



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 08:19 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 wwPDB X-ray Structure Validation Summary 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

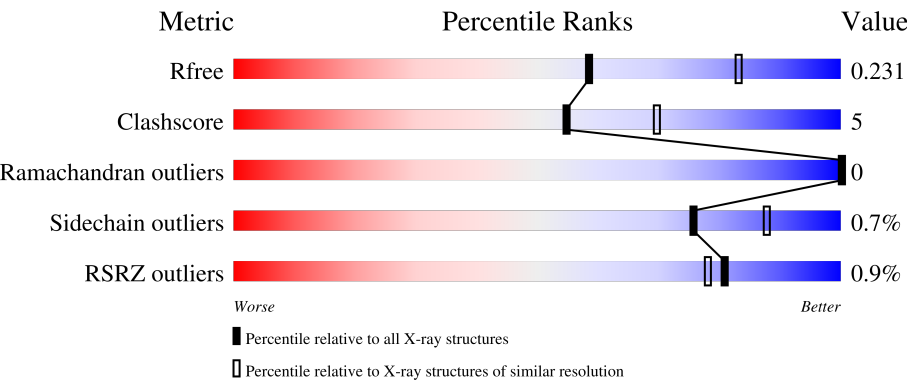
1 Overall quality at a glance i

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%

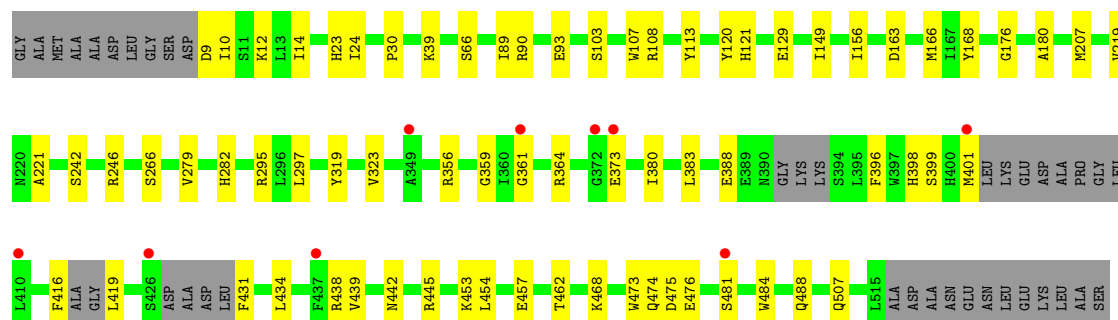
ENTRY-COMPOSITION INFOmissingINFO

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.

