



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:20 PM UTC

PDB ID : 5LLY / pdb_00005lly
Title : Photosensory Module of Bacteriophytochrome linked Diguanylyl Cyclase from
Idiomarina species A28L
Authors : Gourinchas, G.; Winkler, A.
Deposited on : 2016-07-28
Resolution : 2.40 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

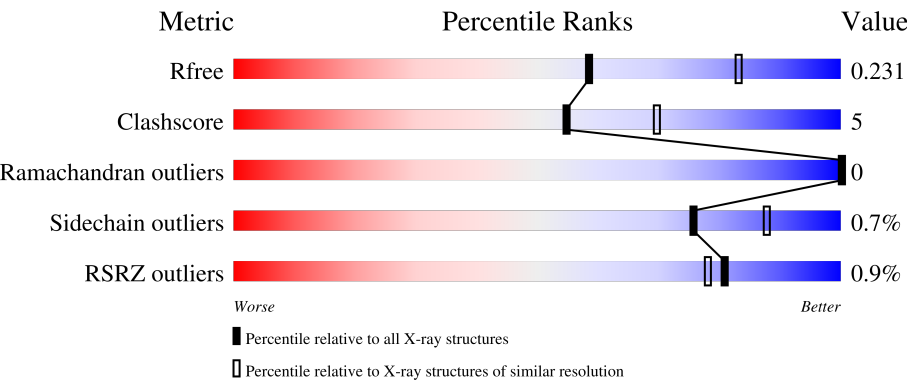
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

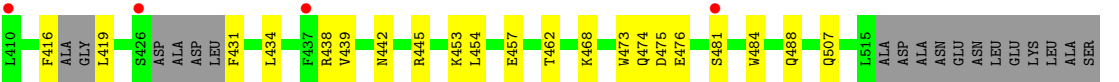
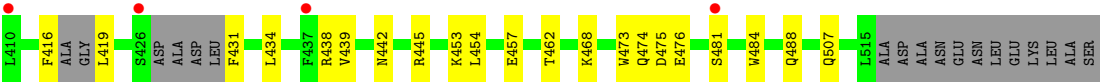
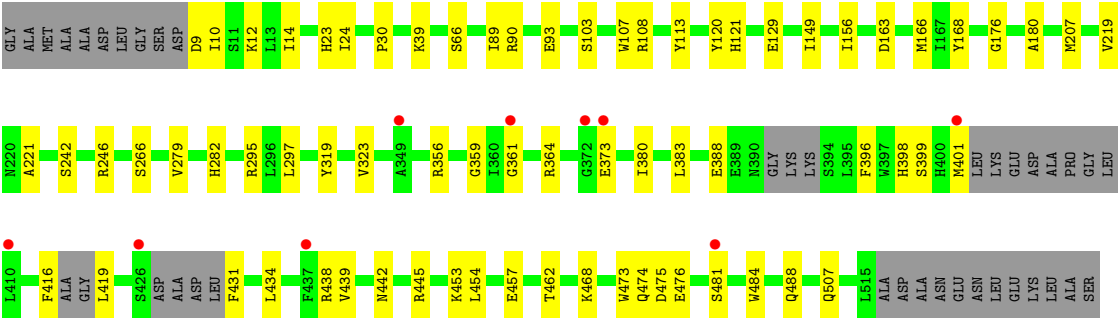
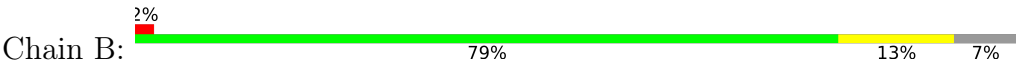
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	529	% 84%12%.
1	B	529	2% 79%13%7%
1	C	529	% 84%12%.
1	D	529	% 81%14%5%

ENTRY-COMPOSITION INFOmissingINFO



● Molecule 1: Diguanylate cyclase (GGDEF) domain-containing protein



3 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	83.50Å 129.00Å 122.01Å 90.00° 96.34° 90.00°	Depositor
Resolution (Å)	48.13 – 2.40 48.13 – 2.40	Depositor EDS
% Data completeness (in resolution range)	93.0 (48.13-2.40) 93.0 (48.13-2.40)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.56 (at 2.39Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.177 , 0.230 (Not available) , 0.231	Depositor DCC
R_{free} test set	4668 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	48.8	Xtriage
Anisotropy	0.395	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 49.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	16833	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.24% 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.

4 Model quality [i](#)

4.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, CL, LBV

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	0.34	1/4227 (0.0%)	0.53	0/5741
1	B	0.34	0/4083	0.52	0/5543
1	C	0.32	0/4229	0.52	0/5742
1	D	0.34	0/4150	0.56	0/5639
All	All	0.33	1/16689 (0.0%)	0.53	0/22665

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	20	GLU	C-N	5.77	1.47	1.33

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

4.2 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	4129	0	4063	35	0
1	B	3983	0	3913	42	0
1	C	4124	0	4075	36	0
1	D	4051	0	3978	43	0
2	A	43	0	34	0	0
2	B	43	0	33	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	43	0	34	0	0
2	D	43	0	35	3	0
3	A	2	0	0	0	0
3	B	2	0	0	1	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
4	A	6	0	8	1	0
4	C	6	0	8	1	0
5	A	79	0	0	1	0
5	B	92	0	0	1	0
5	C	84	0	0	2	0
5	D	99	0	0	0	0
All	All	16833	0	16181	155	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 5.

