:PRO:HD2	2.01	0.42
1:C:160:SER:C	1:C:163:PRO:HD2	2.43	0.42
1:A:270:ARG:O	1:A:274:ILE:HG13	2.18	0.42
1:B:49:ASN:OD1	1:B:51:SER:HB3	2.19	0.42
1:C:162:VAL:HB	1:C:163:PRO:HD3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:56:ILE:CD1	1:B:356:LEU:CD1	2.97	0.42
1:C:201:GLU:OE1	1:C:202:GLU:HG2	2.18	0.42
1:A:36:TRP:N	1:A:37:PRO:CD	2.83	0.42
1:A:88:ARG:O	1:A:92:MET:HG3	2.20	0.42
1:C:44:GLN:HG3	1:C:45:PRO:HD2	2.02	0.42
1:A:99:GLN:O	1:A:100:ALA:C	2.62	0.42
1:B:279:HIS:CD2	1:B:289:LEU:HD11	2.55	0.42
1:A:308:ILE:HB	1:A:309:PRO:HD3	2.00	0.42
1:B:71:GLN:N	1:B:72:PRO:CD	2.83	0.42
1:B:252:ALA:HB1	1:B:253:PRO:HD2	2.01	0.41
1:B:289:LEU:HD12	1:B:289:LEU:H	1.85	0.41
1:A:38:GLU:OE2	1:B:147:SER:OG	2.39	0.41
1:B:276:HIS:O	1:B:279:HIS:N	2.53	0.41
1:C:180:SER:C	1:C:182:LYS:H	2.27	0.41
1:C:278:LEU:HB3	1:C:284:LEU:HD13	2.02	0.41
1:B:308:ILE:HB	1:B:309:PRO:HD3	2.02	0.41
1:B:295:GLN:O	1:B:297:TYR:N	2.54	0.41
1:C:353:VAL:O	1:C:357:GLU:HG3	2.20	0.41
1:B:277:GLU:C	1:B:279:HIS:N	2.78	0.41
1:B:319:HIS:NE2	1:B:321:ILE:HG21	2.35	0.41
1:A:105:GLU:HG3	4:A:511:HOH:O	2.20	0.41
1:A:181:LEU:O	1:A:182:LYS:CB	2.68	0.41
1:B:47:ILE:HG23	1:B:357:GLU:OE2	2.21	0.41
1:B:288:SER:OG	1:B:290:GLU:HB3	2.21	0.41
1:C:192:SER:OG	1:C:193:LEU:N	2.53	0.40
1:B:38:GLU:O	1:B:40:LYS:N	2.55	0.40
1:B:270:ARG:HH21	1:B:274:ILE:HG13	1.86	0.40
1:C:36:TRP:CG	1:C:37:PRO:HD3	2.56	0.40
1:C:52:ALA:O	1:C:53:LEU:C	2.64	0.40
1:A:149:TRP:CE2	1:A:150:ASN:ND2	2.89	0.40

All (1) 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:B:50:SER:OG	1:B:277:GLU:OE1[4_565]	2.06	0.14

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	319/329 (97%)	300 (94%)	18 (6%)	1 (0%)	36	44
1	B	319/329 (97%)	284 (89%)	30 (9%)	5 (2%)	7	6
1	C	319/329 (97%)	294 (92%)	23 (7%)	2 (1%)	21	25
All	All	957/987 (97%)	878 (92%)	71 (7%)	8 (1%)	16	18

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	254	ASN
1	B	302	VAL
1	B	296	ASN
1	B	360	HIS
1	B	334	ASP
1	C	299	TYR
1	C	326	PRO
1	A	150	ASN

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	284/290 (98%)	257 (90%)	27 (10%)	8	9
1	B	284/290 (98%)	258 (91%)	26 (9%)	8	10
1	C	284/290 (98%)	262 (92%)	22 (8%)	12	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	852/870 (98%)	777 (91%)	75 (9%)	9 11

