



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 17, 2025 – 04:05 PM EST

PDB ID : 9PW8 / pdb_00009pw8
Title : Fem-1 homolog B (FEM1B) in complex with VU0417412
Authors : Katinas, J.M.; Fesik, S.W.
Deposited on : 2025-08-04
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 : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
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) : 2.46

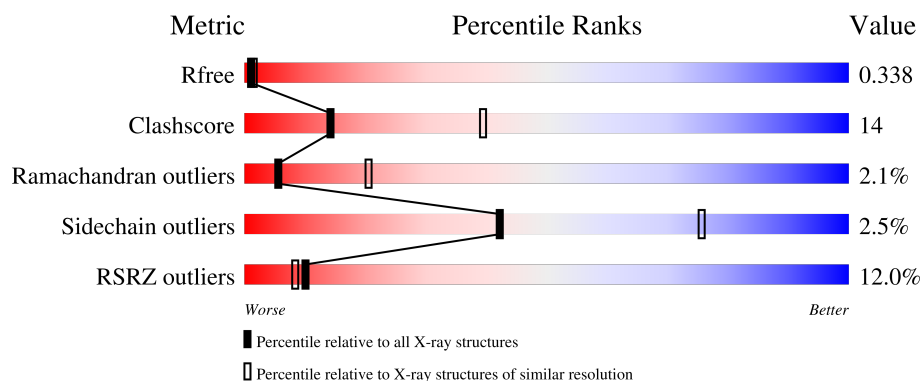
1 Overall quality at a glance

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}	164625	3657 (2.80-2.80)
Clashscore	180529	4123 (2.80-2.80)
Ramachandran outliers	177936	4071 (2.80-2.80)
Sidechain outliers	177891	4073 (2.80-2.80)
RSRZ outliers	164620	3659 (2.80-2.80)

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	357	<div> <div>12%</div> <div>64%</div> <div>26%</div> <div>• • 7%</div> </div>
1	B	357	<div> <div>11%</div> <div>71%</div> <div>21%</div> <div>• 6%</div> </div>

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 5034 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 Protein fem-1 homolog B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	333	Total	C	N	O	S	0	0	0
			2490	1578	435	466	11			
1	B	336	Total	C	N	O	S	0	0	0
			2514	1593	440	469	12			

There are 40 discrepancies between the modelled and reference sequences:

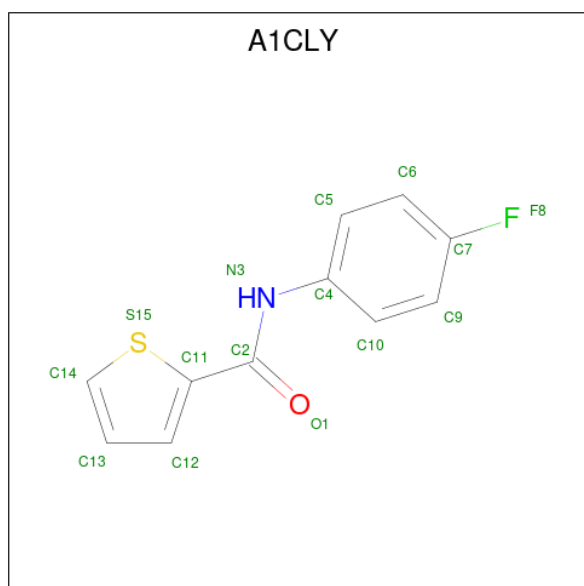
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP Q9UK73
A	0	HIS	-	expression tag	UNP Q9UK73
A	338	GLY	-	expression tag	UNP Q9UK73
A	339	GLY	-	expression tag	UNP Q9UK73
A	340	GLY	-	expression tag	UNP Q9UK73
A	341	SER	-	expression tag	UNP Q9UK73
A	342	GLY	-	expression tag	UNP Q9UK73
A	343	GLY	-	expression tag	UNP Q9UK73
A	344	GLY	-	expression tag	UNP Q9UK73
A	345	SER	-	expression tag	UNP Q9UK73
A	346	LYS	-	expression tag	UNP Q9UK73
A	347	LYS	-	expression tag	UNP Q9UK73
A	348	ARG	-	expression tag	UNP Q9UK73
A	349	LEU	-	expression tag	UNP Q9UK73
A	350	LEU	-	expression tag	UNP Q9UK73
A	351	LEU	-	expression tag	UNP Q9UK73
A	352	GLY	-	expression tag	UNP Q9UK73
A	353	LEU	-	expression tag	UNP Q9UK73
A	354	ASP	-	expression tag	UNP Q9UK73
A	355	ARG	-	expression tag	UNP Q9UK73
B	-1	GLY	-	expression tag	UNP Q9UK73
B	0	HIS	-	expression tag	UNP Q9UK73
B	338	GLY	-	expression tag	UNP Q9UK73
B	339	GLY	-	expression tag	UNP Q9UK73
B	340	GLY	-	expression tag	UNP Q9UK73

