



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 18, 2025 – 12:09 PM EST

PDB ID : 9PQG / pdb_00009pqg
Title : Co-crystal structure of feline coronavirus UU23 main protease with Ibuzatrelvir
Authors : Maryam, A.; Shaqra, A.M.; Iyer, V.; Jung, K.; Schiffer, C.A.
Deposited on : 2025-07-22
Resolution : 2.27 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

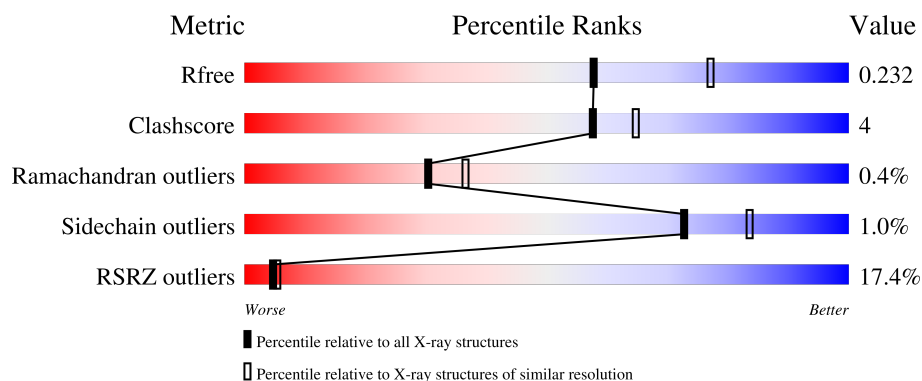
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.27 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	8487 (2.30-2.26)
Clashscore	180529	9437 (2.30-2.26)
Ramachandran outliers	177936	9341 (2.30-2.26)
Sidechain outliers	177891	9342 (2.30-2.26)
RSRZ outliers	164620	8487 (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	302	<div> <div>87%</div> <div>12%</div> <div>.</div> </div>
1	B	302	<div> <div>3%</div> <div>88%</div> <div>11%</div> <div>.</div> </div>
1	C	302	<div> <div>8%</div> <div>91%</div> <div>8%</div> <div>.</div> </div>
1	D	302	<div> <div>56%</div> <div>85%</div> <div>8%</div> <div>6%</div> </div>

2 Entry composition [i](#)

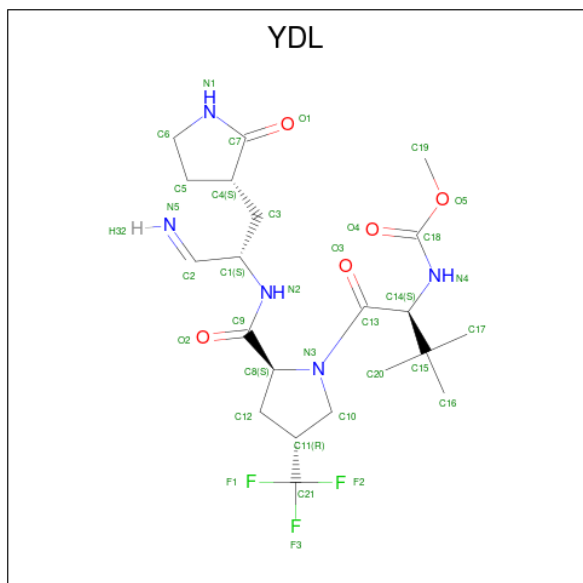
There are 3 unique types of molecules in this entry. The entry contains 18011 atoms, of which 8317 are hydrogens and 0 are deuteriums.

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 Peptidase C30.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	302	Total	C	H	N	O	S	0	6	0
			4628	1490	2270	405	445	18			
1	B	302	Total	C	H	N	O	S	0	3	0
			4549	1471	2228	393	439	18			
1	C	300	Total	C	H	N	O	S	0	3	0
			4492	1457	2198	382	438	17			
1	D	283	Total	C	H	N	O	S	0	1	0
			3375	1169	1497	329	368	12			

- Molecule 2 is N-(methoxycarbonyl)-3-methyl-L-valyl-(4R)-N-{(1Z,2S)-1-imino-3-[(3S)-2-oxopyrrolidin-3-yl]propan-2-yl}-4-(trifluoromethyl)-L-prolinamide (CCD ID: YDL) (formula: $C_{21}H_{32}F_3N_5O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	F	H	N	O	0	0
			65	21	3	31	5	5		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	B	1	Total	C	F	H	N	O	0	0
			65	21	3	31	5	5		
2	C	1	Total	C	F	H	N	O	0	0
			65	21	3	31	5	5		
2	D	1	Total	C	F	H	N	O	0	0
			65	21	3	31	5	5		

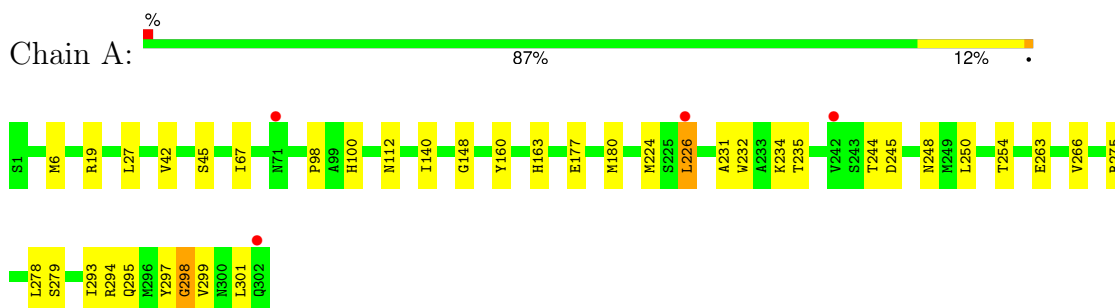
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	269	Total	O	0	0
			269	269		
3	B	216	Total	O	0	0
			216	216		
3	C	171	Total	O	0	0
			171	171		
3	D	51	Total	O	0	0
			51	51		

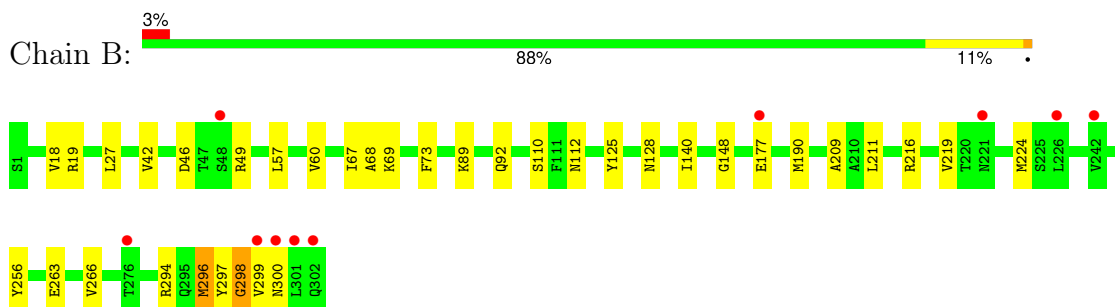
3 Residue-property plots [i](#)

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.