All (155) 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:17:CYS:SG	2:D:601:LBV:HBA3	1.24	1.71
1:D:17:CYS:HG	2:D:601:LBV:HBA3	1.23	0.94
1:B:399:SER:OG	1:B:401:MET:SD	2.44	0.75
1:B:380:ILE:HA	1:B:383:LEU:HD12	1.71	0.73
1:D:17:CYS:SG	2:D:601:LBV:HBA1	2.30	0.69
1:D:424:LEU:HB2	1:D:432:SER:HB3	1.75	0.68
1:C:10:ILE:HD12	1:C:453:LYS:HE3	1.77	0.67
1:C:504:ASP:OD2	5:C:701:HOH:O	2.15	0.65
1:B:398:HIS:HA	1:B:419:LEU:O	1.97	0.64
1:D:473:TRP:CZ3	1:D:475:ASP:HB3	2.34	0.62
1:C:454:LEU:HD21	1:C:468:LYS:HE3	1.84	0.60
1:C:381:ASN:OD1	1:B:89:ILE:HG21	2.02	0.59
1:D:374:THR:HG22	1:D:375:PRO:O	2.01	0.59
1:B:163:ASP:OD2	5:B:701:HOH:O	2.17	0.58
1:B:89:ILE:O	1:B:108:ARG:NH2	2.37	0.58
1:A:103:SER:HB2	1:A:120:TYR:HB2	1.86	0.58
1:A:251:LEU:HD22	1:A:466:PRO:HD3	1.85	0.58
1:B:207:MET:HG2	1:B:246:ARG:NH2	2.19	0.57
1:D:26:ASN:HA	1:D:226:LEU:HD12	1.87	0.57
1:C:107:TRP:CE2	1:C:242:SER:HB2	2.40	0.57
1:A:65:LEU:HD12	1:A:68:ILE:HD12	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:166:MET:HE1	1:B:282:HIS:CE1	2.41	0.55
1:A:14:ILE:HG12	1:A:464:LEU:HD22	1.89	0.54
1:B:107:TRP:CE2	1:B:242:SER:HB2	2.42	0.54
1:B:168:TYR:CZ	1:B:176:GLY:HA3	2.42	0.53
1:B:356:ARG:HD2	1:B:488:GLN:HE22	1.73	0.53
1:A:216:ILE:HG12	1:A:248:VAL:HG21	1.91	0.52
1:D:341:HIS:HD2	1:D:369:THR:OG1	1.93	0.51
1:D:406:ALA:HB1	1:D:409:LEU:HD12	1.92	0.51
1:D:32:GLY:HA2	1:D:54:TYR:CZ	2.46	0.51
1:A:168:TYR:CZ	1:A:176:GLY:HA3	2.45	0.51
1:B:454:LEU:HD11	1:B:468:LYS:HE3	1.93	0.51
1:A:248:VAL:HB	1:A:253:MET:HE2	1.94	0.50
1:C:207:MET:HE2	1:C:246:ARG:NH2	2.26	0.50
1:D:383:LEU:HD23	1:D:409:LEU:HD13	1.93	0.50
1:D:382:LYS:HG2	1:D:409:LEU:HD22	1.94	0.50
1:B:356:ARG:HB2	1:B:438:ARG:HH21	1.77	0.50
1:D:16:ALA:HB3	1:D:464:LEU:HD11	1.93	0.49
1:D:266:SER:HA	1:D:279:VAL:O	2.13	0.49
1:C:291:ARG:O	1:C:295:ARG:HG2	2.12	0.49
1:D:295:ARG:HH11	1:D:295:ARG:HG3	1.78	0.48
1:C:171:ASP:OD2	1:C:175:ASN:HB2	2.12	0.48
1:B:39:LYS:HG3	1:B:113:TYR:CZ	2.48	0.48
1:D:90:ARG:HB2	1:D:93:GLU:OE1	2.13	0.48
1:D:164:ARG:HD3	1:D:166:MET:SD	2.53	0.48
1:A:441:GLN:OE1	1:A:482:GLN:NE2	2.46	0.48
1:D:320:MET:O	1:D:324:GLN:HG2	2.13	0.48
1:D:156:ILE:HB	1:D:165:VAL:HG11	1.96	0.48
1:C:59:ASP:HB3	1:C:62:ILE:HG12	1.96	0.48
1:D:374:THR:CG2	1:D:380:ILE:HD11	2.44	0.48
1:D:177:ARG:HD3	1:D:194:HIS:NE2	2.29	0.47
1:A:87:SER:O	1:A:89:ILE:HG13	2.14	0.47
1:D:49:ALA:HB2	1:D:227:HIS:CD2	2.49	0.47
1:B:416:PHE:HA	1:B:439:VAL:HA	1.95	0.47
1:A:394:SER:HB2	1:A:396:PHE:O	2.14	0.47
1:C:341[A]:HIS:ND1	1:C:369:THR:OG1	2.37	0.47
1:B:156:ILE:HG23	1:B:297:LEU:HD22	1.97	0.47
1:A:454:LEU:HD11	1:A:468:LYS:HE3	1.96	0.47
1:C:65:LEU:HD21	1:C:227:HIS:CG	2.49	0.47
1:C:207:MET:HE2	1:C:246:ARG:HH21	1.79	0.47
1:D:152:LEU:O	1:D:156:ILE:HG12	2.15	0.46
1:A:153:THR:HG22	1:A:167:ILE:HG13	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:398:HIS:HB2	1:B:484:TRP:CD1	2.50	0.46
1:D:363:LEU:HD13	1:D:384:VAL:HG21	1.98	0.46
1:A:383:LEU:HD23	1:A:409:LEU:HG	1.97	0.46
1:C:133:GLN:O	1:C:137:GLN:HG3	2.15	0.46
1:A:78:PRO:O	1:A:82:ILE:HG13	2.16	0.46
1:B:361:GLY:O	1:B:434:LEU:HD12	2.15	0.46
1:A:393:LYS:HE3	1:A:393:LYS:HB2	1.82	0.45
1:B:359:GLY:HA3	1:B:373:GLU:O	2.17	0.45
1:B:10:ILE:HG12	1:B:453:LYS:HE2	1.98	0.45
1:D:90:ARG:HE	1:D:93:GLU:CD	2.23	0.45
1:C:168:TYR:CZ	1:C:176:GLY:HA3	2.52	0.45
1:B:129:GLU:OE1	1:B:129:GLU:N	2.44	0.45
1:C:323:VAL:O	1:C:327:ARG:HG3	2.17	0.45
1:D:50:ASN:O	1:D:53:GLU:HG2	2.16	0.45
1:D:425:LYS:HG3	1:D:430:LEU:HD12	1.99	0.44
1:A:402:LEU:HD11	1:A:419:LEU:HB2	1.99	0.44
1:A:132:PHE:CD2	4:A:604:GOL:H32	2.52	0.44
1:C:50:ASN:O	1:C:53:GLU:HG2	2.17	0.44
1:B:442:ASN:ND2	1:B:476:GLU:OE2	2.38	0.44
1:B:445:ARG:O	1:B:474:GLN:HA	2.18	0.44
1:B:473:TRP:CZ3	1:B:475:ASP:HB3	2.53	0.44
1:C:402:LEU:HD13	1:C:410:LEU:HD11	2.00	0.44
1:B:10:ILE:O	1:B:14:ILE:HG13	2.18	0.44
1:D:207:MET:HE2	1:D:246:ARG:NH2	2.33	0.43
1:D:469:SER:OG	1:D:471:GLU:HG3	2.18	0.43
1:A:28:ILE:HG13	1:A:224:GLN:HB2	2.00	0.43
1:A:55:PHE:CZ	1:A:117:VAL:HG21	2.53	0.43
1:B:9:ASP:HB3	1:B:12:LYS:HD2	2.00	0.43
1:A:166:MET:HG2	1:A:181:GLU:HG3	2.00	0.43
1:C:132:PHE:CZ	1:C:296:LEU:HA	2.53	0.43
1:B:23:HIS:CD2	1:B:24:ILE:HG23	2.53	0.43
1:B:90:ARG:NE	1:B:93:GLU:OE1	2.35	0.43
1:C:291:ARG:HA	1:C:294:ARG:HD2	2.00	0.43
1:A:107:TRP:CE2	1:A:242:SER:HB2	2.53	0.43
1:B:388:GLU:HG3	1:B:431:PHE:CZ	2.54	0.43
1:A:398:HIS:HA	1:A:419:LEU:O	2.19	0.43
1:D:89:ILE:O	1:D:108:ARG:NH2	2.52	0.43
1:C:454:LEU:O	1:C:464:LEU:HD12	2.19	0.43
1:B:149:ILE:HD12	1:B:180:ALA:HB2	2.01	0.43
1:B:319:TYR:O	1:B:323:VAL:HG23	2.18	0.43
1:A:445:ARG:NH2	1:A:475:ASP:OD2	2.42	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:166:MET:HE3	1:C:166:MET:HB2	1.89	0.43
1:C:401:MET:SD	1:C:480:LYS:HE2	2.59	0.42
1:B:457:GLU:OE1	1:B:462:THR:HG22	2.18	0.42
1:A:340:SER:O	1:A:344:VAL:HG23	2.20	0.42
1:A:510:LEU:HG	1:A:514:GLN:HE21	1.83	0.42
1:B:266:SER:HA	1:B:279:VAL:O	2.19	0.42
1:D:202:ALA:HA	1:D:205:ARG:NH1	2.35	0.42
1:A:218:ASP:HB3	1:A:221:ALA:HB2	2.00	0.42
1:A:434:LEU:HD12	1:A:434:LEU:HA	1.89	0.42
1:C:38:GLU:HG3	1:C:45:VAL:HG11	2.01	0.42
1:D:290:GLY:O	1:D:294:ARG:HG3	2.20	0.42
1:A:335:ASP:C	1:A:337:LYS:H	2.27	0.42
1:C:398:HIS:HA	1:C:419:LEU:O	2.20	0.42
1:D:401:MET:HG2	1:D:480:LYS:HG2	2.02	0.42
1:C:24:ILE:HG22	1:C:238:VAL:O	2.19	0.42
1:C:368:LEU:HD21	1:C:380:ILE:HD12	2.00	0.42
1:D:31:PHE:CD1	1:D:217:PRO:HG2	2.54	0.42
1:D:231:LYS:HE2	1:D:231:LYS:HB3	1.73	0.42
1:A:47:ALA:HB3	1:A:229:ILE:HD11	2.01	0.42
1:A:90:ARG:HD2	1:A:93:GLU:OE2	2.20	0.41
1:D:168:TYR:CZ	1:D:176:GLY:HA3	2.55	0.41
1:B:438:ARG:HB3	1:B:481:SER:HB2	2.02	0.41
1:C:266:SER:HA	1:C:279:VAL:O	2.20	0.41
1:C:387:LEU:O	1:C:391:GLY:N	2.37	0.41
1:D:77:LEU:HD11	1:D:115:ILE:HD13	2.02	0.41
1:A:9:ASP:OD1	1:A:10:ILE:N	2.53	0.41
1:A:95:ILE:O	1:A:105:LEU:HA	2.20	0.41
1:C:253:MET:O	1:C:257:ARG:HG3	2.19	0.41
1:C:441:GLN:OE1	1:C:482:GLN:NE2	2.51	0.41
1:D:132:PHE:CD2	4:C:604:GOL:H12	2.55	0.41
1:A:295:ARG:NH2	5:A:706:HOH:O	2.48	0.41
1:A:363:LEU:O	1:A:432:SER:HA	2.21	0.41
1:B:103:SER:HB2	1:B:120:TYR:HB2	2.03	0.41
1:D:185:GLN:C	1:D:187:PHE:H	2.28	0.41
1:D:323:VAL:HG22	1:D:354:LEU:HD11	2.01	0.41
1:D:177:ARG:HD3	1:D:194:HIS:CE1	2.56	0.41
1:C:30:PRO:CG	1:C:221:ALA:HB1	2.51	0.41
1:B:166:MET:HE3	1:B:166:MET:HB2	1.86	0.41
1:C:493:ARG:HD3	5:C:776:HOH:O	2.22	0.40
1:B:120:TYR:CG	1:B:121:HIS:N	2.88	0.40
1:B:438:ARG:HD2	1:B:484:TRP:CZ2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:345:ILE:HD13	1:C:345:ILE:HA	1.89	0.40
1:C:511:LEU:HA	1:C:511:LEU:HD23	1.89	0.40
1:B:364:ARG:NH2	1:B:507:GLN:OE1	2.51	0.40
1:A:409:LEU:HD12	1:A:409:LEU:HA	1.91	0.40
1:C:422:ILE:HG21	1:C:493:ARG:HA	2.03	0.40
1:D:18:ASP:HA	1:D:203:GLN:OE1	2.22	0.40
1:B:30:PRO:HG3	1:B:221:ALA:HB1	2.03	0.40
1:B:295:ARG:NH1	3:B:602:CL:CL	2.88	0.40
1:D:340:SER:HB2	1:D:499:LEU:HD22	2.03	0.40
1:C:399:SER:O	1:C:418:GLY:HA2	2.22	0.40
1:B:295:ARG:HH11	1:B:295:ARG:HG3	1.86	0.40