- Chain D: 
-
- Q185 L186 L187 H194 T200 P201 A202 Q203 A204 R205 A206 K207 P217 L226 H227 K231 R246 S249 S266 V279 G290 R294 R295 K320 V323 Q324 S340 H341 L354 L363 T369 T374 P375 L380 K381 K382 V384 F396
- L401 A406 L409 L424 K425 L430 L431 S432 V456 L464 S469 F470 E471 A472 V473 V474 D475 E476 V477 K480 L499 D517 A518 A519 A520 A521 A522 A523 A524 A525 A526 A527 A528 A529 A530 A531 A532 A533 A534 A535 A536 A537 A538 A539 A540 A541 A542 A543 A544 A545 A546 A547 A548 A549 A550 A551 A552 A553 A554 A555 A556 A557 A558 A559 A560 A561 A562 A563 A564 A565 A566 A567 A568 A569 A570 A571 A572 A573 A574 A575 A576 A577 A578 A579 A580 A581 A582 A583 A584 A585 A586 A587 A588 A589 A590 A591 A592 A593 A594 A595 A596 A597 A598 A599 A600 A601 A602 A603 A604 A605 A606 A607 A608 A609 A610 A611 A612 A613 A614 A615 A616 A617 A618 A619 A620 A621 A622 A623 A624 A625 A626 A627 A628 A629 A630 A631 A632 A633 A634 A635 A636 A637 A638 A639 A640 A641 A642 A643 A644 A645 A646 A647 A648 A649 A650 A651 A652 A653 A654 A655 A656 A657 A658 A659 A660 A661 A662 A663 A664 A665 A666 A667 A668 A669 A670 A671 A672 A673 A674 A675 A676 A677 A678 A679 A680 A681 A682 A683 A684 A685 A686 A687 A688 A689 A690 A691 A692 A693 A694 A695 A696 A697 A698 A699 A700 A701 A702 A703 A704 A705 A706 A707 A708 A709 A710 A711 A712 A713 A714 A715 A716 A717 A718 A719 A720 A721 A722 A723 A724 A725 A726 A727 A728 A729 A730 A731 A732 A733 A734 A735 A736 A737 A738 A739 A740 A741 A742 A743 A744 A745 A746 A747 A748 A749 A750 A751 A752 A753 A754 A755 A756 A757 A758 A759 A760 A761 A762 A763 A764 A765 A766 A767 A768 A769 A770 A771 A772 A773 A774 A775 A776 A777 A778 A779 A780 A781 A782 A783 A784 A785 A786 A787 A788 A789 A790 A791 A792 A793 A794 A795 A796 A797 A798 A799 A800 A801 A802 A803 A804 A805 A806 A807 A808 A809 A810 A811 A812 A813 A814 A815 A816 A817 A818 A819 A820 A821 A822 A823 A824 A825 A826 A827 A828 A829 A830 A831 A832 A833 A834 A835 A836 A837 A838 A839 A840 A841 A842 A843 A844 A845 A846 A847 A848 A849 A850 A851 A852 A853 A854 A855 A856 A857 A858 A859 A860 A861 A862 A863 A864 A865 A866 A867 A868 A869 A870 A871 A872 A873 A874 A875 A876 A877 A878 A879 A880 A881 A882 A883 A884 A885 A886 A887 A888 A889 A890 A891 A892 A893 A894 A895 A896 A897 A898 A899 A900 A901 A902 A903 A904 A905 A906 A907 A908 A909 A910 A911 A912 A913 A914 A915 A916 A917 A918 A919 A920 A921 A922 A923 A924 A925 A926 A927 A928 A929 A930 A931 A932 A933 A934 A935 A936 A937 A938 A939 A940 A941 A942 A943 A944 A945 A946 A947 A948 A949 A950 A951 A952 A953 A954 A955 A956 A957 A958 A959 A960 A961 A962 A963 A964 A965 A966 A967 A968 A969 A970 A971 A972 A973 A974 A975 A976 A977 A978 A979 A980 A981 A982 A983 A984 A985 A986 A987 A988 A989 A990 A991 A992 A993 A994 A995 A996 A997 A998 A999

- Chain A:
-
- | Residue | Information Content (bits) |
|---------|----------------------------|
| GLY | 0.00 |
| ALA | 0.00 |
| MET | 0.00 |
| ALA | 0.00 |
| ALA | 0.00 |
| ASP | 0.00 |
| LEU | 0.00 |
| GLY | 0.00 |
| SER | 0.00 |
| ASP | 0.00 |
| D9 | 0.00 |
| I10 | 0.00 |
| I14 | 0.00 |
| E20 | 0.00 |
| I28 | 0.00 |
| A47 | 0.00 |
| F65 | 0.00 |
| L65 | 0.00 |
| I68 | 0.00 |
| P78 | 0.00 |
| I82 | 0.00 |
| S87 | 0.00 |
| A88 | 0.00 |
| I89 | 0.00 |
| R90 | 0.00 |
| E93 | 0.00 |
| P94 | 0.00 |
| I95 | 0.00 |
| S103 | 0.00 |
| F104 | 0.00 |
| L105 | 0.00 |
| G106 | 0.00 |
| W107 | 0.00 |
| V117 | 0.00 |
| Y120 | 0.00 |
| H121 | 0.00 |
| F132 | 0.00 |
| T153 | 0.00 |
| M166 | 0.00 |
| I167 | 0.00 |
| Y168 | 0.00 |
| C176 | 0.00 |

- Chain C: 
- GLY
ALA
MET
ALA
ALA
ASP
LEU
GLY
SER
SER
ASP
ASP
I10
I24
P30
E38
V46
N50
E63
D69
I62
L65
W107
F132
Q133
Q137
M166
I167
Y168
D171
N175
G176
L186
M207
A221
H227
V238
S242
P246
- M253
R257
S266
V279
R291
R294
R295
L296
V323
R327
H341
I345
L368
T369
I380
N381
L387
G391
H398
S399
Q400
M401
L402
L410
G418
L419
I422
K426
SER
ASP
ASP
L430
V439
A440
Q441
K453
L454



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.

The worst 5 of 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

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 ⓘ

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

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	474	GLN
1	C	439	VAL
1	B	396	PHE
1	B	66	SER
1	B	219	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	230	HIS
1	C	442	ASN
1	C	381	ASN
1	C	514	GLN
1	D	474	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%)
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-

The worst 5 of 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

The worst 5 of 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

There are no chirality outliers.