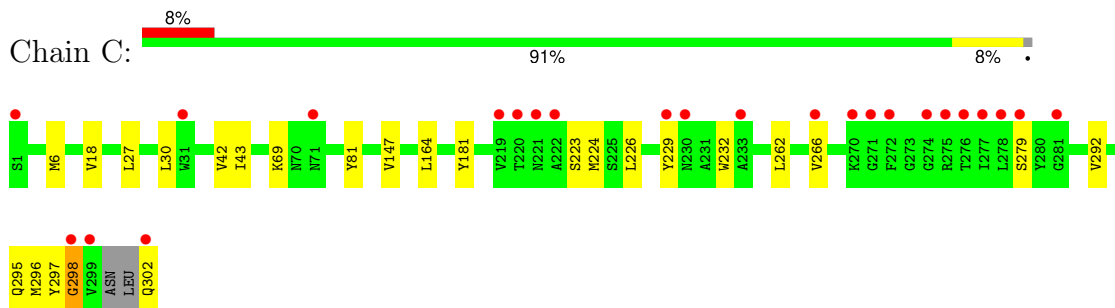
• Molecule 1: Peptidase C30



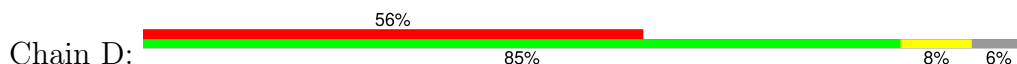
• Molecule 1: Peptidase C30

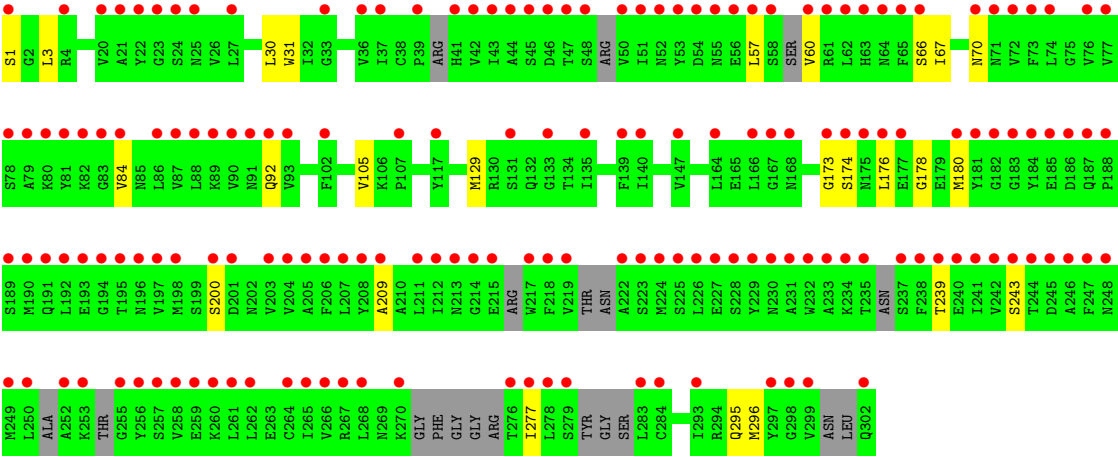


• Molecule 1: Peptidase C30



• Molecule 1: Peptidase C30





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	80.66Å 97.75Å 204.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.18 – 2.27 34.18 – 2.27	Depositor EDS
% Data completeness (in resolution range)	100.0 (34.18-2.27) 99.9 (34.18-2.27)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.76 (at 2.27Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.210 , 0.232 0.211 , 0.232	Depositor DCC
R_{free} test set	2000 reflections (2.14%)	wwPDB-VP
Wilson B-factor (Å ²)	28.9	Xtriage
Anisotropy	0.570	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 57.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	18011	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.20% 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: YDL

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	0.15	0/2405	0.35	0/3257
1	B	0.40	0/2368	0.65	1/3211 (0.0%)
1	C	0.17	0/2341	0.37	0/3176
1	D	0.32	0/1899	0.50	1/2583 (0.0%)
All	All	0.28	0/9013	0.48	2/12227 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	173	GLY	CA-C-O	-6.58	114.70	121.61
1	B	177	GLU	N-CA-C	-5.04	107.19	113.38

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	2358	2270	2316	26	0
1	B	2321	2228	2274	26	0
1	C	2294	2198	2226	16	0
1	D	1878	1497	1539	13	1
2	A	34	31	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	34	31	0	0	0
2	C	34	31	0	1	0
2	D	34	31	0	0	0
3	A	269	0	0	2	0
3	B	216	0	0	1	0
3	C	171	0	0	0	1
3	D	51	0	0	0	0
All	All	9694	8317	8355	76	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 4.

All (76) 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:D:57:LEU:O	1:D:60:VAL:N	2.16	0.79
1:B:297:TYR:O	1:B:299:VAL:HG23	1.83	0.76
1:B:27:LEU:HD21	1:B:42:VAL:HB	1.74	0.68
1:D:84:VAL:HG21	1:D:180:MET:CE	2.29	0.62
1:A:163:HIS:CG	1:A:180:MET:HE1	2.36	0.61
1:C:232:TRP:CD2	1:C:266:VAL:HG22	2.39	0.58
1:C:27:LEU:HD21	1:C:42:VAL:HB	1.86	0.58
1:B:224:MET:HE1	1:B:266:VAL:HG21	1.85	0.57
1:C:43:ILE:HD11	1:C:81:TYR:OH	2.06	0.56
1:C:30:LEU:HD13	1:C:147[B]:VAL:HG21	1.88	0.56
1:C:224:MET:HE1	1:C:266:VAL:CG2	2.36	0.55
1:A:27:LEU:HD21	1:A:42:VAL:HB	1.89	0.55
1:B:297:TYR:O	1:B:298:GLY:C	2.49	0.55
1:C:297:TYR:O	1:C:298:GLY:C	2.51	0.54
1:C:224:MET:HE1	1:C:266:VAL:HG21	1.90	0.54
1:A:297:TYR:O	1:A:299:VAL:HG22	2.08	0.54
1:A:250:LEU:O	1:A:254:THR:HG23	2.09	0.53
1:A:293:ILE:HG22	1:A:299:VAL:HG23	1.92	0.52
1:A:297:TYR:O	1:A:298:GLY:C	2.52	0.52
1:B:224:MET:HE3	1:B:263:GLU:HA	1.91	0.51
1:C:226:LEU:HD23	1:C:262:LEU:HD11	1.92	0.51
1:D:66:SER:C	1:D:67:ILE:HD13	2.36	0.50
1:D:84:VAL:HG21	1:D:180:MET:HE2	1.92	0.50
1:C:229:TYR:CG	1:C:262:LEU:HD22	2.46	0.50
1:B:112:ASN:O	1:B:148:GLY:HA2	2.13	0.49
1:B:224:MET:HE1	1:B:266:VAL:CG2	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:TRP:CD2	1:A:266:VAL:HG22	2.47	0.49
1:C:229:TYR:CD2	1:C:262:LEU:HD22	2.48	0.49
1:D:174:SER:HB3	1:D:180:MET:HE2	1.95	0.49
1:D:200:SER:H	1:D:239:THR:HG22	1.78	0.48
1:B:110:SER:OG	1:B:128:ASN:OD1	2.24	0.48
1:A:231:ALA:HA	1:A:234:LYS:HE2	1.96	0.48
1:A:294:ARG:HD3	1:A:301:LEU:HA	1.96	0.48
1:A:275[A]:ARG:NH2	3:A:507:HOH:O	2.46	0.48
1:B:57:LEU:O	1:B:60:VAL:HG12	2.14	0.47
1:B:294:ARG:O	1:B:298:GLY:HA2	2.13	0.47
1:B:68:ALA:HB2	1:B:73:PHE:CD2	2.49	0.47
1:B:209:ALA:HB1	1:B:296[B]:MET:HE3	1.95	0.47
1:C:30:LEU:HD13	1:C:147[A]:VAL:HG11	1.95	0.47
1:D:105:VAL:HG23	1:D:129:MET:HE3	1.96	0.47
1:A:112:ASN:O	1:A:148:GLY:HA2	2.15	0.46
1:B:68:ALA:HB2	1:B:73:PHE:CE2	2.51	0.46
1:B:190:MET:HE1	1:C:181:TYR:CD1	2.51	0.46
1:B:219:VAL:HG21	1:B:256:TYR:CE1	2.50	0.46
1:C:164:LEU:HD13	2:C:401:YDL:C19	2.46	0.46
1:A:245:ASP:HA	1:A:248:ASN:OD1	2.16	0.45
1:C:18:VAL:HG12	1:C:69:LYS:HB2	1.98	0.45
1:A:6:MET:HE1	1:A:295:GLN:HG2	1.98	0.44
1:D:84:VAL:HG22	1:D:178:GLY:O	2.16	0.44
1:B:209:ALA:HB1	1:B:296[A]:MET:HE2	1.98	0.44
1:D:209:ALA:HB1	1:D:296:MET:HE2	1.99	0.44
1:A:226:LEU:HD11	1:A:244:THR:CG2	2.48	0.44
1:B:46:ASP:OD2	1:B:49:ARG:HD2	2.17	0.44
1:A:298:GLY:H	1:B:140:ILE:CD1	2.31	0.43
1:A:224:MET:HE1	1:A:266:VAL:HG21	2.00	0.43
1:A:278:LEU:O	1:A:279:SER:HB2	2.17	0.43
1:B:299:VAL:O	1:B:300:ASN:C	2.60	0.43
1:C:6:MET:HE2	1:C:295:GLN:HG3	2.01	0.43
1:B:19:ARG:O	1:B:67:ILE:HA	2.19	0.43
1:A:19:ARG:O	1:A:67:ILE:HA	2.19	0.42
1:D:3:LEU:HA	1:D:295:GLN:OE1	2.19	0.42
1:A:293:ILE:CG2	1:A:299:VAL:HG23	2.50	0.42
1:D:30:LEU:HD23	1:D:176:LEU:HD11	2.00	0.42
1:A:148:GLY:HA3	1:A:160:TYR:HB3	2.02	0.42
1:D:31:TRP:CZ2	1:D:92:GLN:HG2	2.54	0.42
1:D:3:LEU:HD12	1:D:295:GLN:CD	2.44	0.42
1:C:292:VAL:O	1:C:296:MET:HG2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:PRO:O	1:A:100:HIS:HD2	2.02	0.41
1:B:18:VAL:HG12	1:B:69:LYS:HB2	2.02	0.41
1:A:140:ILE:CD1	1:B:298:GLY:H	2.31	0.41
1:A:177:GLU:OE1	3:A:501:HOH:O	2.22	0.41
1:A:6:MET:HG2	1:B:125:TYR:HB3	2.02	0.41
1:A:224:MET:HE3	1:A:263:GLU:HA	2.03	0.41
1:A:140:ILE:HD11	1:B:298:GLY:H	1.86	0.41
1:B:211:LEU:O	1:B:216:ARG:NH2	2.53	0.40
1:B:92:GLN:NE2	3:B:508:HOH:O	2.54	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:D:1:SER:OG	3:C:511:HOH:O[3_644]	2.17	0.03