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	GLU
1	A	41	ASN
1	A	51	SER
1	A	55	GLN
1	A	58	GLU
1	A	64	GLU
1	A	67	GLN
1	A	89	GLN
1	A	105	GLU
1	A	107	ASP
1	A	110	LEU
1	A	132	LYS
1	A	137	LEU
1	A	147	SER
1	A	150	ASN
1	A	176	LYS
1	A	179	LEU
1	A	205	LEU
1	A	208	SER
1	A	233	ARG
1	A	238	LEU
1	A	242	ASP
1	A	247	LEU
1	A	284	LEU
1	A	297	TYR
1	A	302	VAL
1	A	312	ARG
1	B	44	GLN
1	B	49	ASN
1	B	50	SER
1	B	56	ILE
1	B	60	THR
1	B	64	GLU
1	B	119	SER
1	B	130	THR
1	B	147	SER
1	B	151	ASN

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Mol	Chain	Res	Type
1	B	158	THR
1	B	160	SER
1	B	180	SER
1	B	205	LEU
1	B	206	HIS
1	B	208	SER
1	B	210	GLN
1	B	242	ASP
1	B	256	THR
1	B	272	GLN
1	B	277	GLU
1	B	286	ASP
1	B	296	ASN
1	B	342	SER
1	B	343	THR
1	B	357	GLU
1	C	34	SER
1	C	40	LYS
1	C	50	SER
1	C	58	GLU
1	C	84	SER
1	C	95	ILE
1	C	112	GLN
1	C	177	LYS
1	C	179	LEU
1	C	205	LEU
1	C	206	HIS
1	C	208	SER
1	C	210	GLN
1	C	263	ASN
1	C	281	LEU
1	C	289	LEU
1	C	290	GLU
1	C	297	TYR
1	C	312	ARG
1	C	337	GLU
1	C	341	GLU
1	C	342	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	GLN
1	A	90	HIS
1	A	128	ASN
1	B	112	GLN
1	C	41	ASN
1	C	112	GLN
1	C	218	HIS
1	C	228	HIS

5.3.3 RNA [i](#)

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](#)

Of 6 ligands modelled in this entry, 3 are monoatomic - leaving 3 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	A1EFY	B	402	2	20,20,20	2.16	4 (20%)	27,27,27	3.01	7 (25%)
3	A1EFY	C	402	2	20,20,20	2.07	4 (20%)	27,27,27	3.75	4 (14%)
3	A1EFY	A	402	2	20,20,20	2.45	6 (30%)	27,27,27	3.48	12 (44%)

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	A1EFY	B	402	2	-	4/15/15/15	0/2/2/2
3	A1EFY	C	402	2	-	6/15/15/15	0/2/2/2
3	A1EFY	A	402	2	-	5/15/15/15	0/2/2/2

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	402	A1EFY	C07-N11	-5.55	1.28	1.37
3	A	402	A1EFY	C08-N09	-5.36	1.28	1.37
3	B	402	A1EFY	C07-N11	-5.05	1.28	1.37
3	A	402	A1EFY	C07-N11	-4.84	1.29	1.37
3	C	402	A1EFY	S02-N04	4.82	1.68	1.61
3	B	402	A1EFY	S02-N04	4.77	1.68	1.61
3	B	402	A1EFY	C08-N09	-4.72	1.29	1.37
3	A	402	A1EFY	S02-N04	4.09	1.67	1.61
3	A	402	A1EFY	C10-N11	-3.93	1.28	1.35
3	C	402	A1EFY	C08-N09	-3.60	1.31	1.37
3	A	402	A1EFY	O03-S02	-3.26	1.39	1.43
3	A	402	A1EFY	O01-S02	-3.06	1.40	1.43
3	B	402	A1EFY	C10-N11	-2.80	1.30	1.35
3	C	402	A1EFY	C10-N11	-2.07	1.31	1.35