5 of 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

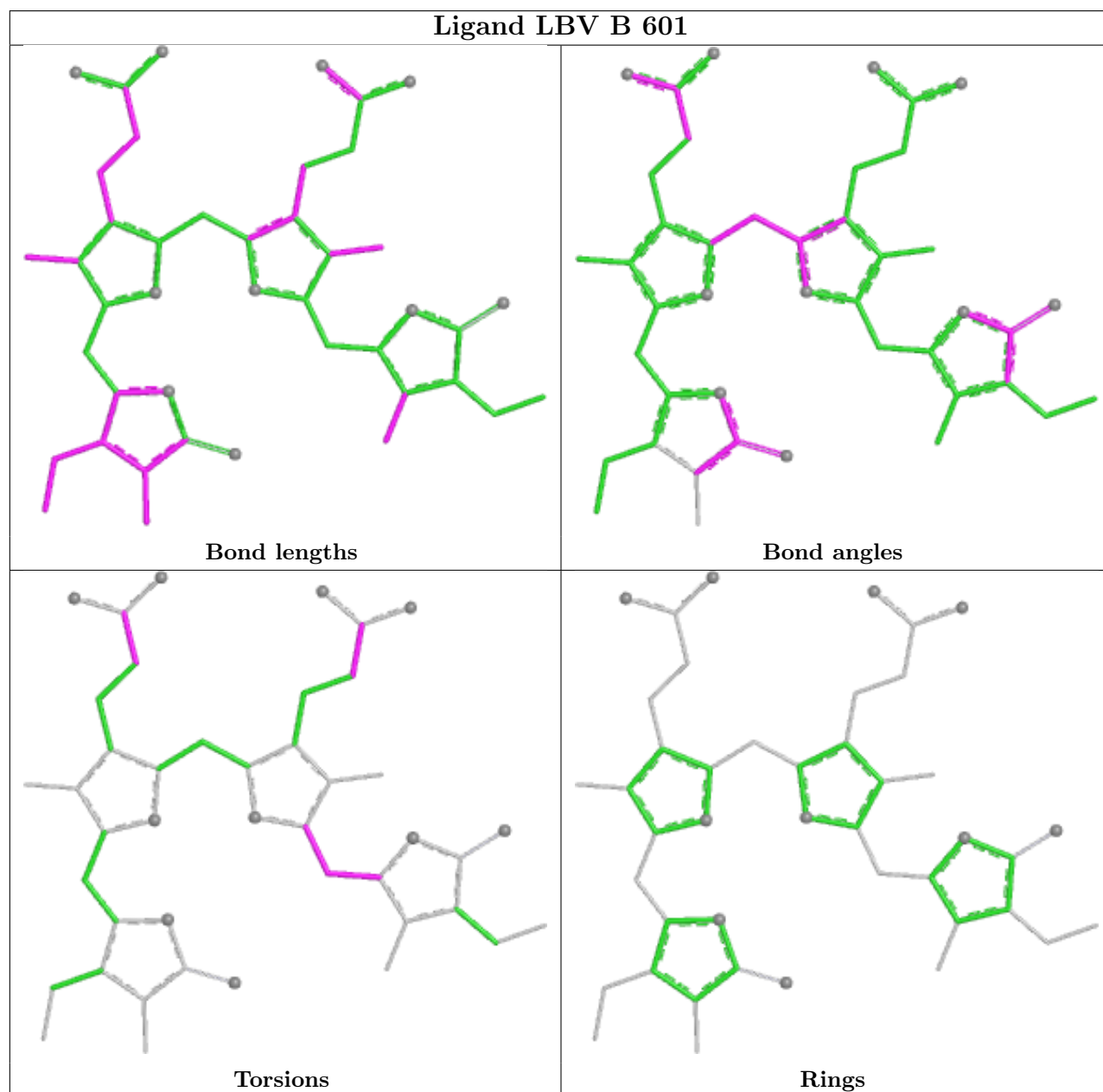
There are no ring outliers.