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	306/302 (101%)	293 (96%)	12 (4%)	1 (0%)	37	45
1	B	303/302 (100%)	290 (96%)	12 (4%)	1 (0%)	37	45
1	C	300/302 (99%)	288 (96%)	11 (4%)	1 (0%)	37	45
1	D	261/302 (86%)	246 (94%)	13 (5%)	2 (1%)	16	19
All	All	1170/1208 (97%)	1117 (96%)	48 (4%)	5 (0%)	30	36

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	298	GLY

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Mol	Chain	Res	Type
1	B	298	GLY
1	C	298	GLY
1	D	70	ASN
1	D	277	ILE

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	258/254 (102%)	255 (99%)	3 (1%)	67	79
1	B	253/254 (100%)	250 (99%)	3 (1%)	67	79
1	C	248/254 (98%)	245 (99%)	3 (1%)	67	79
1	D	153/254 (60%)	152 (99%)	1 (1%)	81	89
All	All	912/1016 (90%)	902 (99%)	10 (1%)	73	81

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	SER
1	A	226	LEU
1	A	235	THR
1	B	89	LYS
1	B	296[A]	MET
1	B	296[B]	MET
1	C	223	SER
1	C	279	SER
1	C	302	GLN
1	D	243	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	100	HIS
1	B	100	HIS

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Mol	Chain	Res	Type
1	B	236	ASN
1	C	100	HIS
1	C	153	ASN
1	C	269	ASN
1	D	202	ASN
1	D	269	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 ⓘ

4 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	YDL	B	401	1	33,35,35	4.23	17 (51%)	41,52,52	2.53	17 (41%)
2	YDL	D	401	1	33,35,35	4.32	20 (60%)	41,52,52	2.74	16 (39%)
2	YDL	C	401	1	33,35,35	4.29	16 (48%)	41,52,52	2.42	15 (36%)
2	YDL	A	401	1	33,35,35	4.23	18 (54%)	41,52,52	2.35	14 (34%)

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	YDL	B	401	1	-	7/38/62/62	0/2/2/2
2	YDL	D	401	1	-	6/38/62/62	0/2/2/2
2	YDL	C	401	1	-	4/38/62/62	0/2/2/2
2	YDL	A	401	1	-	2/38/62/62	0/2/2/2

All (71) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	YDL	C10-N3	-13.19	1.27	1.47
2	D	401	YDL	C12-C8	-13.08	1.30	1.53
2	C	401	YDL	C12-C8	-13.02	1.30	1.53
2	B	401	YDL	C12-C8	-12.90	1.30	1.53
2	A	401	YDL	C12-C8	-12.86	1.31	1.53
2	B	401	YDL	C10-N3	-12.78	1.28	1.47
2	D	401	YDL	C10-N3	-12.65	1.28	1.47
2	A	401	YDL	C10-N3	-12.60	1.28	1.47
2	C	401	YDL	C8-N3	7.62	1.62	1.47
2	A	401	YDL	C8-N3	7.59	1.61	1.47
2	B	401	YDL	C8-N3	7.54	1.61	1.47
2	D	401	YDL	C8-N3	7.43	1.61	1.47
2	A	401	YDL	C5-C4	-7.29	1.33	1.54
2	B	401	YDL	C5-C4	-7.27	1.33	1.54
2	C	401	YDL	C5-C4	-7.24	1.33	1.54
2	D	401	YDL	C5-C4	-7.13	1.34	1.54
2	D	401	YDL	C5-C6	5.18	1.60	1.53
2	A	401	YDL	C5-C6	5.14	1.60	1.53
2	C	401	YDL	C5-C6	4.98	1.60	1.53
2	B	401	YDL	C5-C6	4.90	1.60	1.53
2	D	401	YDL	C4-C7	4.76	1.63	1.52
2	B	401	YDL	C4-C7	4.67	1.63	1.52
2	A	401	YDL	C4-C7	4.64	1.63	1.52
2	C	401	YDL	C4-C7	4.61	1.63	1.52
2	D	401	YDL	O5-C18	4.07	1.41	1.34
2	D	401	YDL	O3-C13	-3.70	1.15	1.22
2	C	401	YDL	O3-C13	-3.68	1.15	1.22
2	A	401	YDL	O3-C13	-3.53	1.16	1.22
2	B	401	YDL	O3-C13	-3.51	1.16	1.22
2	A	401	YDL	O5-C18	3.31	1.39	1.34
2	C	401	YDL	O5-C18	3.31	1.39	1.34
2	D	401	YDL	C7-N1	2.98	1.36	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	YDL	O5-C18	2.98	1.39	1.34
2	D	401	YDL	C8-C9	2.97	1.59	1.52
2	A	401	YDL	C20-C15	2.90	1.59	1.53
2	C	401	YDL	C20-C15	2.87	1.59	1.53
2	C	401	YDL	C7-N1	2.87	1.36	1.33
2	D	401	YDL	C20-C15	2.85	1.59	1.53
2	C	401	YDL	C8-C9	2.83	1.59	1.52
2	B	401	YDL	C8-C9	2.75	1.59	1.52
2	B	401	YDL	C20-C15	2.73	1.59	1.53
2	A	401	YDL	C8-C9	2.70	1.59	1.52
2	D	401	YDL	C13-N3	2.70	1.40	1.34
2	A	401	YDL	C7-N1	2.66	1.36	1.33
2	A	401	YDL	C6-N1	2.65	1.51	1.46
2	B	401	YDL	C6-N1	2.63	1.51	1.46
2	D	401	YDL	C6-N1	2.62	1.51	1.46
2	B	401	YDL	C21-C11	-2.61	1.47	1.50
2	C	401	YDL	C6-N1	2.60	1.51	1.46
2	B	401	YDL	C7-N1	2.58	1.36	1.33
2	A	401	YDL	C13-N3	2.55	1.40	1.34
2	C	401	YDL	O4-C18	-2.55	1.17	1.21
2	D	401	YDL	O4-C18	-2.55	1.17	1.21
2	D	401	YDL	C15-C14	2.51	1.59	1.55
2	C	401	YDL	O2-C9	-2.50	1.18	1.23
2	A	401	YDL	O2-C9	-2.50	1.18	1.23
2	B	401	YDL	O2-C9	-2.48	1.18	1.23
2	D	401	YDL	C14-N4	2.46	1.49	1.45
2	A	401	YDL	O4-C18	-2.45	1.17	1.21
2	A	401	YDL	C21-C11	-2.43	1.47	1.50
2	B	401	YDL	O4-C18	-2.42	1.17	1.21
2	C	401	YDL	C21-C11	-2.36	1.47	1.50
2	D	401	YDL	C3-C4	2.32	1.58	1.53
2	B	401	YDL	C13-N3	2.28	1.39	1.34
2	D	401	YDL	C21-C11	-2.25	1.47	1.50
2	D	401	YDL	O2-C9	-2.23	1.19	1.23
2	C	401	YDL	C3-C4	2.20	1.58	1.53
2	B	401	YDL	C3-C4	2.14	1.58	1.53
2	D	401	YDL	F1-C21	2.13	1.38	1.33
2	A	401	YDL	C3-C4	2.12	1.58	1.53
2	A	401	YDL	F2-C21	2.01	1.38	1.33