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	402	A1EFY	O03-S02-O01	-16.77	99.16	119.52
3	A	402	A1EFY	O03-S02-O01	-14.36	102.08	119.52
3	B	402	A1EFY	O03-S02-O01	-13.51	103.11	119.52
3	C	402	A1EFY	O03-S02-C12	6.96	116.76	107.98
3	A	402	A1EFY	O03-S02-C12	5.47	114.88	107.98
3	C	402	A1EFY	C17-O16-C15	-4.15	108.59	117.50
3	A	402	A1EFY	C12-S02-N04	3.94	112.99	107.54
3	C	402	A1EFY	O03-S02-N04	3.45	112.41	107.03
3	A	402	A1EFY	O01-S02-N04	3.36	112.25	107.03
3	A	402	A1EFY	C19-C12-S02	3.34	123.42	119.76
3	B	402	A1EFY	O03-S02-C12	3.30	112.14	107.98
3	A	402	A1EFY	C05-C06-C07	3.26	117.06	112.28
3	B	402	A1EFY	C12-S02-N04	3.23	112.00	107.54
3	A	402	A1EFY	C06-C05-N04	-2.76	107.33	110.91
3	B	402	A1EFY	C06-C05-N04	-2.53	107.62	110.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	402	A1EFY	C08-N09-C10	2.38	110.62	105.94
3	B	402	A1EFY	C08-C07-N11	2.36	108.44	105.65
3	A	402	A1EFY	N11-C10-N09	-2.33	106.68	111.00
3	B	402	A1EFY	O01-S02-N04	2.33	110.65	107.03
3	A	402	A1EFY	C07-C08-N09	-2.32	105.57	109.73
3	B	402	A1EFY	N11-C10-N09	-2.22	106.88	111.00
3	A	402	A1EFY	C13-C12-S02	-2.20	117.34	119.76
3	A	402	A1EFY	C08-C07-N11	2.01	108.02	105.65

There are no chirality outliers.

All (15) torsion outliers are listed below:

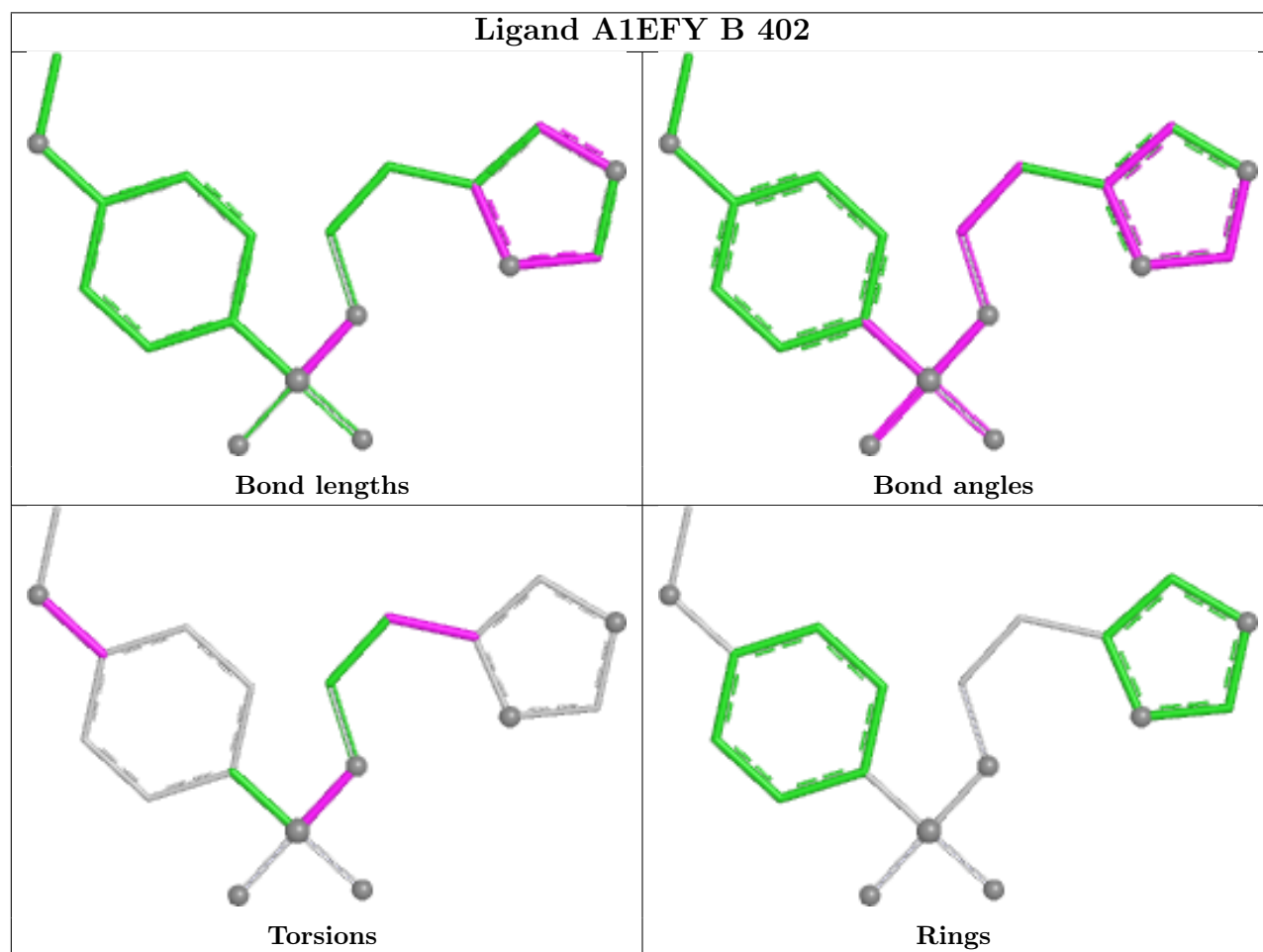
Mol	Chain	Res	Type	Atoms
3	C	402	A1EFY	N04-C05-C06-C07
3	B	402	A1EFY	C18-C15-O16-C17
3	B	402	A1EFY	C14-C15-O16-C17
3	C	402	A1EFY	C14-C15-O16-C17
3	C	402	A1EFY	C18-C15-O16-C17
3	A	402	A1EFY	C05-N04-S02-O01
3	C	402	A1EFY	C05-N04-S02-O03
3	C	402	A1EFY	C05-N04-S02-C12
3	A	402	A1EFY	C05-N04-S02-C12
3	A	402	A1EFY	C14-C15-O16-C17
3	C	402	A1EFY	C05-N04-S02-O01
3	A	402	A1EFY	C18-C15-O16-C17
3	B	402	A1EFY	C05-N04-S02-O03
3	A	402	A1EFY	C05-C06-C07-C08
3	B	402	A1EFY	C05-C06-C07-C08