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Chain	Residue	Modelled	Actual	Comment	Reference
B	341	SER	-	expression tag	UNP Q9UK73
B	342	GLY	-	expression tag	UNP Q9UK73
B	343	GLY	-	expression tag	UNP Q9UK73
B	344	GLY	-	expression tag	UNP Q9UK73
B	345	SER	-	expression tag	UNP Q9UK73
B	346	LYS	-	expression tag	UNP Q9UK73
B	347	LYS	-	expression tag	UNP Q9UK73
B	348	ARG	-	expression tag	UNP Q9UK73
B	349	LEU	-	expression tag	UNP Q9UK73
B	350	LEU	-	expression tag	UNP Q9UK73
B	351	LEU	-	expression tag	UNP Q9UK73
B	352	GLY	-	expression tag	UNP Q9UK73
B	353	LEU	-	expression tag	UNP Q9UK73
B	354	ASP	-	expression tag	UNP Q9UK73
B	355	ARG	-	expression tag	UNP Q9UK73

- Molecule 2 is N-(4-fluorophenyl)thiophene-2-carboxamide (CCD ID: A1CLY) (formula: $C_{11}H_8FNOS$) (labeled as "Ligand of Interest" by depositor).

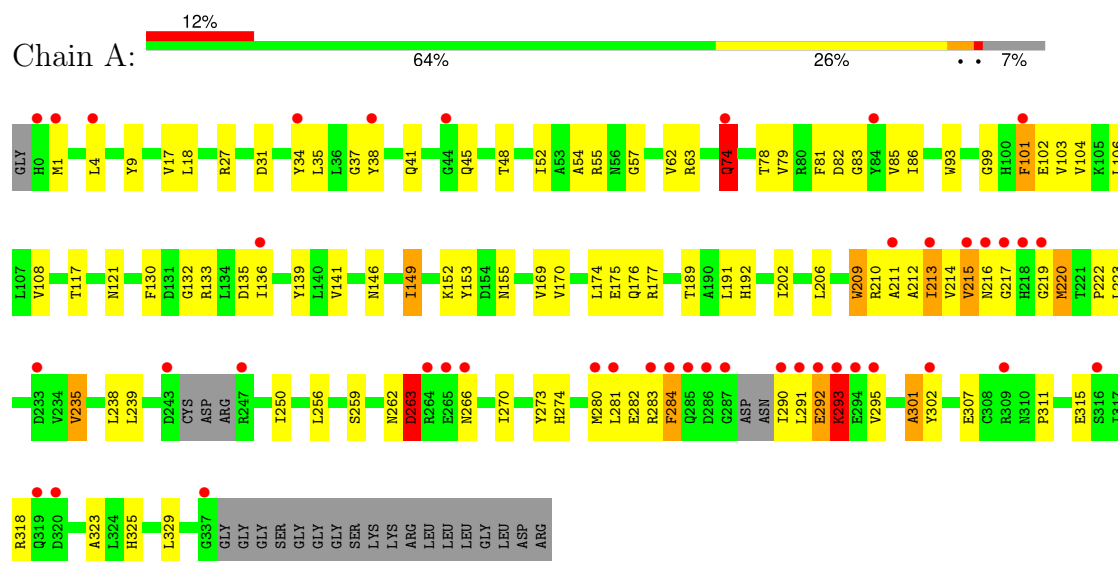


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	S	0	0
			15	11	1	1	1	1		
2	B	1	Total	C	F	N	O	S	0	0
			15	11	1	1	1	1		