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	401	YDL	C15-C14-N4	-7.44	100.33	111.94
2	C	401	YDL	O5-C18-N4	6.70	122.05	110.77
2	B	401	YDL	O5-C18-N4	6.55	121.80	110.77
2	D	401	YDL	C13-C14-N4	6.35	115.10	107.40
2	D	401	YDL	C12-C8-N3	5.87	110.16	103.17
2	A	401	YDL	O5-C18-N4	5.85	120.61	110.77
2	A	401	YDL	C12-C8-N3	5.57	109.80	103.17
2	B	401	YDL	C12-C8-N3	5.39	109.59	103.17
2	C	401	YDL	C14-C13-N3	5.05	124.50	118.46
2	B	401	YDL	C19-O5-C18	-4.95	109.90	115.63
2	C	401	YDL	C12-C8-N3	4.87	108.96	103.17
2	D	401	YDL	C9-C8-N3	-4.83	99.31	112.50
2	A	401	YDL	C20-C15-C14	4.57	119.07	109.71
2	D	401	YDL	C20-C15-C14	4.38	118.68	109.71
2	D	401	YDL	O5-C18-N4	4.21	117.86	110.77
2	B	401	YDL	C14-C13-N3	4.11	123.37	118.46
2	A	401	YDL	C14-C13-N3	4.01	123.26	118.46
2	C	401	YDL	O4-C18-N4	-3.97	118.36	124.86
2	D	401	YDL	F2-C21-C11	-3.95	107.70	112.60
2	B	401	YDL	O5-C18-O4	-3.93	118.89	124.62
2	A	401	YDL	F3-C21-C11	-3.89	107.79	112.60
2	B	401	YDL	F1-C21-C11	-3.88	107.79	112.60
2	C	401	YDL	F3-C21-C11	-3.83	107.86	112.60
2	C	401	YDL	O5-C18-O4	-3.67	119.28	124.62
2	D	401	YDL	C10-N3-C8	-3.54	107.14	111.83
2	B	401	YDL	O4-C18-N4	-3.49	119.15	124.86
2	A	401	YDL	C16-C15-C14	-3.41	102.74	109.71
2	A	401	YDL	O5-C18-O4	-3.36	119.72	124.62
2	C	401	YDL	C13-C14-N4	-3.33	103.36	107.40
2	A	401	YDL	O4-C18-N4	-3.26	119.53	124.86
2	B	401	YDL	F2-C21-C11	-3.04	108.84	112.60
2	C	401	YDL	O3-C13-N3	-3.00	116.00	121.38
2	A	401	YDL	F1-C21-C11	-2.99	108.90	112.60
2	D	401	YDL	O5-C18-O4	-2.97	120.30	124.62
2	B	401	YDL	C20-C15-C16	2.91	114.49	108.80
2	C	401	YDL	C20-C15-C17	2.89	114.44	108.80
2	A	401	YDL	C10-N3-C8	-2.83	108.09	111.83
2	D	401	YDL	C14-C13-N3	2.81	121.82	118.46
2	C	401	YDL	C19-O5-C18	-2.76	112.44	115.63
2	B	401	YDL	F3-C21-C11	-2.76	109.19	112.60
2	D	401	YDL	F3-C21-C11	-2.71	109.24	112.60
2	C	401	YDL	F1-C21-C11	-2.65	109.31	112.60
2	D	401	YDL	F1-C21-C11	-2.63	109.35	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	YDL	C6-N1-C7	-2.58	108.32	113.79
2	A	401	YDL	F2-C21-C11	-2.58	109.41	112.60
2	D	401	YDL	C17-C15-C16	-2.58	103.78	108.80
2	B	401	YDL	C10-N3-C8	-2.56	108.44	111.83
2	C	401	YDL	C6-N1-C7	-2.55	108.39	113.79
2	B	401	YDL	C16-C15-C14	-2.55	104.50	109.71
2	B	401	YDL	C17-C15-C14	2.51	114.84	109.71
2	B	401	YDL	C6-N1-C7	-2.51	108.48	113.79
2	D	401	YDL	C6-N1-C7	-2.47	108.55	113.79
2	C	401	YDL	F2-C21-C11	-2.47	109.55	112.60
2	A	401	YDL	C2-C1-N2	-2.43	105.91	110.37
2	B	401	YDL	C9-C8-N3	-2.41	105.91	112.50
2	B	401	YDL	C2-C1-N2	-2.37	106.01	110.37
2	C	401	YDL	C17-C15-C16	-2.27	104.37	108.80
2	C	401	YDL	C9-C8-N3	-2.23	106.40	112.50
2	D	401	YDL	C8-C9-N2	2.21	121.37	116.52
2	A	401	YDL	C9-C8-N3	-2.20	106.49	112.50
2	B	401	YDL	C15-C14-C13	-2.09	110.45	113.23
2	D	401	YDL	F3-C21-F2	2.05	111.32	106.87

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	YDL	N4-C18-O5-C19
2	A	401	YDL	O4-C18-O5-C19
2	B	401	YDL	C13-C14-C15-C17
2	B	401	YDL	C13-C14-C15-C20
2	B	401	YDL	N4-C14-C15-C17
2	B	401	YDL	N4-C14-C15-C20
2	C	401	YDL	N4-C18-O5-C19
2	C	401	YDL	O4-C18-O5-C19
2	B	401	YDL	N4-C14-C15-C16
2	B	401	YDL	C13-C14-C15-C16
2	D	401	YDL	O4-C18-O5-C19
2	D	401	YDL	O5-C18-N4-C14
2	B	401	YDL	O3-C13-C14-C15
2	C	401	YDL	O3-C13-C14-C15
2	D	401	YDL	O3-C13-C14-C15
2	D	401	YDL	N3-C13-C14-C15
2	D	401	YDL	N4-C18-O5-C19
2	C	401	YDL	N3-C13-C14-C15