There are no symmetry-related clashes.

4.3 Torsion angles [i](#)

4.3.1 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	B	340/529 (64%)	333 (98%)	7 (2%)	0	100	100
1	D	86/529 (16%)	83 (96%)	3 (4%)	0	100	100
All	All	426/1058 (40%)	416 (98%)	10 (2%)	0	100	100

There are no Ramachandran outliers to report.

4.3.2 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	448/457 (98%)	446 (100%)	2 (0%)	84	92
1	B	435/457 (95%)	432 (99%)	3 (1%)	76	88
1	C	447/457 (98%)	445 (100%)	2 (0%)	84	92
1	D	439/457 (96%)	433 (99%)	6 (1%)	59	79
All	All	1769/1828 (97%)	1756 (99%)	13 (1%)	76	88

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	24	ILE
1	D	186	LEU
1	D	200	ILE
1	D	249	SER
1	D	396	PHE
1	D	456	VAL
1	A	278	ILE
1	A	474	GLN
1	C	439	VAL
1	C	469	SER
1	B	66	SER
1	B	219	VAL
1	B	396	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	63	HIS
1	D	92	ASN
1	D	121	HIS
1	D	131	GLN
1	D	341	HIS
1	D	441	GLN
1	D	474	GLN
1	D	482	GLN
1	A	137	GLN
1	A	169	GLN
1	A	441	GLN
1	A	474	GLN
1	A	482	GLN
1	A	507	GLN

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Mol	Chain	Res	Type
1	C	230	HIS
1	C	338	HIS
1	C	381	ASN
1	C	442	ASN
1	C	514	GLN
1	B	43	GLN
1	B	121	HIS
1	B	157	GLN
1	B	224	GLN
1	B	488	GLN

4.3.3 RNA ⓘ

There are no RNA molecules in this entry.

4.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

4.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

4.6 Ligand geometry ⓘ

Of 14 ligands modelled in this entry, 8 are monoatomic - leaving 6 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	$\# Z > 2$
4	GOL	A	604	-	5,5,5	0.40	0	5,5,5	0.51	0
2	LBV	B	601	1	46,46,46	2.30	16 (34%)	58,67,67	1.40	7 (12%)
2	LBV	C	601	1	46,46,46	2.34	12 (26%)	58,67,67	1.36	10 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	LBV	A	601	1	46,46,46	2.31	11 (23%)	58,67,67	1.35	10 (17%)
2	LBV	D	601	1	46,46,46	2.31	15 (32%)	58,67,67	1.28	6 (10%)
4	GOL	C	604	-	5,5,5	0.36	0	5,5,5	0.28	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
4	GOL	A	604	-	-	3/4/4/4	-
2	LBV	B	601	1	-	8/26/74/74	0/4/4/4
2	LBV	C	601	1	-	8/26/74/74	0/4/4/4
2	LBV	A	601	1	-	8/26/74/74	0/4/4/4
2	LBV	D	601	1	-	8/26/74/74	0/4/4/4
4	GOL	C	604	-	-	1/4/4/4	-