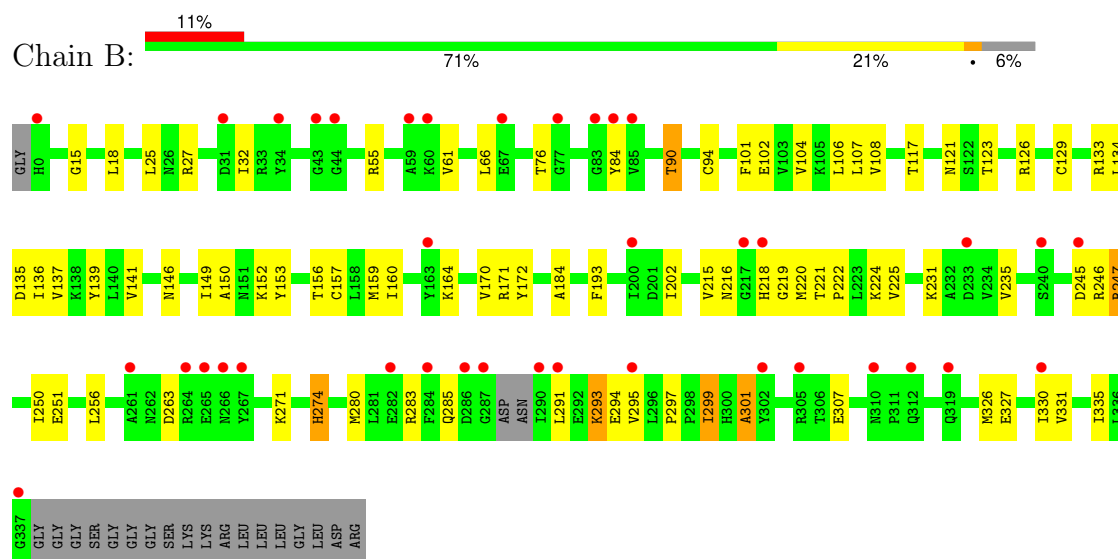
3 Residue-property plots [i](#)

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: Protein fem-1 homolog B



• Molecule 1: Protein fem-1 homolog B



4 Data and refinement statistics

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, α , β , γ	123.71Å 123.71Å 137.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.03 – 2.80 46.03 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.7 (46.03-2.80) 99.5 (46.03-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.26 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, R_{free}	0.299 , 0.338 0.299 , 0.338	Depositor DCC
R_{free} test set	1351 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	65.6	Xtriage
Anisotropy	0.252	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 43.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	5034	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.45% 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: A1CLY

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	0.35	2/2530 (0.1%)	0.75	10/3437 (0.3%)
1	B	0.25	1/2556 (0.0%)	0.66	5/3474 (0.1%)
All	All	0.31	3/5086 (0.1%)	0.71	15/6911 (0.2%)

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	A	0	5

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	293	LYS	CG-CD	6.18	1.71	1.52
1	B	294	GLU	C-N	-5.49	1.22	1.33
1	A	37	GLY	C-O	-5.45	1.20	1.24

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	263	ASP	CB-CG-OD2	-11.19	92.67	118.40
1	B	25	LEU	CA-C-N	-11.01	108.01	123.20
1	B	25	LEU	C-N-CA	-11.01	108.01	123.20
1	A	263	ASP	CB-CG-OD1	10.00	141.41	118.40
1	A	74	GLN	CB-CA-C	-9.46	92.51	110.67
1	B	294	GLU	N-CA-CB	7.93	121.92	109.71
1	A	74	GLN	N-CA-C	-7.26	103.40	111.82
1	A	292	GLU	CA-C-N	6.45	132.86	123.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	292	GLU	C-N-CA	6.45	132.86	123.13
1	A	293	LYS	CB-CG-CD	6.38	125.98	111.30
1	A	220	MET	CA-C-N	-5.70	113.24	122.48
1	A	220	MET	C-N-CA	-5.70	113.24	122.48
1	B	293	LYS	CA-C-N	-5.70	113.03	121.24
1	B	293	LYS	C-N-CA	-5.70	113.03	121.24
1	A	263	ASP	CA-CB-CG	5.58	118.18	112.60

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	209	TRP	Peptide
1	A	262	ASN	Peptide
1	A	263	ASP	Sidechain
1	A	74	GLN	Mainchain,Peptide