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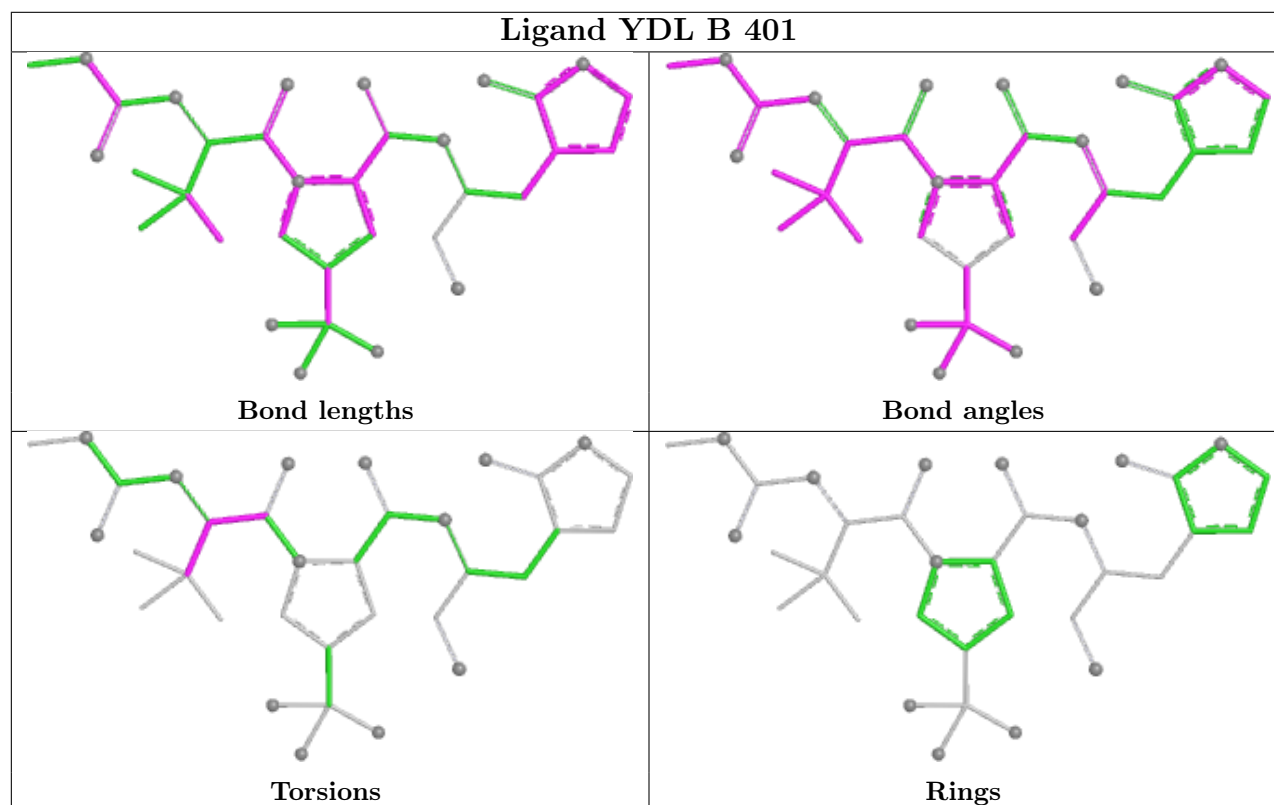
Mol	Chain	Res	Type	Atoms
2	D	401	YDL	O4-C18-N4-C14

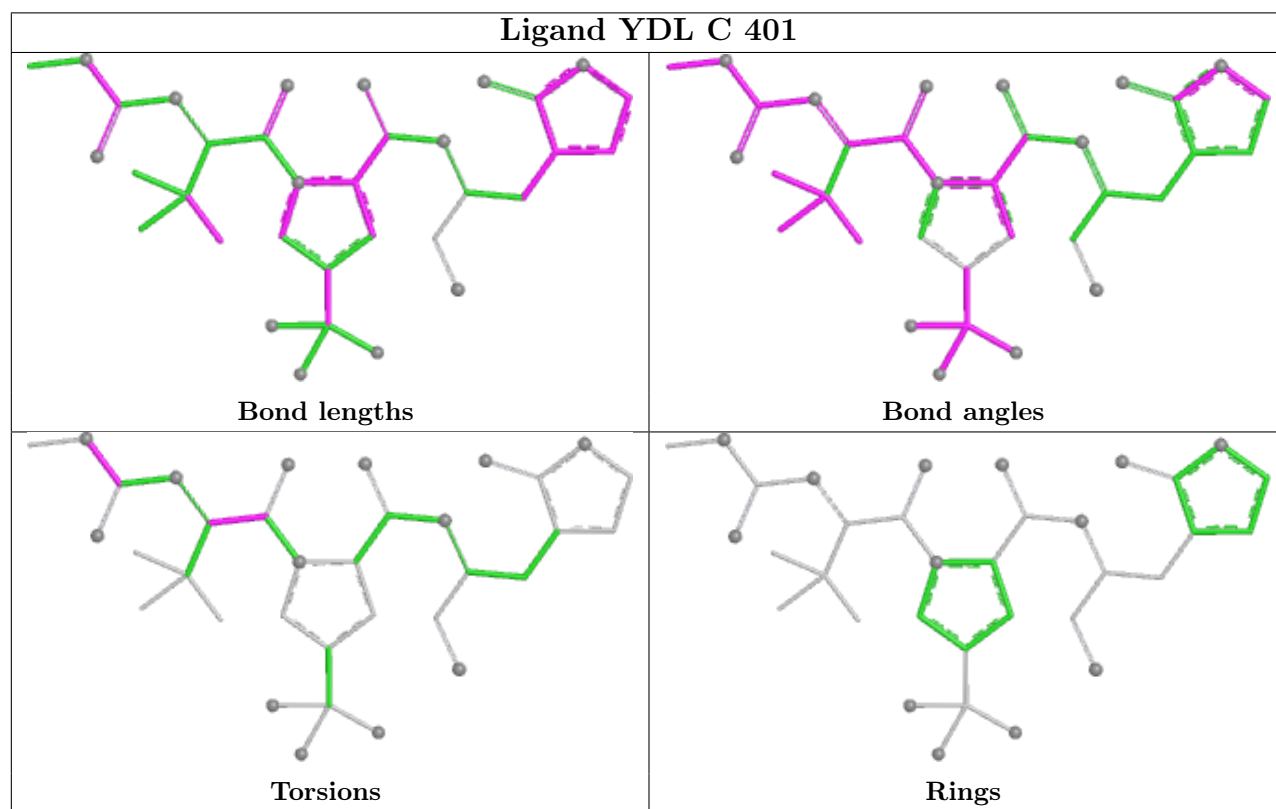
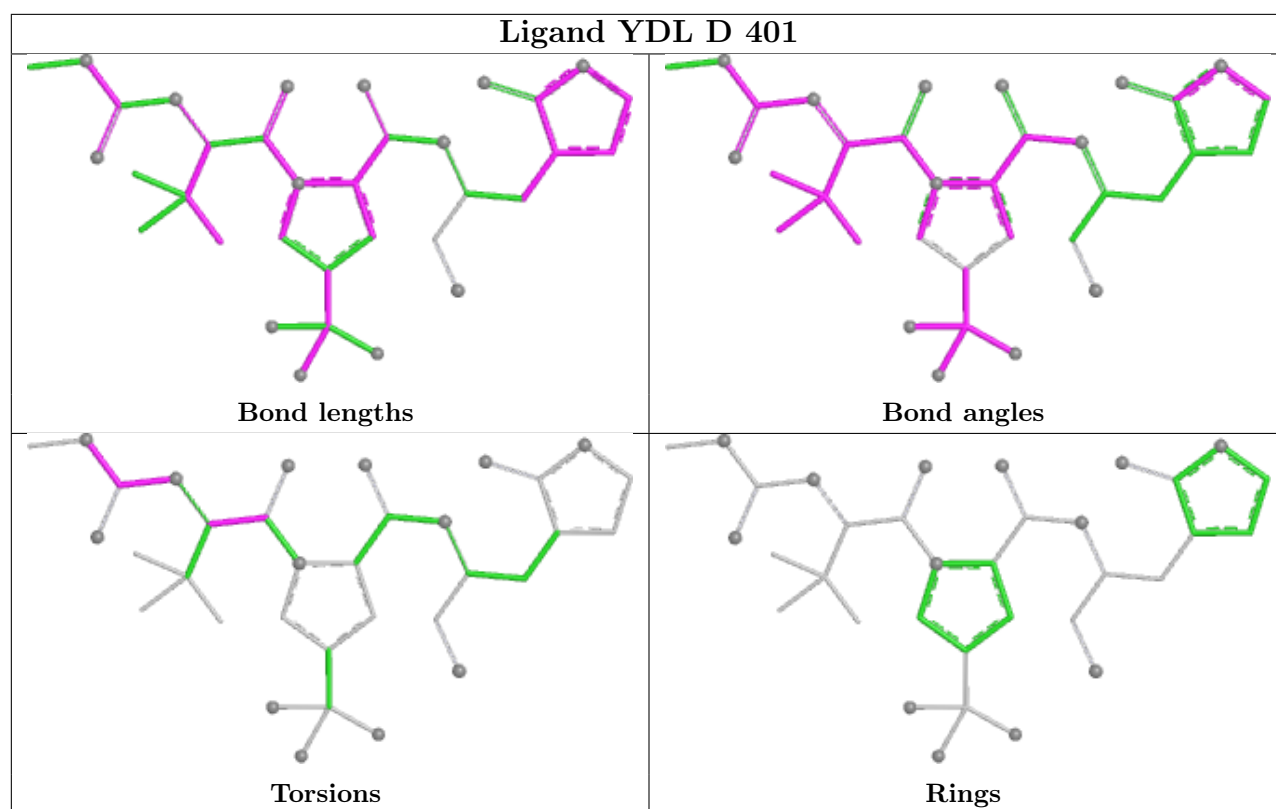
There are no ring outliers.