All (54) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	601	LBV	C2A-C1A	-8.00	1.43	1.52
2	B	601	LBV	C2A-C1A	-7.57	1.43	1.52
2	D	601	LBV	C2A-C1A	-7.52	1.43	1.52
2	A	601	LBV	C2A-C1A	-7.44	1.43	1.52
2	B	601	LBV	C2A-C3A	-6.80	1.42	1.51
2	D	601	LBV	C2A-C3A	-6.29	1.43	1.51
2	A	601	LBV	C2A-C3A	-5.41	1.44	1.51
2	C	601	LBV	CMD-C2D	-5.01	1.40	1.50
2	C	601	LBV	C2A-C3A	-5.00	1.45	1.51
2	A	601	LBV	CMB-C2B	-4.68	1.41	1.50
2	A	601	LBV	CMC-C3C	-4.56	1.41	1.50
2	C	601	LBV	CMB-C2B	-4.44	1.41	1.50
2	C	601	LBV	CMC-C3C	-4.38	1.41	1.50
2	D	601	LBV	CMC-C3C	-4.29	1.42	1.50
2	A	601	LBV	CMD-C2D	-4.06	1.42	1.50
2	B	601	LBV	CMC-C3C	-3.94	1.42	1.50
2	D	601	LBV	CMB-C2B	-3.90	1.42	1.50
2	A	601	LBV	CMA-C2A	-3.80	1.42	1.53
2	D	601	LBV	CMD-C2D	-3.72	1.43	1.50
2	D	601	LBV	CMA-C2A	-3.72	1.42	1.53
2	B	601	LBV	CMD-C2D	-3.65	1.43	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	601	LBV	CAA-C3A	3.58	1.42	1.33
2	C	601	LBV	CMA-C2A	-3.58	1.42	1.53
2	B	601	LBV	CMA-C2A	-3.58	1.42	1.53
2	A	601	LBV	CAB-C3B	-3.42	1.42	1.51
2	A	601	LBV	CAA-C3A	3.41	1.42	1.33
2	B	601	LBV	CMB-C2B	-3.31	1.44	1.50
2	C	601	LBV	CAC-C2C	-3.09	1.43	1.51
2	D	601	LBV	CBB-CGB	-3.06	1.43	1.50
2	C	601	LBV	CBB-CGB	-3.04	1.43	1.50
2	D	601	LBV	CAA-C3A	2.90	1.40	1.33
2	D	601	LBV	CAB-C3B	-2.82	1.44	1.51
2	C	601	LBV	C1D-C2D	-2.78	1.40	1.45
2	B	601	LBV	CAB-C3B	-2.72	1.44	1.51
2	B	601	LBV	C4A-C3A	-2.70	1.40	1.45
2	B	601	LBV	CAA-C3A	2.67	1.40	1.33
2	B	601	LBV	CAC-C2C	-2.67	1.44	1.51
2	B	601	LBV	C4A-N_A	-2.62	1.33	1.37
2	A	601	LBV	CBB-CAB	-2.61	1.42	1.51
2	A	601	LBV	CBB-CGB	-2.60	1.44	1.50
2	D	601	LBV	C1B-C2B	-2.57	1.35	1.41
2	D	601	LBV	C4B-C3B	-2.51	1.37	1.42
2	B	601	LBV	CBB-CGB	-2.44	1.44	1.50
2	D	601	LBV	CAC-C2C	-2.38	1.45	1.51
2	B	601	LBV	C1C-C2C	-2.37	1.42	1.45
2	D	601	LBV	O2B-CGB	-2.37	1.23	1.30
2	D	601	LBV	CAD-C3D	-2.25	1.41	1.47
2	A	601	LBV	O2B-CGB	-2.24	1.23	1.30
2	D	601	LBV	CBB-CAB	-2.15	1.44	1.51
2	B	601	LBV	CBA-CAA	-2.12	1.41	1.49
2	C	601	LBV	CAB-C3B	-2.12	1.45	1.51
2	B	601	LBV	CBB-CAB	-2.09	1.44	1.51
2	B	601	LBV	O1C-CGC	-2.04	1.24	1.30
2	C	601	LBV	CBC-CGC	-2.04	1.45	1.50

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	LBV	O_A-C1A-N_A	-4.54	119.58	124.93
2	A	601	LBV	C4B-CHC-C1C	4.28	137.57	128.22
2	C	601	LBV	C4B-CHC-C1C	3.73	136.36	128.22
2	B	601	LBV	C4B-CHC-C1C	3.45	135.77	128.22
2	C	601	LBV	O_A-C1A-N_A	-3.29	121.05	124.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	601	LBV	C4B-CHC-C1C	3.18	135.16	128.22
2	A	601	LBV	O_A-C1A-C2A	2.80	129.71	126.74
2	B	601	LBV	O_A-C1A-C2A	2.48	129.38	126.74
2	A	601	LBV	O_A-C1A-N_A	-2.48	122.01	124.93
2	A	601	LBV	C2C-C1C-N_C	-2.47	106.55	110.04
2	D	601	LBV	O_D-C4D-N_D	-2.41	119.43	125.08
2	B	601	LBV	O_D-C4D-N_D	-2.41	119.44	125.08
2	C	601	LBV	O1B-CGB-CBB	-2.40	115.50	123.09
2	B	601	LBV	O_D-C4D-C3D	2.39	135.48	129.71
2	C	601	LBV	CMD-C2D-C1D	-2.36	121.28	124.16
2	A	601	LBV	CAA-C3A-C4A	-2.36	123.51	126.36
2	A	601	LBV	CHC-C4B-N_B	2.20	130.27	125.29
2	C	601	LBV	C2C-C1C-N_C	-2.17	106.97	110.04
2	B	601	LBV	O1B-CGB-CBB	-2.16	116.23	123.09
2	A	601	LBV	O_D-C4D-N_D	-2.15	120.03	125.08
2	C	601	LBV	O_A-C1A-C2A	2.13	129.00	126.74
2	D	601	LBV	O_A-C1A-N_A	-2.11	122.44	124.93
2	D	601	LBV	C2C-C1C-N_C	-2.08	107.10	110.04
2	A	601	LBV	CHD-C4C-C3C	2.07	130.19	124.87
2	C	601	LBV	CAA-C3A-C4A	-2.06	123.87	126.36
2	D	601	LBV	O_D-C4D-C3D	2.06	134.67	129.71
2	C	601	LBV	C1C-C2C-C3C	2.05	108.95	106.73
2	C	601	LBV	O2C-CGC-CBC	-2.05	116.59	123.09
2	D	601	LBV	CHD-C4C-C3C	2.04	130.10	124.87
2	A	601	LBV	CAB-CBB-CGB	-2.02	108.32	113.67
2	C	601	LBV	O_D-C4D-N_D	-2.00	120.38	125.08
2	A	601	LBV	C1C-N_C-C4C	2.00	110.19	106.52
2	B	601	LBV	C2C-C1C-N_C	-2.00	107.21	110.04

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	604	GOL	O1-C1-C2-C3
2	C	601	LBV	C2D-C1D-CHD-C4C
2	D	601	LBV	C2D-C1D-CHD-C4C
2	B	601	LBV	C2D-C1D-CHD-C4C
2	D	601	LBV	N_D-C1D-CHD-C4C
2	C	601	LBV	N_D-C1D-CHD-C4C
2	B	601	LBV	N_D-C1D-CHD-C4C
2	D	601	LBV	N_C-C4C-CHD-C1D
2	A	601	LBV	N_C-C4C-CHD-C1D