There are no ring outliers.

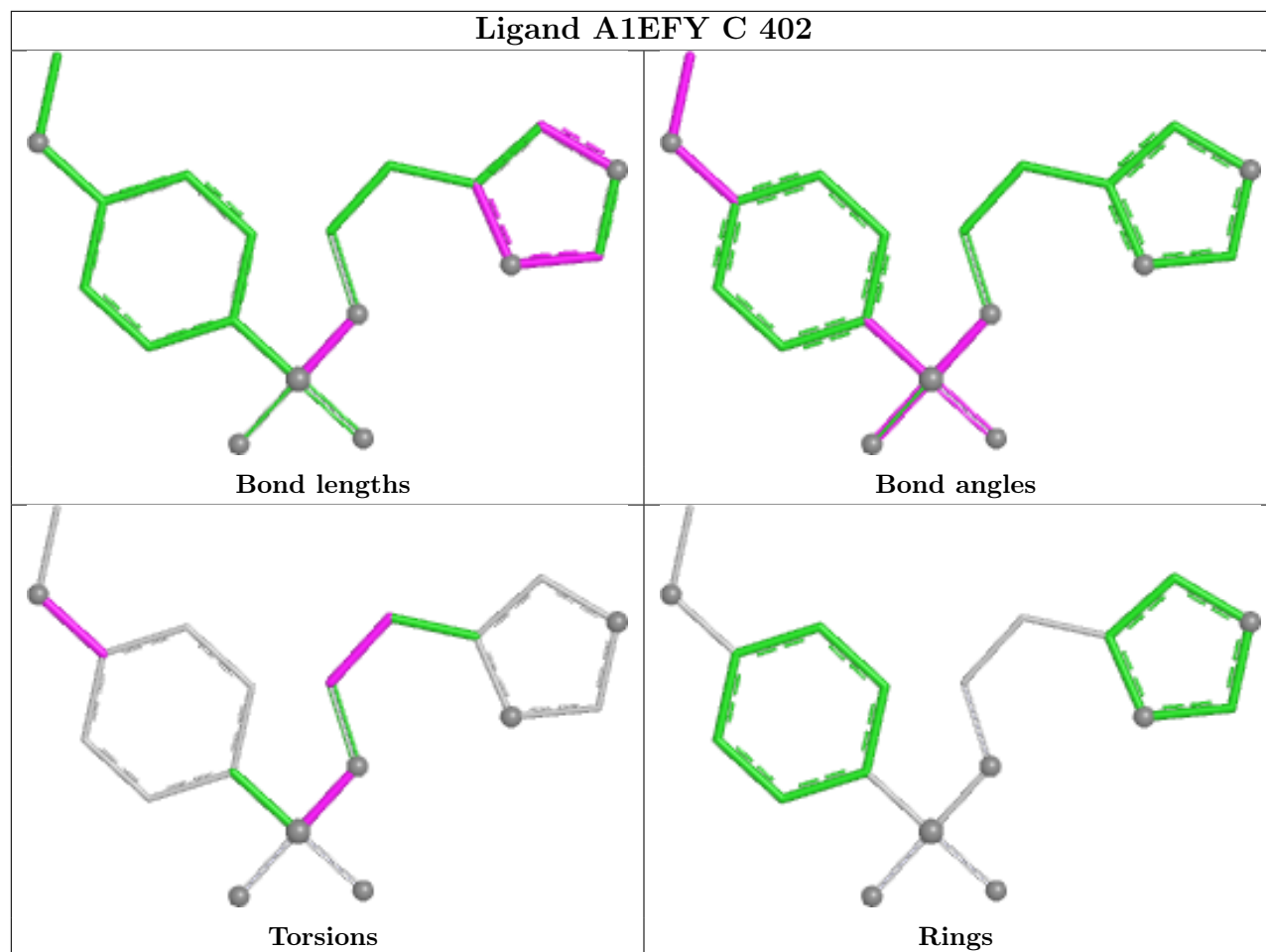
No monomer is involved in short contacts.