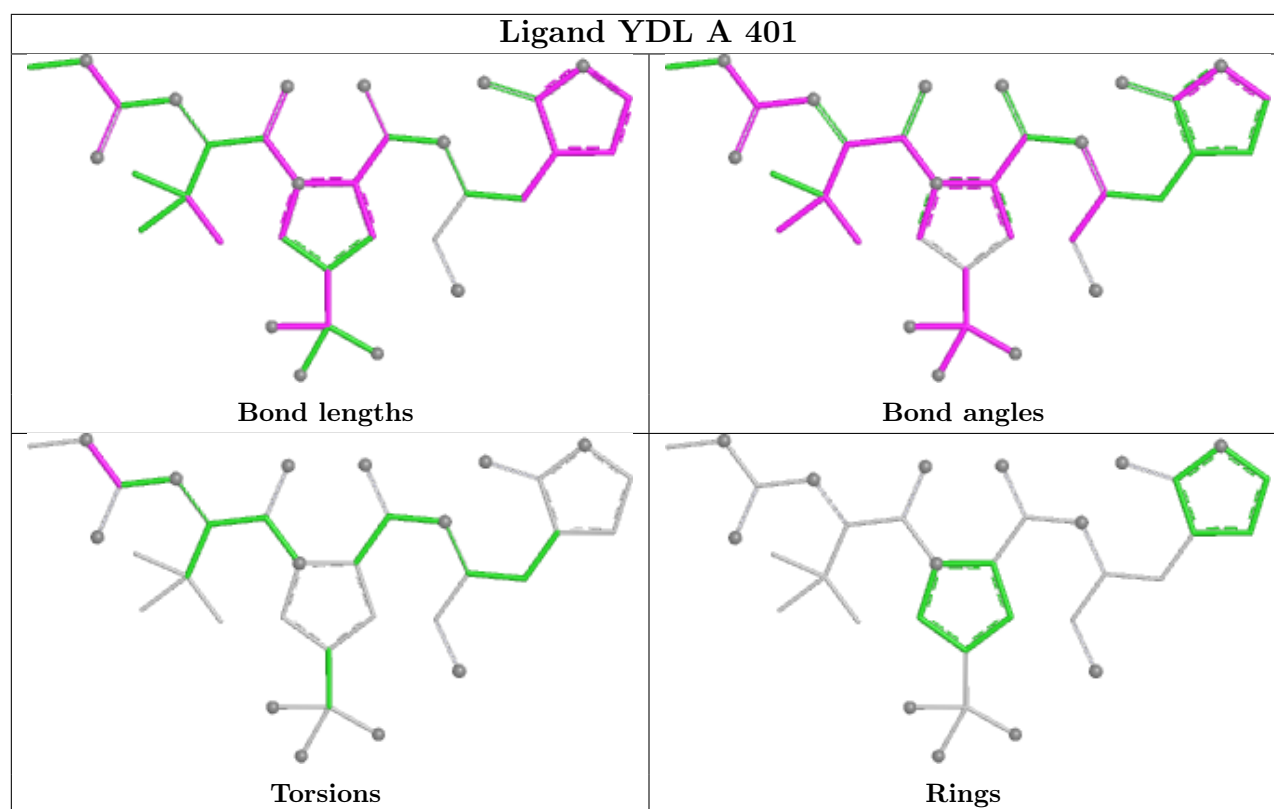
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	401	YDL	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	302/302 (100%)	-0.29	4 (1%) 74 75	14, 30, 52, 100	6 (1%)
1	B	302/302 (100%)	0.02	10 (3%) 49 51	11, 35, 64, 83	3 (0%)
1	C	300/302 (99%)	0.16	24 (8%) 20 21	11, 36, 71, 93	3 (1%)
1	D	283/302 (93%)	2.53	168 (59%) 0 0	30, 77, 117, 141	1 (0%)
All	All	1187/1208 (98%)	0.57	206 (17%) 5 5	11, 38, 99, 141	13 (1%)

All (206) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	212	ILE	7.4
1	D	230	ASN	6.7
1	D	258	VAL	6.7
1	D	256	TYR	6.6
1	D	209	ALA	6.6
1	D	219	VAL	6.5
1	D	56[A]	GLU	6.5
1	D	81	TYR	6.4
1	D	299	VAL	6.2
1	D	197	VAL	6.1
1	D	217	TRP	6.0
1	D	298	GLY	5.5
1	D	238	PHE	5.5
1	D	297	TYR	5.5
1	D	283	LEU	5.4
1	D	48	SER	5.4
1	D	237	SER	5.3
1	D	268	LEU	5.3
1	D	50	VAL	5.3
1	D	62	LEU	5.3
1	D	264	CYS	5.1

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Mol	Chain	Res	Type	RSRZ
1	D	265	ILE	5.1
1	D	279	SER	5.0
1	D	226	LEU	5.0
1	D	195	THR	4.9
1	D	244	THR	4.9
1	D	192	LEU	4.9
1	D	196	ASN	4.9
1	D	228	SER	4.9
1	D	21	ALA	4.8
1	A	71	ASN	4.7
1	D	53	TYR	4.7
1	D	54	ASP	4.7
1	D	250	LEU	4.6
1	D	190	MET	4.6
1	D	64	ASN	4.6
1	D	277	ILE	4.6
1	D	255	GLY	4.6
1	D	206	PHE	4.5
1	C	221	ASN	4.5
1	D	261	LEU	4.5
1	D	215	GLU	4.4
1	D	235	THR	4.4
1	D	45	SER	4.4
1	D	58	SER	4.4
1	D	71	ASN	4.3
1	D	42	VAL	4.3
1	D	225	SER	4.3
1	D	245	ASP	4.2
1	D	200	SER	4.2
1	D	229	TYR	4.2
1	C	31[A]	TRP	4.2
1	D	65	PHE	4.2
1	A	226	LEU	4.1
1	D	302	GLN	4.1
1	D	284	CYS	4.1
1	D	223	SER	4.1
1	D	233	ALA	4.1
1	C	299	VAL	4.1
1	D	41	HIS	4.0
1	A	302	GLN	4.0
1	D	167	GLY	4.0
1	D	270	LYS	4.0