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Mol	Chain	Res	Type	Atoms
2	C	601	LBV	N_C-C4C-CHD-C1D
2	B	601	LBV	N_C-C4C-CHD-C1D
2	D	601	LBV	C3C-C4C-CHD-C1D
2	A	601	LBV	C3C-C4C-CHD-C1D
2	C	601	LBV	C3C-C4C-CHD-C1D
2	B	601	LBV	C3C-C4C-CHD-C1D
4	A	604	GOL	O1-C1-C2-O2
2	A	601	LBV	N_D-C1D-CHD-C4C
2	A	601	LBV	C2D-C1D-CHD-C4C
4	A	604	GOL	O2-C2-C3-O3
4	C	604	GOL	O1-C1-C2-C3
2	C	601	LBV	CAB-CBB-CGB-O2B
2	D	601	LBV	CAB-CBB-CGB-O2B
2	D	601	LBV	CAC-CBC-CGC-O2C
2	D	601	LBV	CAC-CBC-CGC-O1C
2	B	601	LBV	CAC-CBC-CGC-O2C
2	A	601	LBV	CAB-CBB-CGB-O2B
2	D	601	LBV	CAB-CBB-CGB-O1B
2	C	601	LBV	CAB-CBB-CGB-O1B
2	A	601	LBV	CAC-CBC-CGC-O1C
2	A	601	LBV	CAB-CBB-CGB-O1B
2	C	601	LBV	CAC-CBC-CGC-O1C
2	B	601	LBV	CAC-CBC-CGC-O1C
2	B	601	LBV	CAB-CBB-CGB-O2B
2	A	601	LBV	CAC-CBC-CGC-O2C
2	C	601	LBV	CAC-CBC-CGC-O2C
2	B	601	LBV	CAB-CBB-CGB-O1B

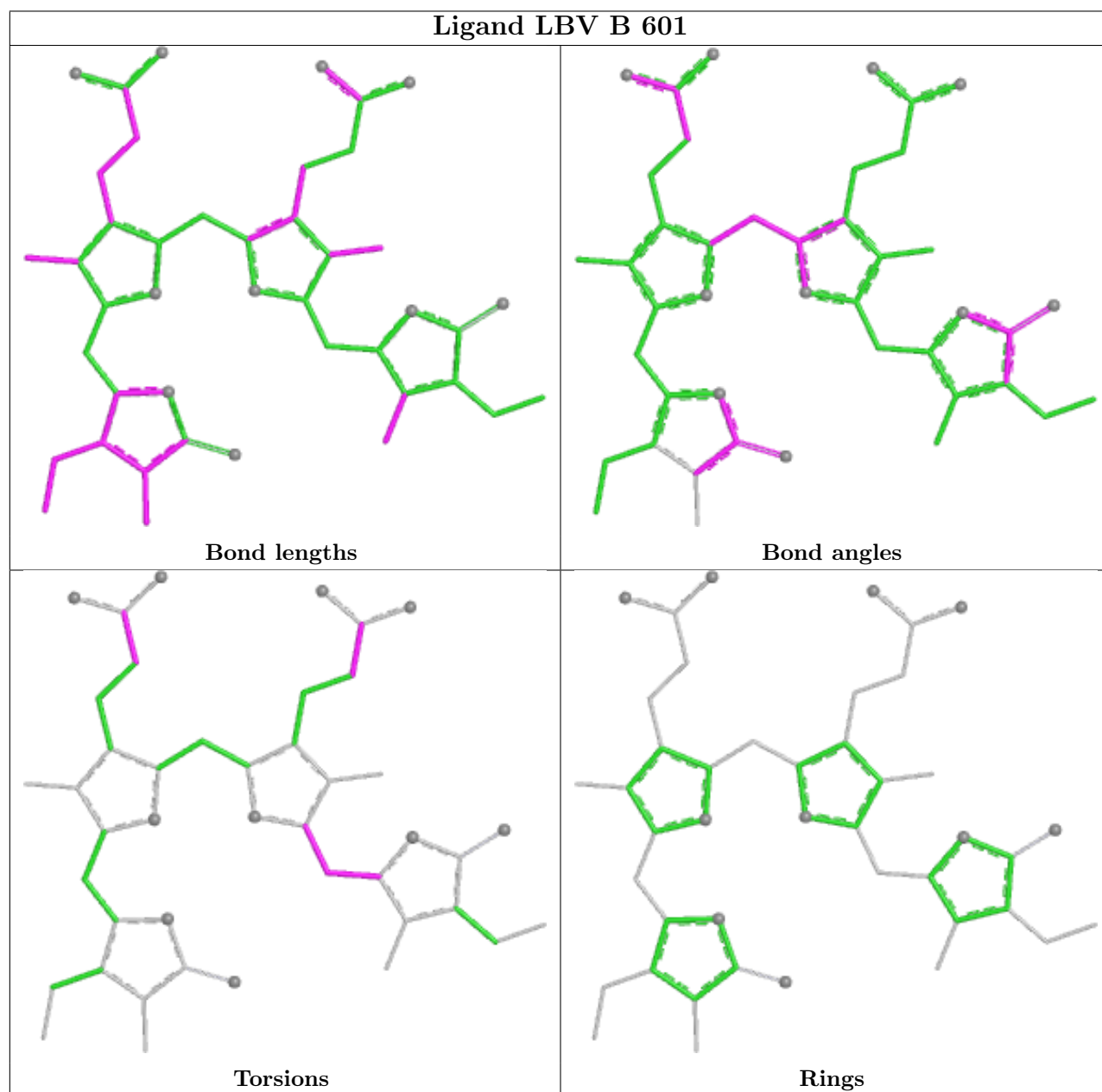
There are no ring outliers.

3 monomers are involved in 5 short contacts:

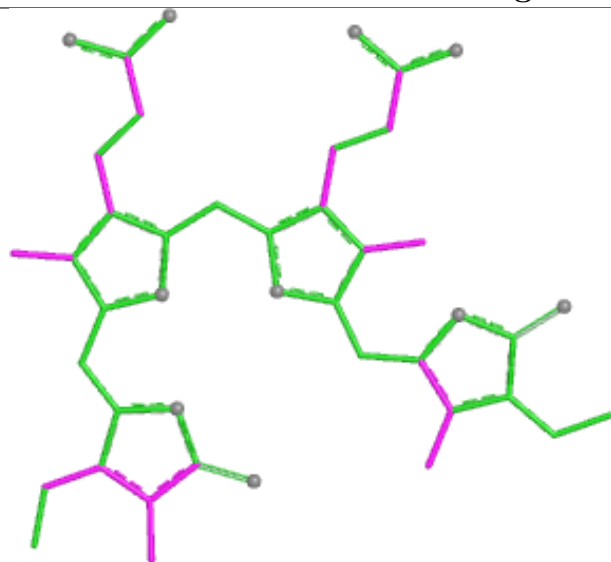
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	604	GOL	1	0
2	D	601	LBV	3	0
4	C	604	GOL	1	0

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

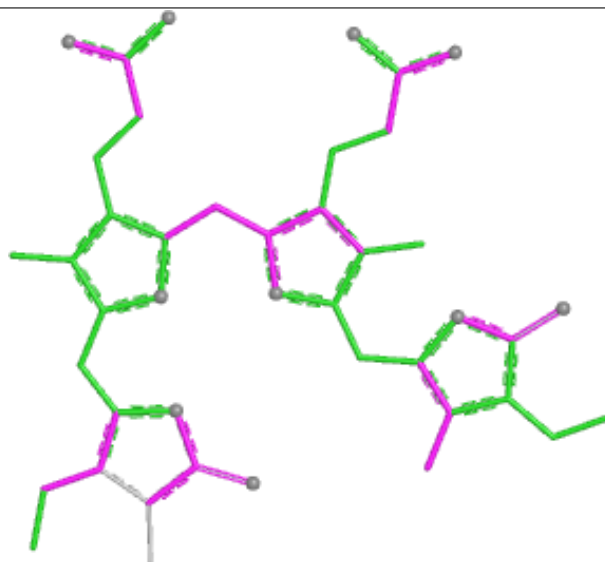
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified 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.