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	2490	0	2421	83	0
1	B	2514	0	2438	60	0
2	A	15	0	0	0	0
2	B	15	0	0	1	0
All	All	5034	0	4859	138	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 (138) 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:101:PHE:HD1	1:A:102:GLU:H	1.21	0.88
1:A:170:VAL:HG11	1:A:202:ILE:HG23	1.61	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:VAL:HG22	1:A:219:GLY:HA2	1.61	0.83
1:A:108:VAL:HG21	1:A:139:TYR:HE2	1.43	0.82
1:B:101:PHE:HD2	1:B:102:GLU:H	1.28	0.81
1:A:284:PHE:HA	1:A:293:LYS:HB3	1.64	0.80
1:B:246:ARG:HH21	1:B:291:LEU:HG	1.45	0.80
1:B:117:THR:HB	1:B:121:ASN:HA	1.65	0.79
1:A:117:THR:HB	1:A:121:ASN:HA	1.65	0.76
1:B:76:THR:HG22	1:B:90:THR:HG22	1.68	0.75
1:A:215:VAL:HG13	1:A:219:GLY:H	1.52	0.74
1:A:295:VAL:HG13	1:A:307:GLU:HB3	1.72	0.70
1:B:280:MET:HA	1:B:283:ARG:HD3	1.73	0.70
1:B:327:GLU:O	1:B:331:VAL:HG23	1.91	0.70
1:A:189:THR:HG23	1:A:191:LEU:H	1.57	0.69
1:A:215:VAL:HA	1:A:220:MET:H	1.58	0.67
1:A:202:ILE:O	1:A:206:LEU:HD12	1.96	0.66
1:B:224:LYS:HE3	1:B:251:GLU:HG2	1.77	0.66
1:A:301:ALA:HA	1:B:218:HIS:HB3	1.77	0.66
1:B:66:LEU:HD11	1:B:107:LEU:HD23	1.78	0.65
1:B:141:VAL:HG11	1:B:172:TYR:HE2	1.60	0.65
1:B:295:VAL:HG23	1:B:307:GLU:HB2	1.79	0.65
1:B:326:MET:O	1:B:330:ILE:HD12	1.97	0.64
1:B:271:LYS:HA	1:B:274:HIS:HB3	1.80	0.63
1:A:263:ASP:OD1	1:A:266:ASN:C	2.42	0.63
1:A:104:VAL:HG11	1:A:136:ILE:HG22	1.80	0.62
1:A:57:GLY:HA2	1:A:103:VAL:HG21	1.82	0.62
1:A:99:GLY:HA2	1:A:136:ILE:HD11	1.82	0.61
1:B:133:ARG:HE	1:B:135:ASP:H	1.49	0.60
1:A:54:ALA:HA	1:A:103:VAL:HG11	1.83	0.60
1:B:108:VAL:HG11	1:B:139:TYR:HE2	1.66	0.60
1:A:146:ASN:HB3	1:A:149:ILE:HG22	1.82	0.60
1:A:215:VAL:HG12	1:A:217:GLY:H	1.67	0.60
1:B:104:VAL:O	1:B:108:VAL:HG12	2.01	0.59
1:A:152:LYS:HD2	1:A:153:TYR:CZ	2.37	0.59
1:A:217:GLY:O	1:B:301:ALA:HB1	2.02	0.59
1:B:159:MET:HE2	1:B:193:PHE:HE2	1.68	0.59
1:A:108:VAL:HG21	1:A:139:TYR:CE2	2.34	0.58
1:B:141:VAL:HG11	1:B:172:TYR:CE2	2.39	0.58
1:A:189:THR:HG22	1:A:192:HIS:ND1	2.20	0.57
1:A:41:GLN:HA	1:A:45:GLN:O	2.05	0.56
1:B:222:PRO:HA	1:B:225:VAL:HG12	1.87	0.56
1:B:55:ARG:HB2	1:B:94:CYS:HB3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:221:THR:HG23	1:B:224:LYS:H	1.71	0.55
1:A:290:ILE:HG22	1:A:291:LEU:H	1.72	0.54
1:B:152:LYS:HD2	1:B:153:TYR:CZ	2.43	0.53
1:B:231:LYS:O	1:B:235:VAL:HG23	2.09	0.53
1:A:63:ARG:HG3	1:A:106:LEU:HD11	1.89	0.53
1:B:104:VAL:HG21	1:B:136:ILE:HD13	1.90	0.53
1:B:216:ASN:HB3	1:B:220:MET:H	1.75	0.52
1:B:295:VAL:CG2	1:B:307:GLU:HB2	2.39	0.52
1:A:263:ASP:CG	1:A:263:ASP:O	2.53	0.51
1:A:4:LEU:HD11	1:A:27:ARG:HH21	1.75	0.51
1:A:17:VAL:HG13	1:A:18:LEU:HD12	1.93	0.51
1:A:259:SER:O	1:A:263:ASP:OD2	2.29	0.50
1:A:34:TYR:HE1	1:A:38:TYR:HD1	1.60	0.50
1:A:213:ILE:HG22	1:A:214:VAL:HG12	1.94	0.49
1:A:235:VAL:O	1:A:239:LEU:HD23	2.12	0.49
1:A:325:HIS:C	1:A:325:HIS:CD2	2.90	0.49
1:A:293:LYS:O	1:A:293:LYS:HG3	2.10	0.49
1:A:212:ALA:HB3	1:A:222:PRO:HG3	1.93	0.49
1:A:215:VAL:CA	1:A:220:MET:H	2.26	0.49
1:B:170:VAL:HG21	1:B:202:ILE:HD13	1.94	0.49
1:A:311:PRO:O	1:A:315:GLU:HG3	2.13	0.48
1:B:247:ARG:O	1:B:250:ILE:HG12	2.14	0.48
1:B:101:PHE:HD2	1:B:102:GLU:N	2.03	0.48
1:A:283:ARG:O	1:A:293:LYS:HE3	2.14	0.48
1:B:146:ASN:O	1:B:149:ILE:HG22	2.13	0.48