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Mol	Chain	Res	Type	RSRZ
1	D	185	GLU	4.0
1	D	22	TYR	3.9
1	D	51	ILE	3.9
1	D	242	VAL	3.8
1	D	257	SER	3.8
1	D	79	ALA	3.8
1	D	70	ASN	3.8
1	D	57	LEU	3.8
1	D	224	MET	3.8
1	D	262	LEU	3.8
1	D	241	ILE	3.8
1	D	52	ASN	3.7
1	D	55	ASN	3.7
1	D	222	ALA	3.7
1	D	247	PHE	3.7
1	D	207	LEU	3.7
1	D	183	GLY	3.7
1	D	60	VAL	3.6
1	D	227	GLU	3.6
1	D	252	ALA	3.6
1	D	36	VAL	3.5
1	D	44	ALA	3.5
1	D	218	PHE	3.5
1	D	173	GLY	3.4
1	D	205	ALA	3.4
1	D	72	VAL	3.4
1	D	239	THR	3.4
1	D	117	TYR	3.3
1	D	63	HIS	3.3
1	D	248	ASN	3.3
1	D	231	ALA	3.3
1	D	232	TRP	3.3
1	D	249	MET	3.3
1	D	83	GLY	3.3
1	D	164	LEU	3.2
1	D	234	LYS	3.2
1	D	82	LYS	3.2
1	D	278	LEU	3.2
1	D	203	VAL	3.1
1	D	201	ASP	3.1
1	D	191	GLN	3.1
1	D	253	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	266	VAL	3.1
1	B	177	GLU	3.1
1	D	24	SER	3.1
1	D	213	ASN	3.1
1	D	208	TYR	3.1
1	C	277	ILE	3.0
1	D	133	GLY	3.0
1	D	214	GLY	3.0
1	D	23	GLY	3.0
1	D	166	LEU	3.0
1	D	267	ARG	3.0
1	D	27	LEU	3.0
1	D	102	PHE	3.0
1	D	246	ALA	3.0
1	C	71	ASN	2.9
1	D	76	VAL	2.9
1	C	302	GLN	2.9
1	D	184	TYR	2.9
1	C	279	SER	2.9
1	D	33	GLY	2.9
1	D	86	LEU	2.9
1	D	131	SER	2.9
1	B	302	GLN	2.9
1	D	90	VAL	2.9
1	D	204	VAL	2.9
1	D	43	ILE	2.9
1	D	25	ASN	2.9
1	D	189	SER	2.9
1	D	243	SER	2.9
1	D	187	GLN	2.9
1	D	177	GLU	2.8
1	C	281	GLY	2.8
1	D	47	THR	2.8
1	B	301	LEU	2.8
1	D	259	GLU	2.7
1	B	242	VAL	2.7
1	D	87	VAL	2.7
1	D	92	GLN	2.7
1	C	275	ARG	2.7
1	D	276	THR	2.7
1	A	242	VAL	2.7
1	D	194	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	48	SER	2.7
1	D	66	SER	2.7
1	B	300	ASN	2.6
1	D	188	PRO	2.6
1	D	46	ASP	2.6
1	D	193	GLU	2.6
1	D	107	PRO	2.6
1	C	270	LYS	2.6
1	C	298	GLY	2.6
1	D	182	GLY	2.6
1	D	293	ILE	2.6
1	C	274	GLY	2.5
1	D	73	PHE	2.5
1	D	88	LEU	2.5
1	D	61	ARG	2.5
1	B	299	VAL	2.5
1	D	168	ASN	2.5
1	D	175	ASN	2.5
1	C	278	LEU	2.4
1	D	139	PHE	2.4
1	D	198	MET	2.4
1	D	20	VAL	2.4
1	C	222	ALA	2.4
1	D	89	LYS	2.4
1	B	221	ASN	2.4
1	D	147	VAL	2.3
1	C	1	SER	2.3
1	D	181	TYR	2.3
1	B	226	LEU	2.3
1	D	135	ILE	2.3
1	C	229	TYR	2.3
1	C	233	ALA	2.3
1	B	276	THR	2.3
1	D	37	ILE	2.3
1	D	78	SER	2.3
1	D	174	SER	2.3
1	D	176	LEU	2.3
1	D	240	GLU	2.3
1	D	74	LEU	2.2
1	C	272	PHE	2.2
1	D	77	VAL	2.2
1	D	39	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	276	THR	2.2
1	D	80	LYS	2.2
1	C	271	GLY	2.2
1	D	180	MET	2.2
1	D	211	LEU	2.2
1	D	1	SER	2.1
1	D	140	ILE	2.1
1	C	219	VAL	2.1
1	C	230	ASN	2.1
1	D	260	LYS	2.1
1	C	266	VAL	2.1
1	D	91	ASN	2.1
1	D	84	VAL	2.0
1	D	93	VAL	2.0
1	C	220	THR	2.0
1	D	4	ARG	2.0
1	D	186	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.

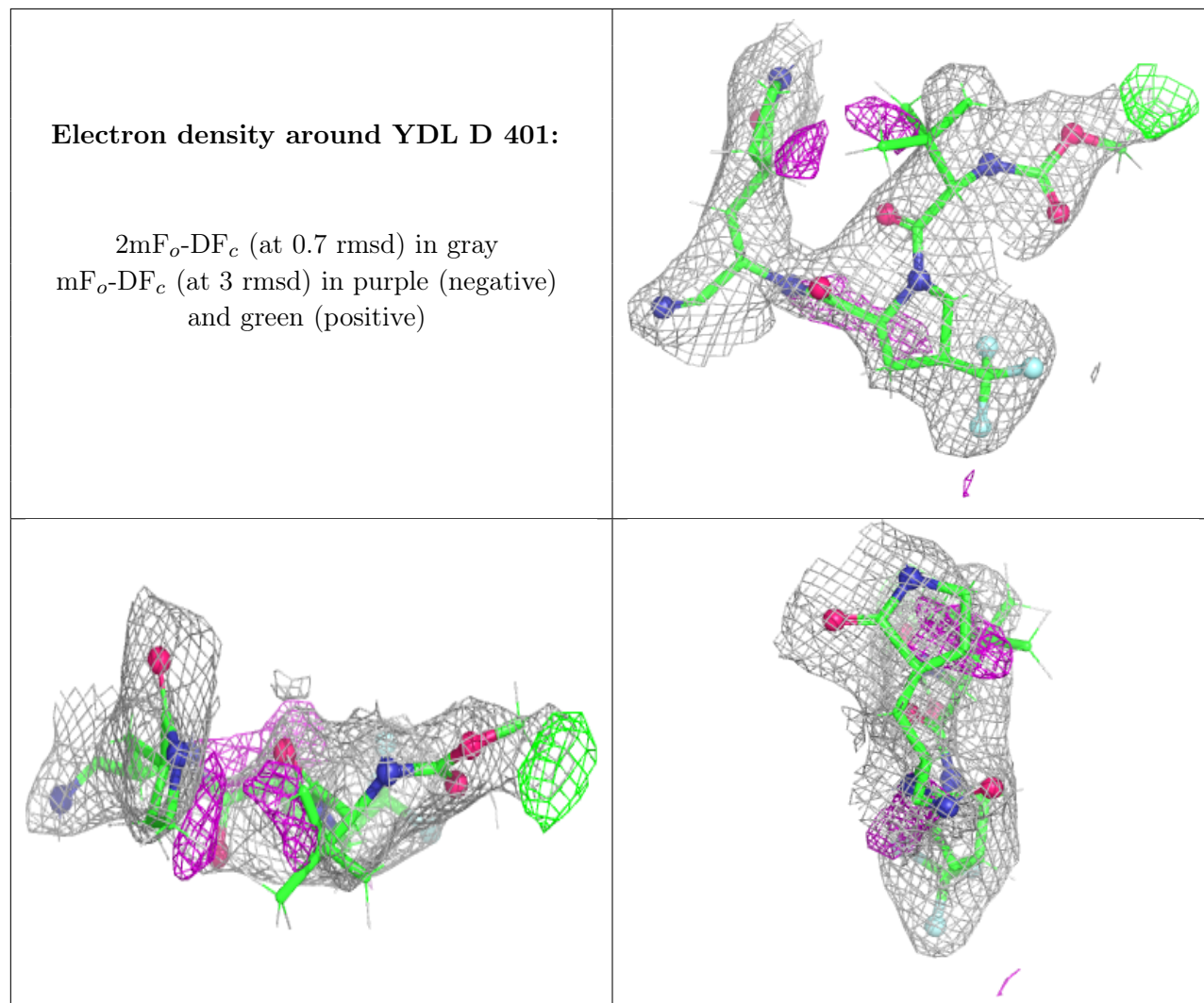
6.4 Ligands [i](#)

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	YDL	D	401	34/34	0.72	0.20	52,74,95,95	0
2	YDL	B	401	34/34	0.91	0.10	18,26,39,40	0
2	YDL	A	401	34/34	0.91	0.09	20,25,35,37	0
2	YDL	C	401	34/34	0.93	0.08	20,27,33,35	0