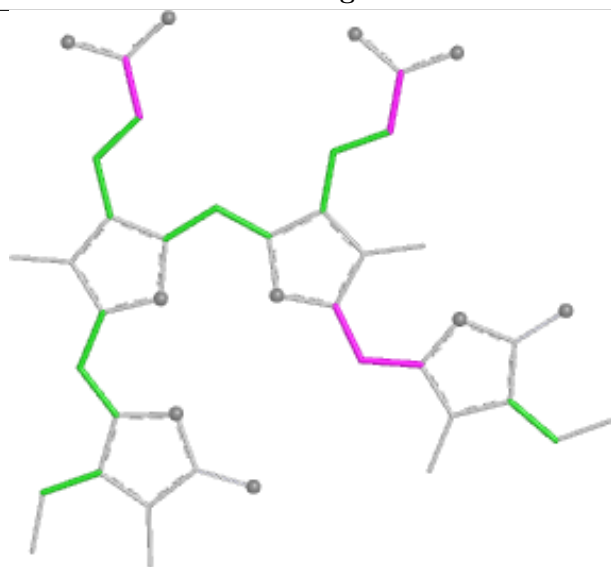
Ligand LBV C 601



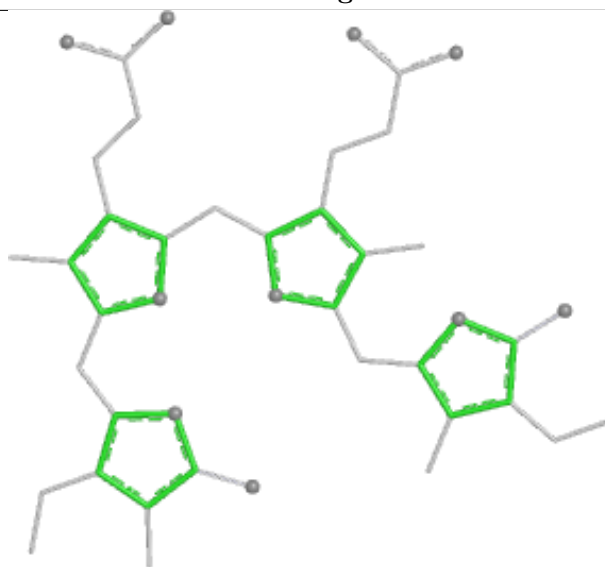
Bond lengths



Bond angles

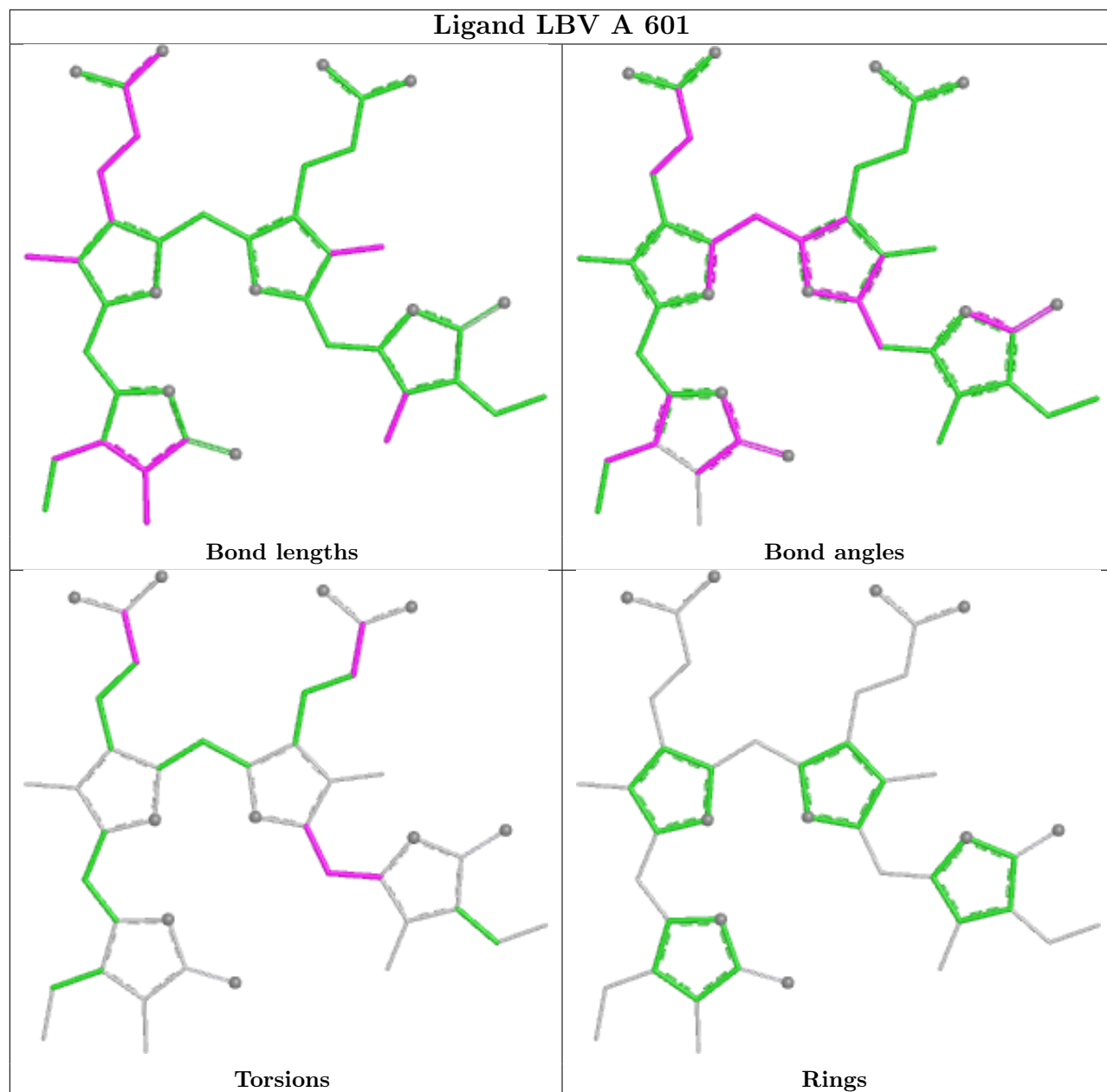


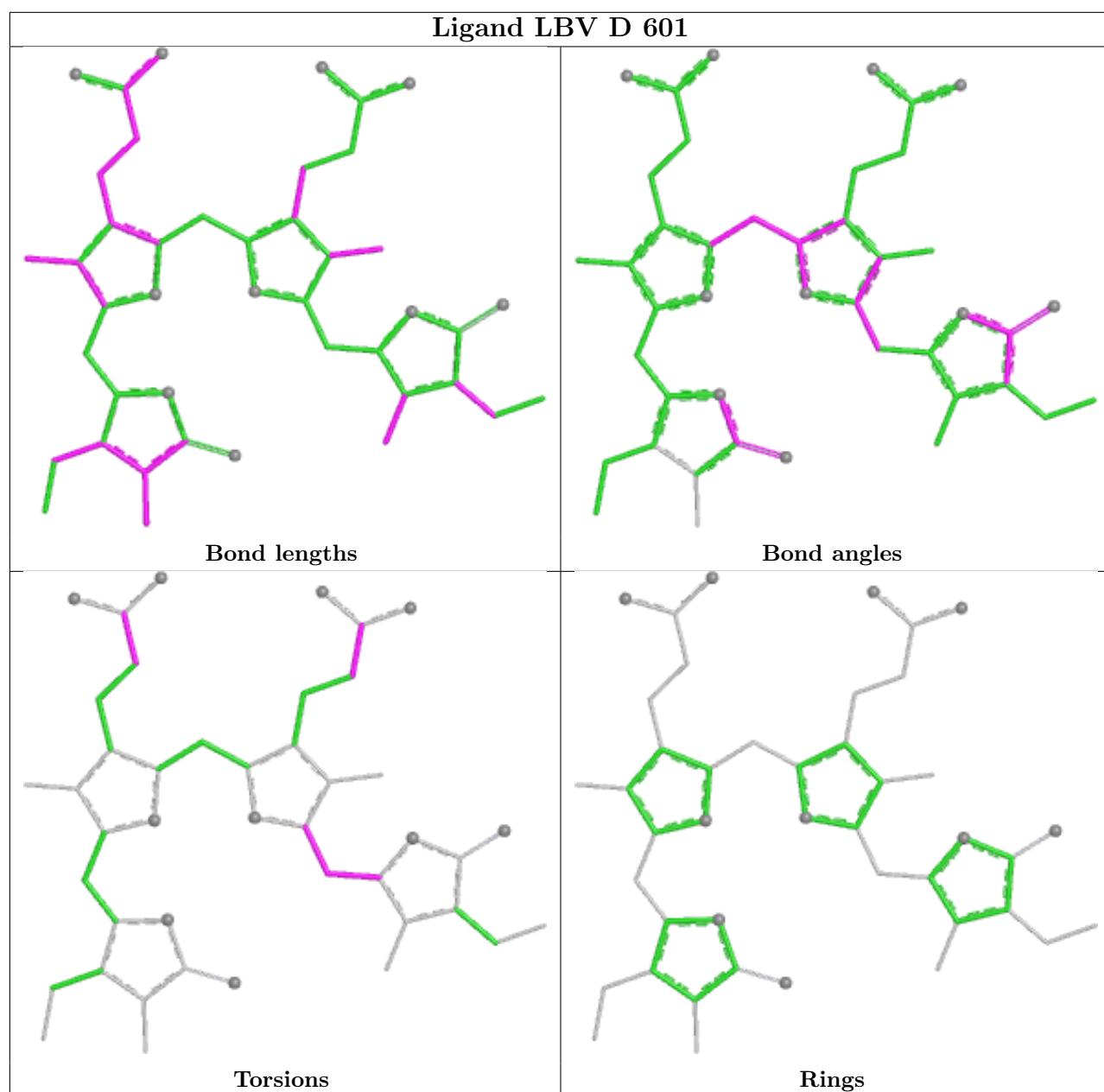
Torsions



Rings

Ligand LBV A 601





4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

5 Fit of model and data [i](#)

5.1 Protein, DNA and RNA chains [i](#)

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	512/529 (96%)	-0.25	3 (0%) 85 83	28, 55, 96, 128	1 (0%)
1	B	490/529 (92%)	-0.15	9 (1%) 67 63	25, 56, 99, 117	3 (0%)
1	C	509/529 (96%)	-0.21	3 (0%) 85 83	27, 55, 96, 132	3 (0%)
1	D	502/529 (94%)	-0.31	3 (0%) 85 83	25, 50, 86, 103	1 (0%)
All	All	2013/2116 (95%)	-0.23	18 (0%) 81 78	25, 54, 95, 132	8 (0%)

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	522	LEU	3.8
1	A	89	ILE	3.2
1	D	186	LEU	3.0
1	C	522	LEU	2.8
1	C	10	ILE	2.7
1	B	401	MET	2.7
1	B	481	SER	2.5
1	B	426	SER	2.4
1	B	361	GLY	2.4
1	C	186	LEU	2.4
1	D	477	VAL	2.4