1:B:216:ASN:N	1:B:220:MET:O	2.47	0.48
1:A:141:VAL:HG11	1:A:176:GLN:HG3	1.96	0.47
1:B:108:VAL:CG1	1:B:139:TYR:HE2	2.26	0.47
1:B:250:ILE:HD12	1:B:283:ARG:HH11	1.80	0.47
1:A:215:VAL:HG12	1:A:217:GLY:N	2.28	0.47
1:A:291:LEU:CG	1:A:292:GLU:H	2.27	0.47
1:A:291:LEU:HG	1:A:292:GLU:H	1.80	0.47
1:A:282:GLU:HB2	1:A:290:ILE:HA	1.96	0.46
1:A:175:GLU:C	1:A:177:ARG:H	2.23	0.46
1:B:331:VAL:O	1:B:335:ILE:HD12	2.16	0.46
1:B:297:PRO:O	1:B:299:ILE:HD13	2.16	0.46
1:A:280:MET:HE2	1:A:280:MET:HB2	1.86	0.46
1:A:31:ASP:O	1:A:35:LEU:HG	2.16	0.45
1:A:189:THR:HG23	1:A:191:LEU:N	2.26	0.45
1:B:27:ARG:HB2	1:B:32:ILE:HG13	1.99	0.45
1:B:283:ARG:NH2	1:B:293:LYS:HB3	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:VAL:HG11	1:A:136:ILE:CG2	2.44	0.45
1:B:137:VAL:O	1:B:141:VAL:HG12	2.17	0.45
1:A:174:LEU:HD13	1:A:209:TRP:CD1	2.53	0.44
1:A:1:MET:HB3	1:A:34:TYR:CE2	2.51	0.44
1:A:192:HIS:HB3	1:A:216:ASN:OD1	2.17	0.44
1:B:123:THR:HG21	1:B:149:ILE:HG21	1.99	0.44
1:A:78:THR:HG22	1:A:85:VAL:HG12	1.98	0.44
1:A:273:TYR:CE2	1:A:318:ARG:HG3	2.52	0.44
1:A:323:ALA:HB2	1:B:153:TYR:OH	2.17	0.44
1:B:123:THR:HG21	1:B:149:ILE:CG2	2.47	0.44
1:B:215:VAL:HG22	1:B:216:ASN:O	2.18	0.44
1:A:81:PHE:HB3	1:A:82:ASP:H	1.61	0.44
1:A:223:LEU:HD11	1:A:239:LEU:CD2	2.48	0.43
1:A:270:ILE:HG13	1:B:84:TYR:CZ	2.53	0.43
1:A:284:PHE:CA	1:A:293:LYS:HB3	2.42	0.43
1:B:133:ARG:HH21	1:B:134:LEU:HB3	1.83	0.43
1:B:299:ILE:HG22	1:B:301:ALA:HB3	2.01	0.43
1:B:235:VAL:HG11	1:B:256:LEU:HD22	2.00	0.43
1:A:74:GLN:OE1	1:A:74:GLN:N	2.52	0.43
1:A:130:PHE:C	1:A:130:PHE:CD1	2.96	0.43
1:A:215:VAL:N	1:A:220:MET:O	2.50	0.43
1:B:15:GLY:HA2	1:B:61:VAL:HG21	2.00	0.43
1:B:170:VAL:HG11	1:B:202:ILE:HG23	2.00	0.43
1:A:291:LEU:HD12	1:A:292:GLU:H	1.84	0.43
1:A:133:ARG:HA	1:A:133:ARG:HD2	1.57	0.43
1:A:302:TYR:CE2	1:A:329:LEU:HB3	2.54	0.43
1:A:235:VAL:HG11	1:A:256:LEU:HD22	2.01	0.42
1:B:126:ARG:HH21	2:B:401:A1CLY:C13	2.31	0.42
1:A:104:VAL:HG21	1:A:136:ILE:HG21	2.01	0.42
1:A:133:ARG:HH21	1:A:135:ASP:CG	2.26	0.42
1:A:325:HIS:O	1:A:325:HIS:HD2	2.03	0.42
1:A:132:GLY:HA2	1:A:169:VAL:HG21	2.01	0.42
1:A:209:TRP:CD1	1:A:209:TRP:N	2.88	0.42
1:B:224:LYS:HZ2	1:B:224:LYS:HG3	1.64	0.42
1:A:86:ILE:HG21	1:A:93:TRP:CH2	2.54	0.42
1:B:150:ALA:HB2	1:B:156:THR:HG22	2.01	0.42
1:A:223:LEU:HD13	1:A:238:LEU:HB2	2.02	0.42
1:B:160:ILE:O	1:B:164:LYS:HG2	2.20	0.42
1:A:62:VAL:HG21	1:A:103:VAL:HG13	2.02	0.41
1:A:250:ILE:HD11	1:A:281:LEU:HD12	2.02	0.41
1:A:101:PHE:CD1	1:A:102:GLU:N	2.79	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:TYR:CZ	1:A:52:ILE:HD13	2.55	0.41
1:A:81:PHE:C	1:A:83:GLY:H	2.28	0.41
1:A:282:GLU:CB	1:A:290:ILE:HA	2.51	0.41
1:B:159:MET:HE1	1:B:184:ALA:HB2	2.02	0.41
1:B:101:PHE:CD2	1:B:102:GLU:N	2.82	0.41
1:A:55:ARG:HD3	1:A:79:VAL:HG21	2.03	0.41
1:B:129:CYS:SG	1:B:157:CYS:HB3	2.61	0.41
1:B:102:GLU:O	1:B:106:LEU:HD23	2.21	0.41
1:B:246:ARG:NH2	1:B:291:LEU:HG	2.25	0.41
1:A:293:LYS:O	1:A:293:LYS:CG	2.67	0.41
1:A:301:ALA:CA	1:B:218:HIS:HB3	2.50	0.41
1:B:159:MET:HE2	1:B:193:PHE:CE2	2.52	0.40
1:A:48:THR:O	1:A:52:ILE:HG12	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	327/357 (92%)	293 (90%)	26 (8%)	8 (2%)	5	18
1	B	332/357 (93%)	303 (91%)	23 (7%)	6 (2%)	7	24
All	All	659/714 (92%)	596 (90%)	49 (7%)	14 (2%)	5	20