3 monomers are involved in 5 short contacts:

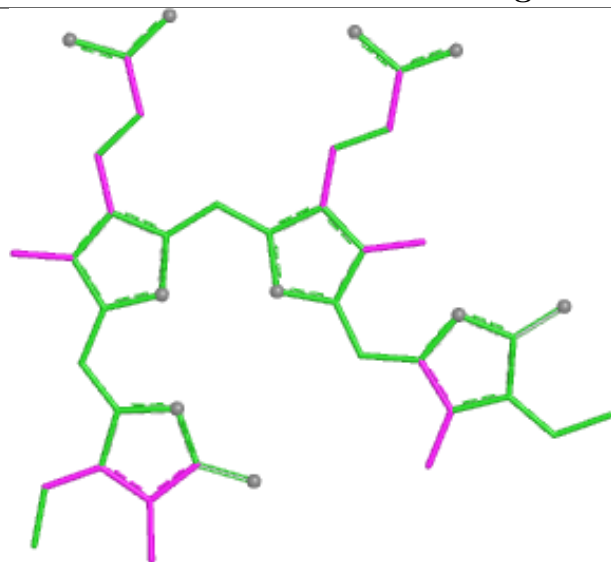
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	604	GOL	1	0
2	D	601	LBV	3	0
4	C	604	GOL	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

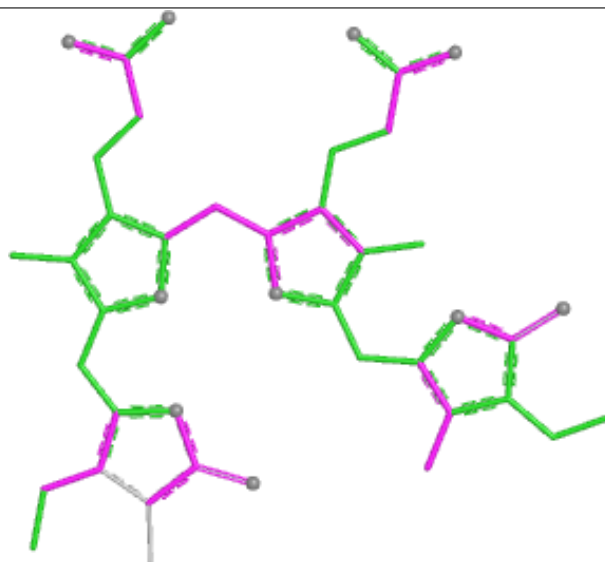
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 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.