1	B	437	PHE	2.3
1	A	121	HIS	2.3
1	B	410	LEU	2.3
1	B	372	GLY	2.2
1	D	16	ALA	2.1
1	B	373	GLU	2.1
1	B	349	ALA	2.0

5.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.4 Ligands ⓘ

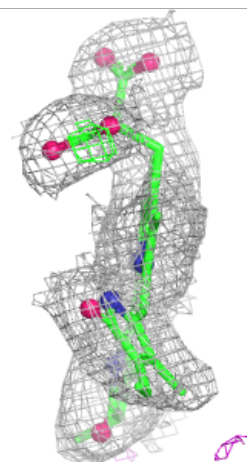
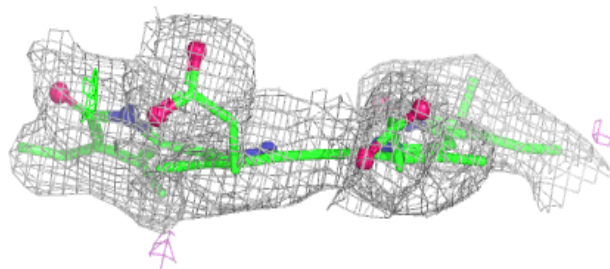
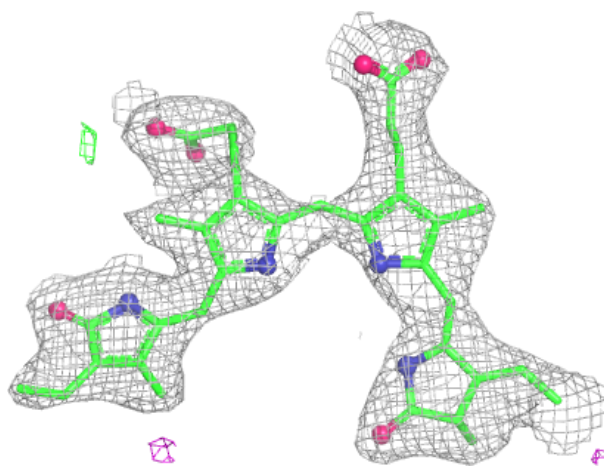
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	LBV	A	601	43/43	0.94	0.09	44,56,65,69	0
2	LBV	C	601	43/43	0.94	0.09	38,50,56,68	0
3	CL	A	603	1/1	0.94	0.15	90,90,90,90	0
2	LBV	D	601	43/43	0.95	0.08	33,39,50,56	0
2	LBV	B	601	43/43	0.96	0.06	33,40,45,53	0
3	CL	C	603	1/1	0.96	0.11	80,80,80,80	0
3	CL	B	603	1/1	0.96	0.08	43,43,43,43	0
4	GOL	A	604	6/6	0.96	0.08	38,54,54,60	0
3	CL	D	602	1/1	0.97	0.06	52,52,52,52	0
4	GOL	C	604	6/6	0.97	0.06	46,57,61,63	0
3	CL	B	602	1/1	0.98	0.05	40,40,40,40	0
3	CL	C	602	1/1	0.98	0.05	54,54,54,54	0
3	CL	A	602	1/1	0.99	0.05	42,42,42,42	0
3	CL	D	603	1/1	0.99	0.03	37,37,37,37	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.