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	211	ALA
1	A	213	ILE
1	A	263	ASP
1	A	284	PHE
1	B	247	ARG

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Mol	Chain	Res	Type
1	B	285	GLN
1	A	210	ARG
1	A	215	VAL
1	A	274	HIS
1	A	301	ALA
1	B	245	ASP
1	B	301	ALA
1	B	299	ILE
1	B	219	GLY

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	242/285 (85%)	235 (97%)	7 (3%)	37	71
1	B	244/285 (86%)	239 (98%)	5 (2%)	50	81
All	All	486/570 (85%)	474 (98%)	12 (2%)	42	75

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	74	GLN
1	A	101	PHE
1	A	149	ILE
1	A	155	ASN
1	A	235	VAL
1	A	263	ASP
1	A	293	LYS
1	B	18	LEU
1	B	90	THR
1	B	171	ARG
1	B	263	ASP
1	B	274	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	HIS
1	A	75	GLN
1	A	116	HIS
1	A	155	ASN
1	A	325	HIS
1	B	72	GLN
1	B	74	GLN
1	B	143	ASN
1	B	176	GLN
1	B	262	ASN

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](#)

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	A1CLY	A	401	-	15,16,16	0.43	0	16,21,21	0.98	1 (6%)
2	A1CLY	B	401	-	15,16,16	0.32	0	16,21,21	0.47	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
2	A1CLY	A	401	-	-	0/6/8/8	0/2/2/2
2	A1CLY	B	401	-	-	4/6/8/8	0/2/2/2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	A1CLY	C9-C7-C6	2.05	125.49	122.80

There are no chirality outliers.

All (4) torsion outliers are listed below:

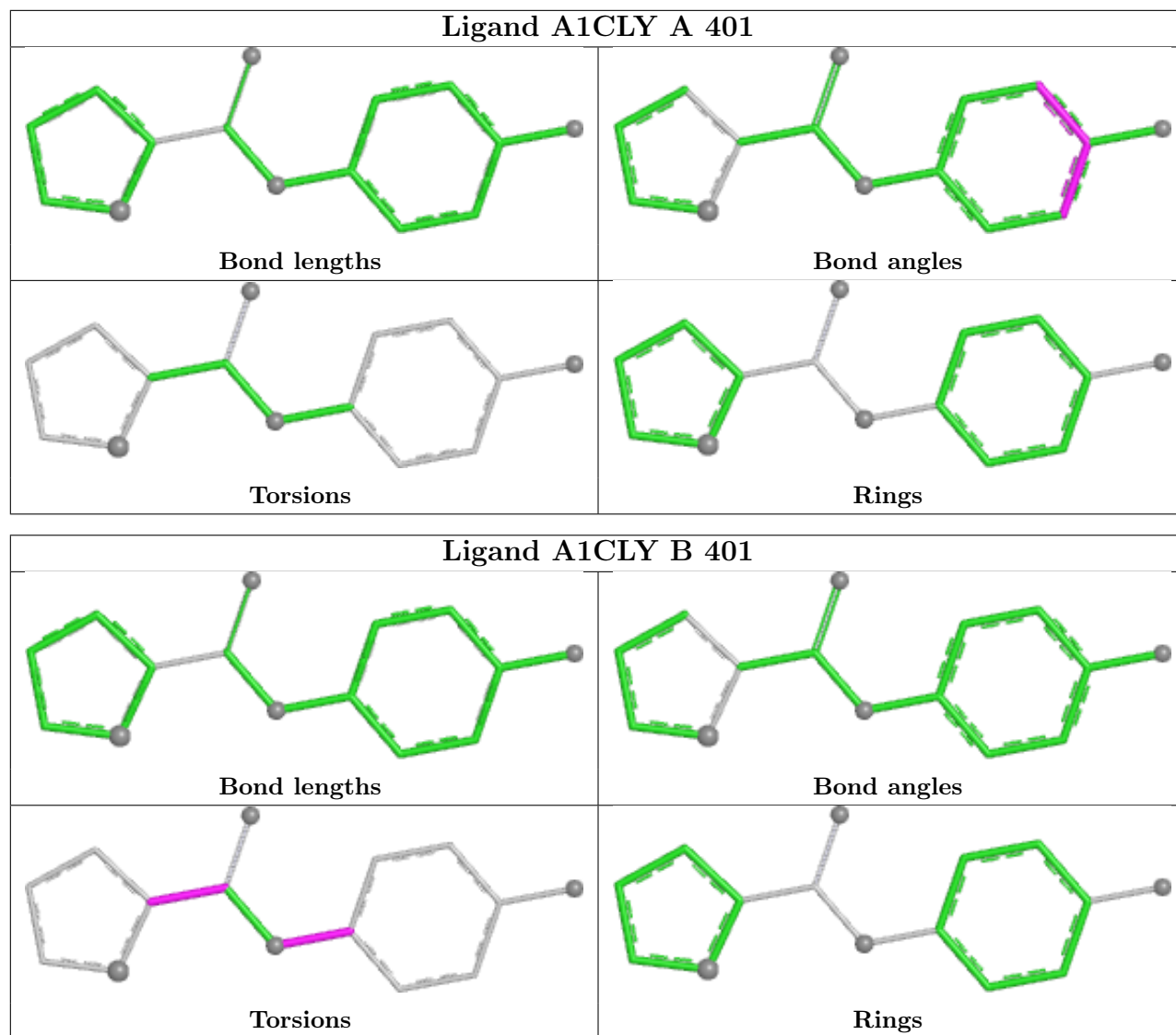
Mol	Chain	Res	Type	Atoms
2	B	401	A1CLY	C12-C11-C2-N3
2	B	401	A1CLY	C12-C11-C2-O1
2	B	401	A1CLY	C10-C4-N3-C2
2	B	401	A1CLY	C5-C4-N3-C2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	A1CLY	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	333/357 (93%)	0.92	42 (12%) 9 8	43, 62, 96, 113	0
1	B	336/357 (94%)	0.91	38 (11%) 11 9	50, 65, 96, 110	0
All	All	669/714 (93%)	0.91	80 (11%) 10 8	43, 64, 96, 113	0