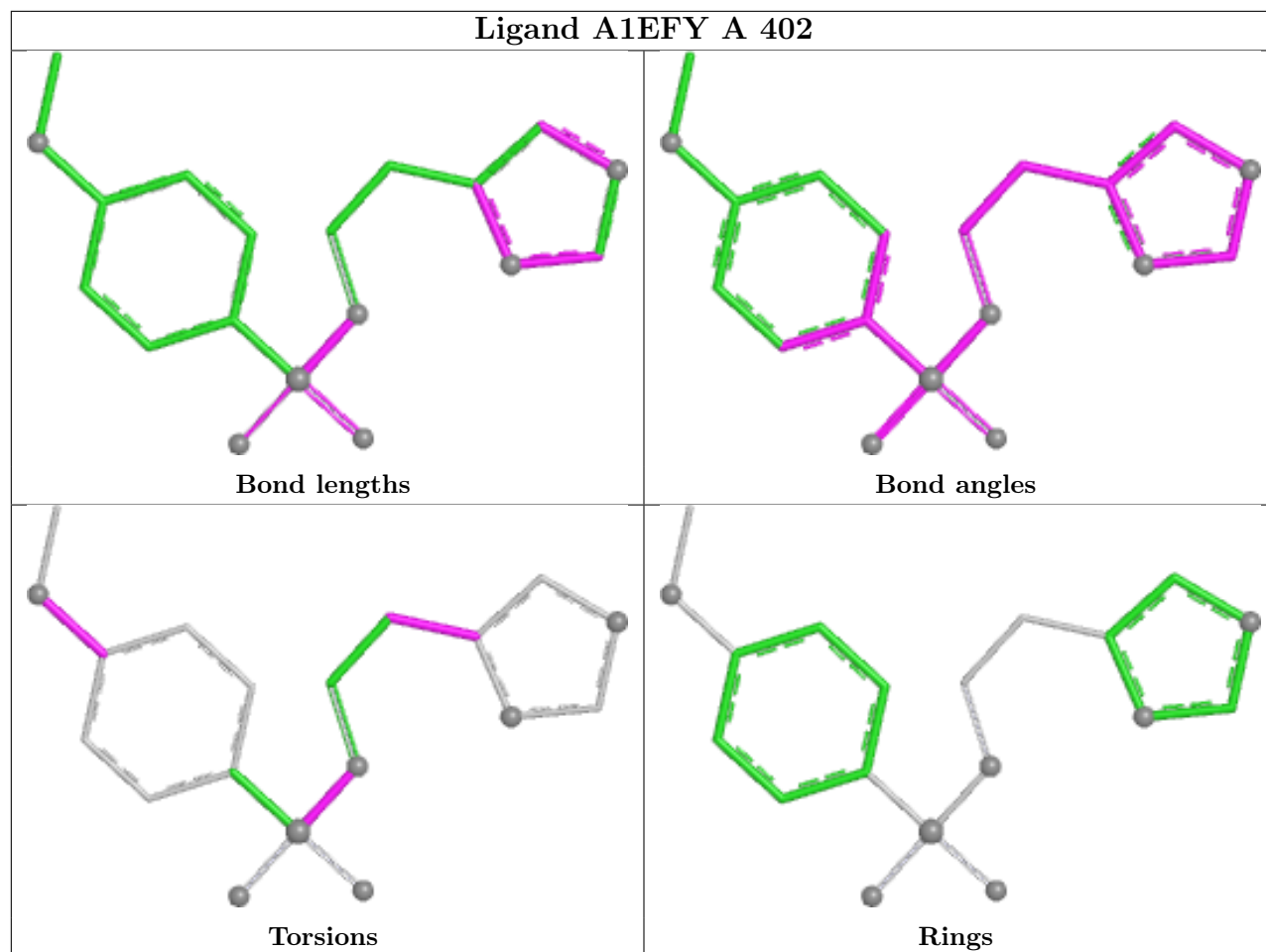
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