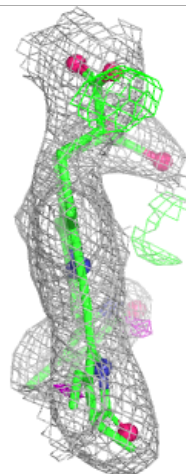
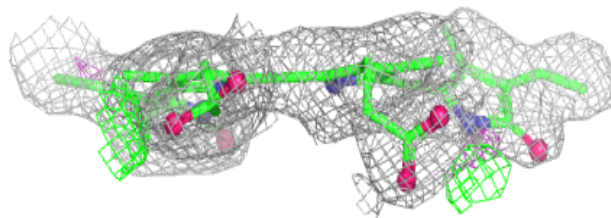
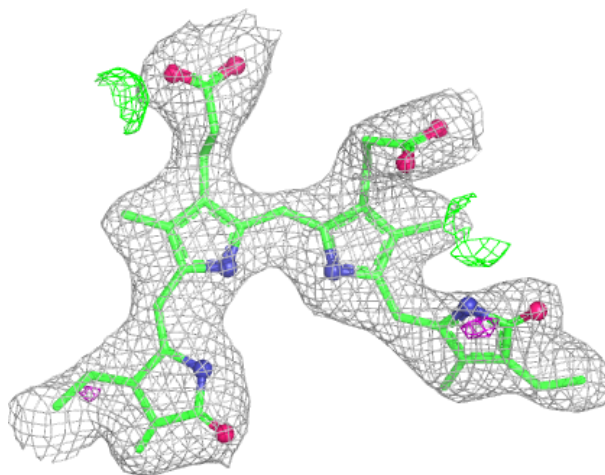
Electron density around LBV A 601:

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



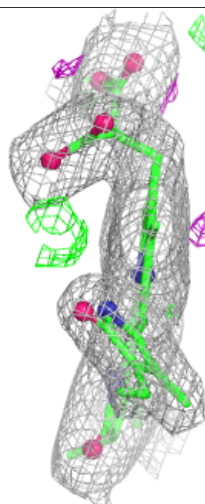
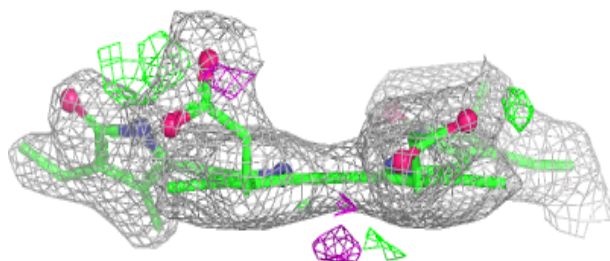
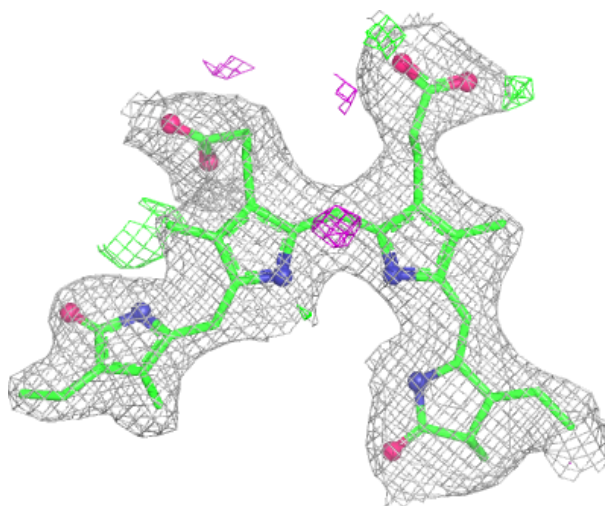
Electron density around LBV C 601:

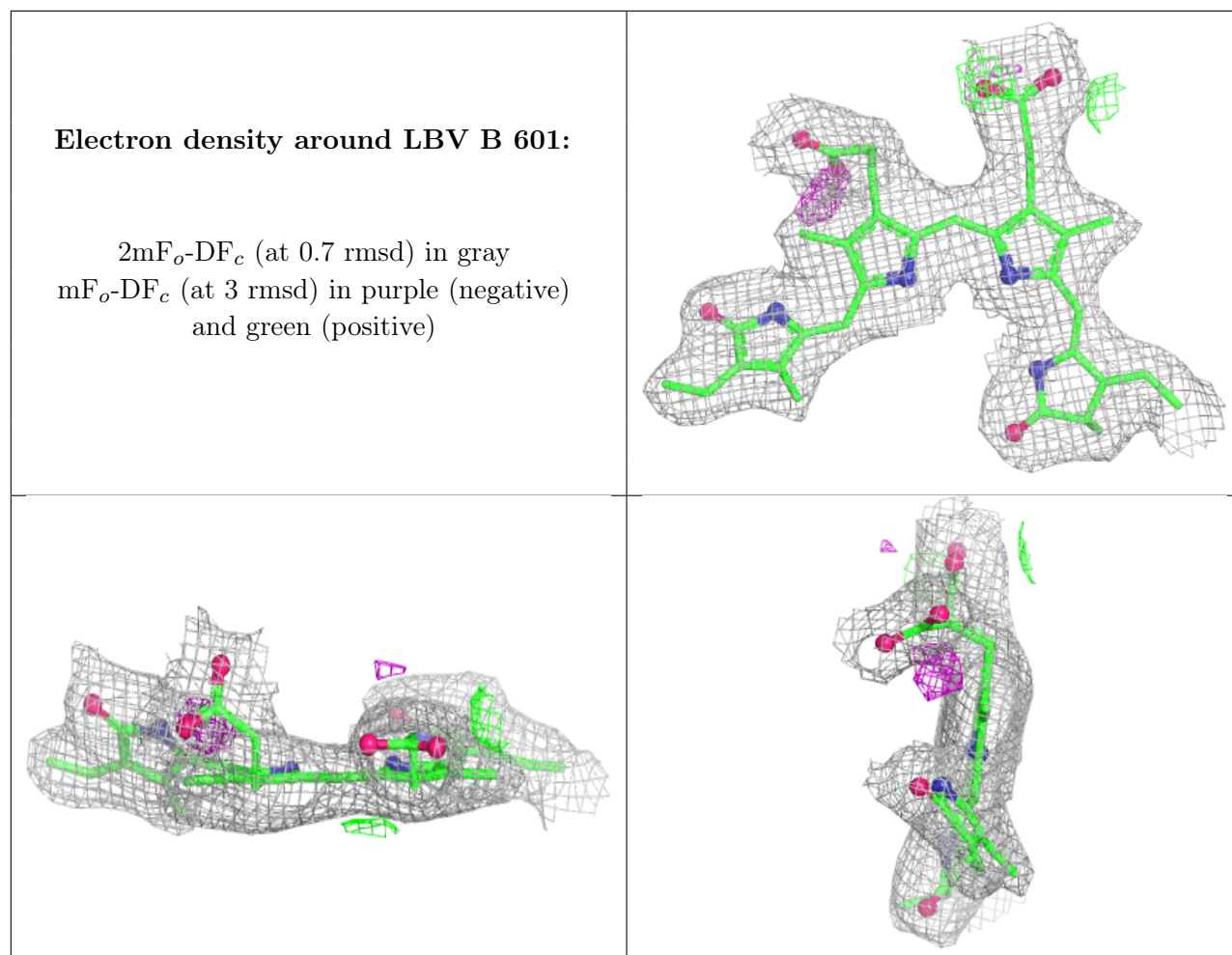
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around LBV D 601:

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





5.5 Other polymers ⓘ

There are no such residues in this entry.