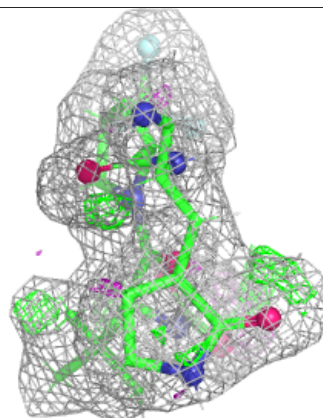
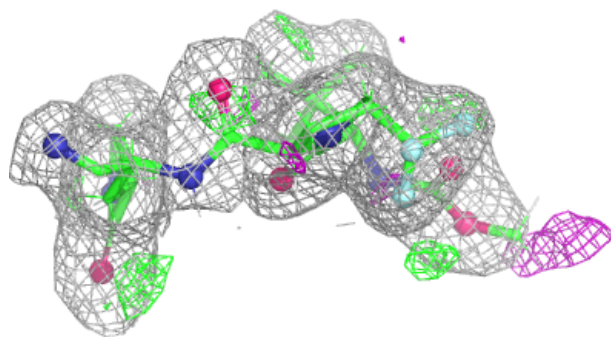
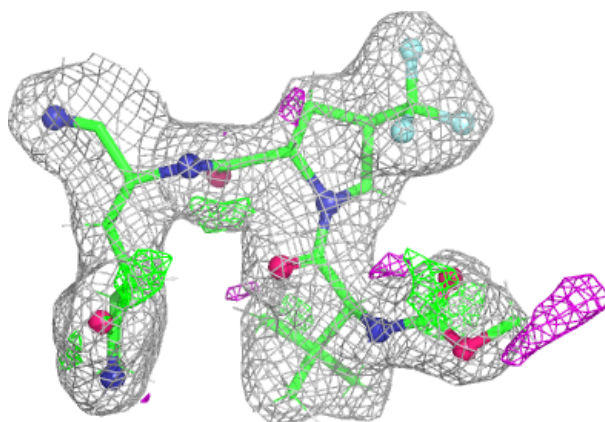
The following is a graphical depiction of the model fit to experimental electron density of all

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.



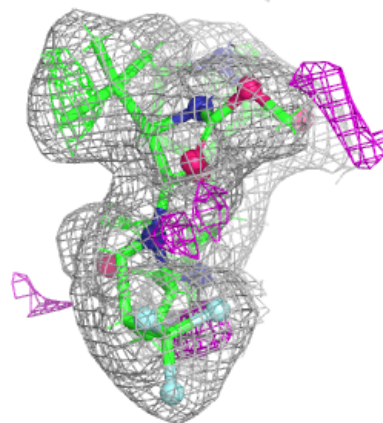
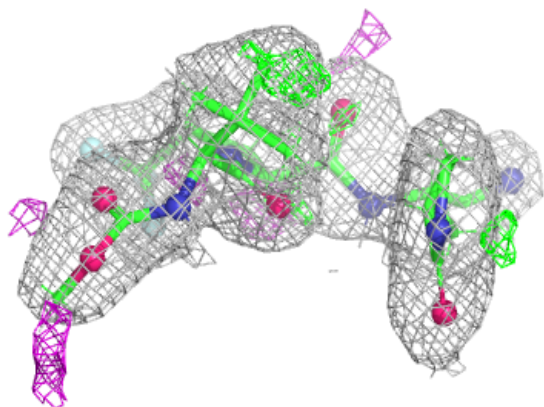
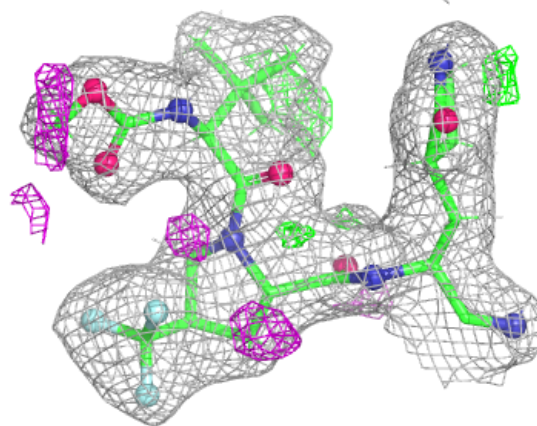
Electron density around YDL B 401:

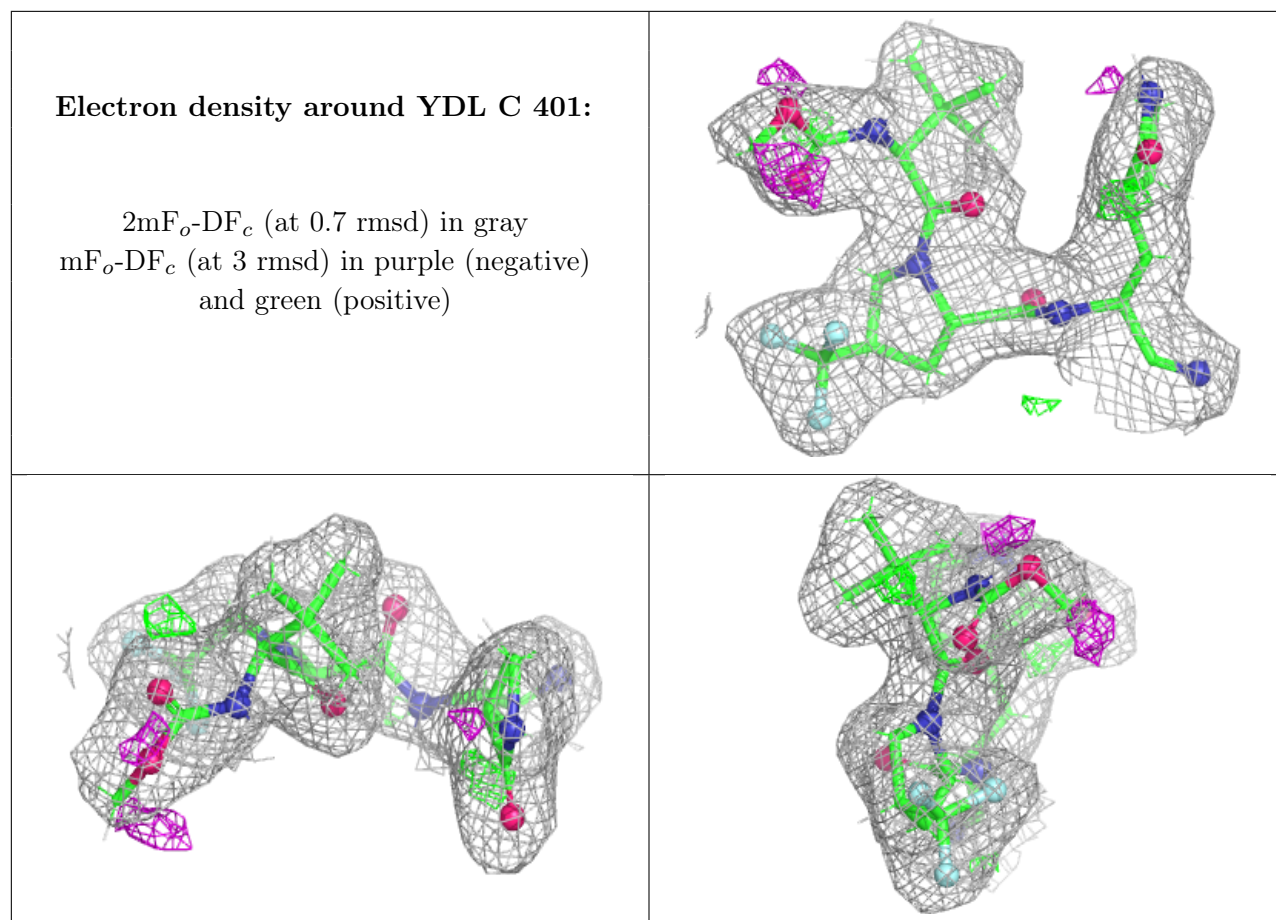
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around YDL 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 ⓘ

There are no such residues in this entry.