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	286	ASP	6.9
1	A	283	ARG	5.1
1	A	293	LYS	4.8
1	B	217	GLY	4.7
1	B	287	GLY	4.7
1	A	217	GLY	4.6
1	B	310	ASN	4.3
1	B	302	TYR	4.2
1	A	290	ILE	4.2
1	A	281	LEU	4.2
1	A	265	GLU	4.1
1	A	291	LEU	4.0
1	A	213	ILE	3.9
1	B	84	TYR	3.9
1	A	295	VAL	3.7
1	B	44	GLY	3.7
1	A	74	GLN	3.6
1	A	309	ARG	3.6
1	A	0	HIS	3.5
1	B	245	ASP	3.4
1	A	216	ASN	3.3
1	A	284	PHE	3.3
1	B	218	HIS	3.3
1	A	266	ASN	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	305	ARG	3.2
1	B	60	LYS	3.2
1	A	243	ASP	3.2
1	A	84	TYR	3.2
1	A	285	GLN	3.0
1	B	43	GLY	3.0
1	A	44	GLY	2.9
1	B	59	ALA	2.9
1	A	302	TYR	2.8
1	B	83	GLY	2.8
1	B	266	ASN	2.8
1	B	267	TYR	2.8
1	B	200	ILE	2.8
1	B	290	ILE	2.8
1	A	337	GLY	2.6
1	B	261	ALA	2.5
1	B	265	GLU	2.5
1	B	319	GLN	2.5
1	A	1	MET	2.4
1	A	280	MET	2.4
1	B	264	ARG	2.4
1	A	316	SER	2.4
1	A	38	TYR	2.3
1	A	4	LEU	2.3
1	A	264	ARG	2.3
1	A	215	VAL	2.3
1	B	291	LEU	2.3
1	B	0	HIS	2.3
1	B	282	GLU	2.3
1	A	136	ILE	2.3
1	A	320	ASP	2.3
1	B	240	SER	2.3
1	A	34	TYR	2.2
1	A	287	GLY	2.2
1	B	163	TYR	2.2
1	A	233	ASP	2.2
1	B	286	ASP	2.2
1	B	34	TYR	2.2
1	A	101	PHE	2.2
1	A	247	ARG	2.2
1	B	233	ASP	2.2
1	B	330	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	67	GLU	2.2
1	A	219	GLY	2.1
1	B	337	GLY	2.1
1	A	292	GLU	2.1
1	B	295	VAL	2.1
1	B	312	GLN	2.1
1	A	211	ALA	2.1
1	A	294	GLU	2.1
1	A	218	HIS	2.1
1	A	319	GLN	2.0
1	B	85	VAL	2.0
1	B	77	GLY	2.0
1	B	284	PHE	2.0
1	B	31	ASP	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](#)

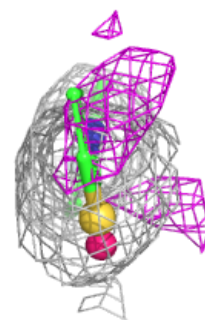
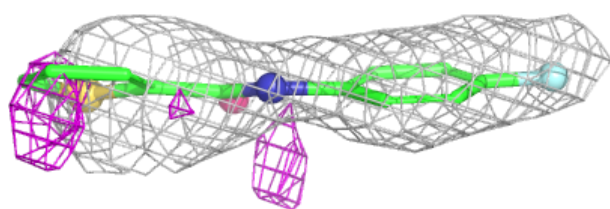
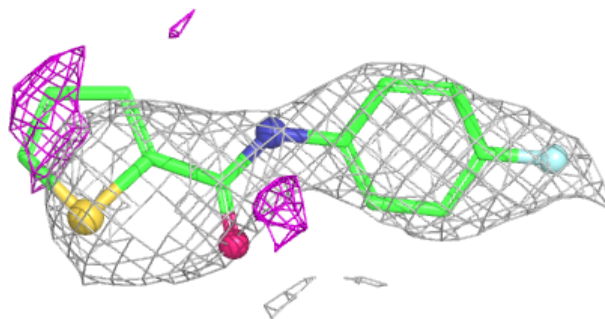
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	A1CLY	A	401	15/15	0.86	0.16	69,73,77,99	0
2	A1CLY	B	401	15/15	0.92	0.11	55,60,68,80	0

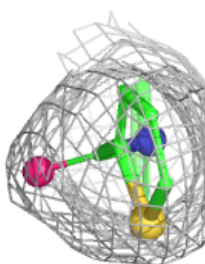
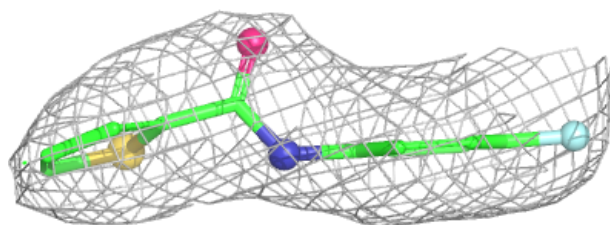
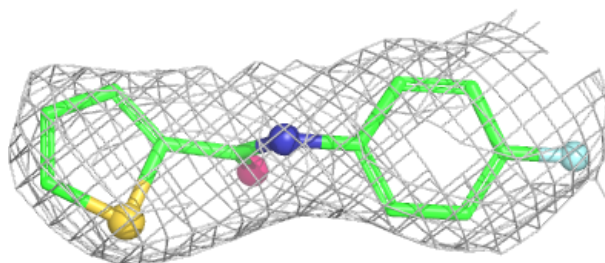
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around A1CLY 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 A1CLY 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.