Ligand A1EFY C 402





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	323/329 (98%)	-0.15	10 (3%) 51 53	26, 49, 87, 122	0
1	B	323/329 (98%)	0.46	19 (5%) 28 29	37, 65, 118, 146	0
1	C	323/329 (98%)	0.22	12 (3%) 45 47	37, 59, 111, 135	0
All	All	969/987 (98%)	0.18	41 (4%) 40 42	26, 57, 109, 146	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	33	ALA	7.1
1	C	33	ALA	5.0
1	A	33	ALA	4.5
1	C	302	VAL	4.3
1	A	297	TYR	4.2
1	C	149	TRP	4.2
1	C	299	TYR	4.0
1	B	299	TYR	4.0
1	C	34	SER	3.9
1	B	297	TYR	3.8
1	B	300	GLY	3.6
1	B	298	SER	3.6
1	C	35	ALA	3.3
1	C	300	GLY	3.3
1	B	34	SER	3.1
1	B	296	ASN	3.1
1	C	297	TYR	3.1
1	B	189	PRO	3.1
1	A	149	TRP	3.0
1	A	189	PRO	2.9
1	A	302	VAL	2.9
1	B	35	ALA	2.8
1	B	281	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	182	LYS	2.7
1	B	283	LEU	2.7
1	B	289	LEU	2.7
1	A	34	SER	2.7
1	B	261	PHE	2.6
1	B	301	GLY	2.6
1	C	301	GLY	2.5
1	A	35	ALA	2.5
1	B	290	GLU	2.4
1	B	257	PHE	2.3
1	B	149	TRP	2.3
1	B	42	TYR	2.3
1	C	53	LEU	2.2
1	C	296	ASN	2.2
1	B	260	PHE	2.2
1	C	189	PRO	2.1
1	A	296	ASN	2.1
1	A	299	TYR	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	A1EFY	B	402	19/19	0.91	0.12	54,69,83,88	0
3	A1EFY	C	402	19/19	0.94	0.12	49,79,102,102	0
3	A1EFY	A	402	19/19	0.95	0.09	31,53,84,84	0
2	ZN	A	401	1/1	0.99	0.05	36,36,36,36	0
2	ZN	B	401	1/1	0.99	0.03	48,48,48,48	0

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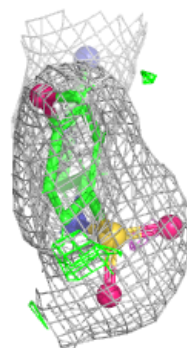
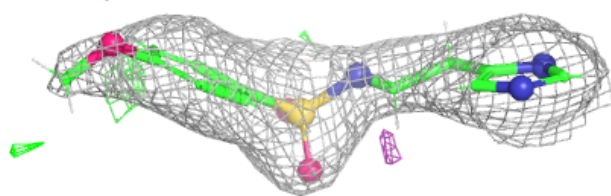
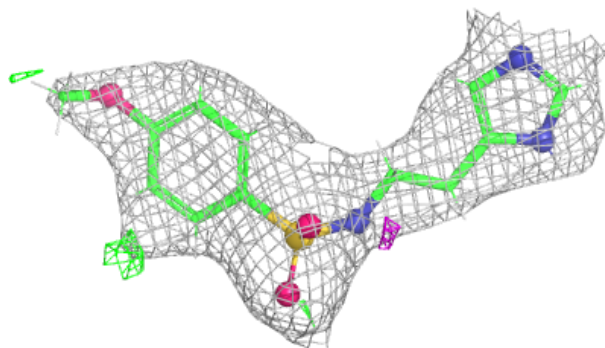
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ZN	C	401	1/1	0.99	0.03	40,40,40,40	0

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.

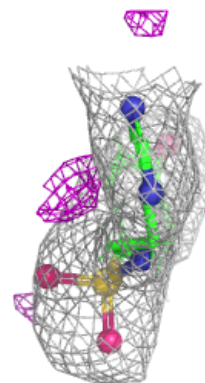
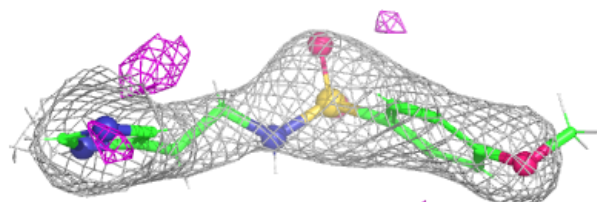
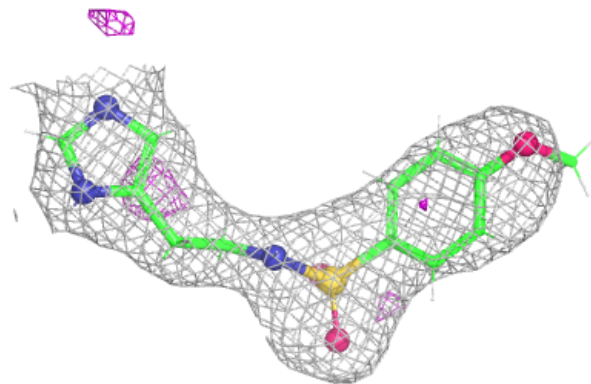
Electron density around A1EFY B 402:

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



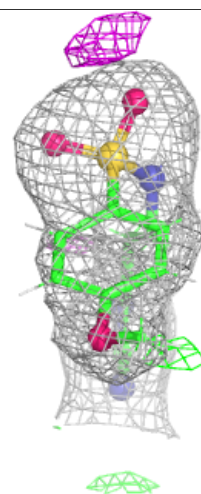
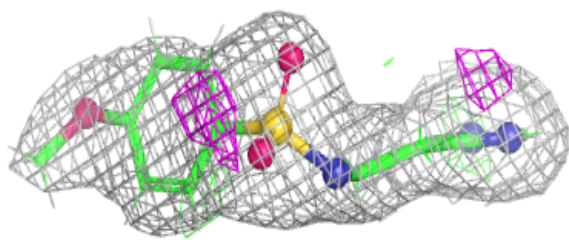
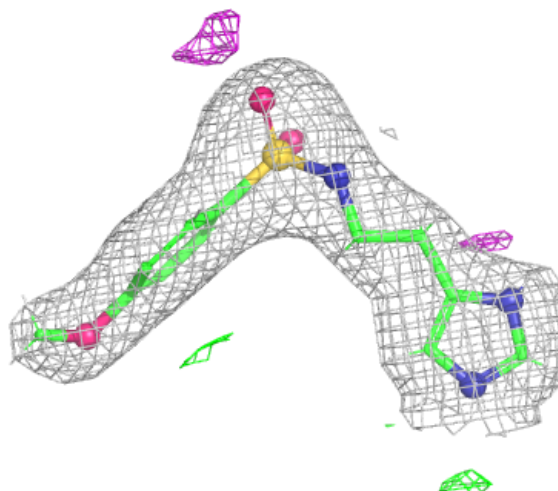
Electron density around A1EFY C 402:

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



Electron density around A1EFY A 402:

$2mF_o-DF_c$ (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.