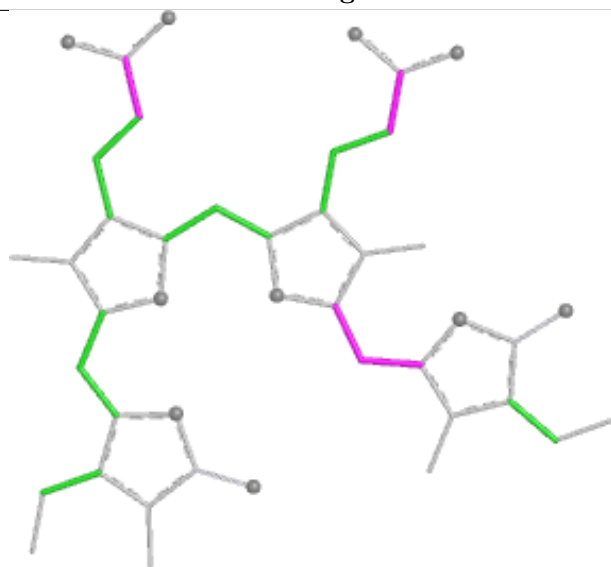
Ligand LBV C 601



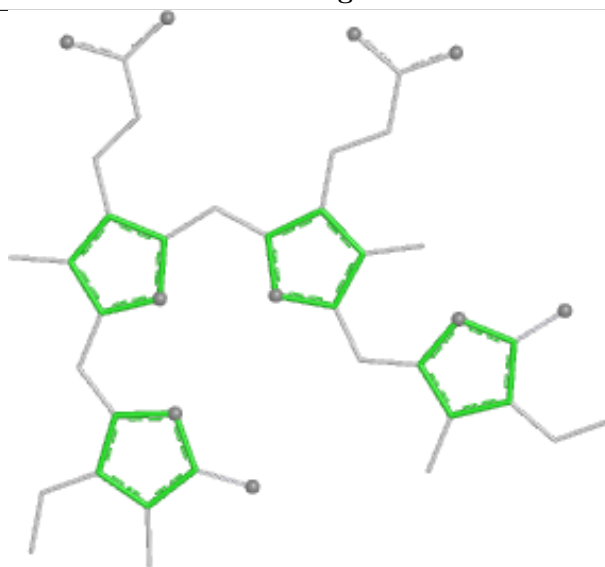
Bond lengths



Bond angles

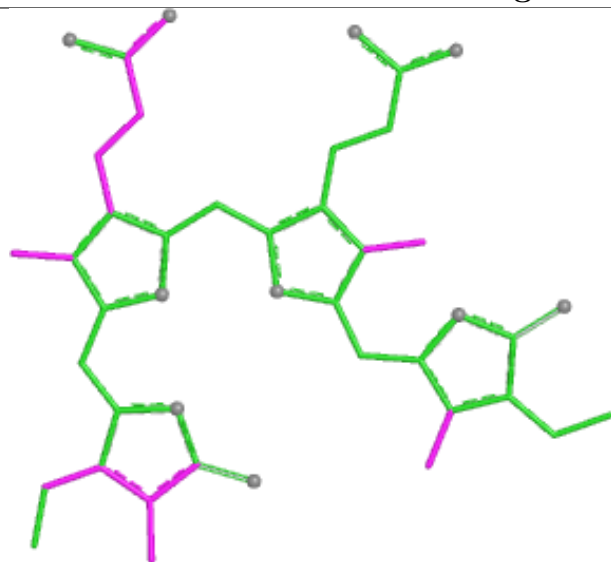


Torsions

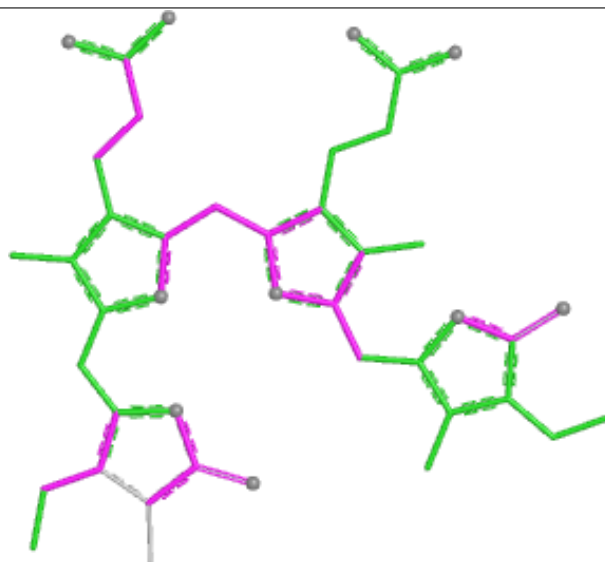


Rings

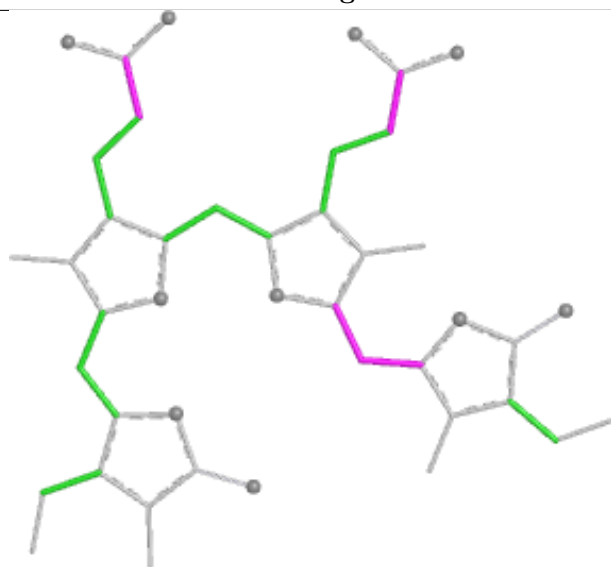
Ligand LBV A 601



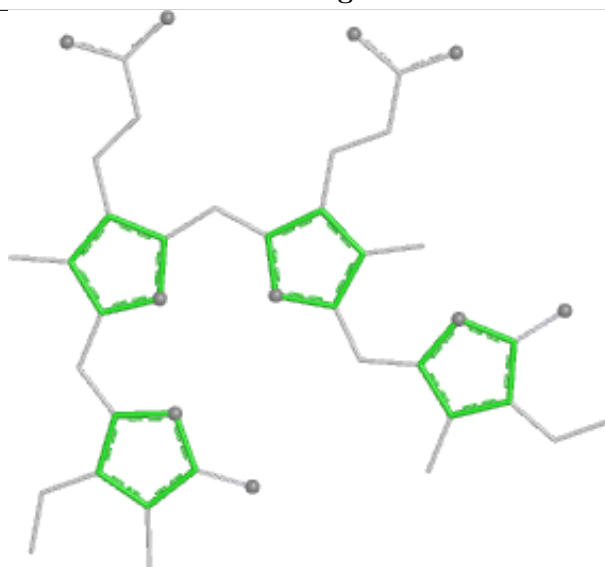
Bond lengths



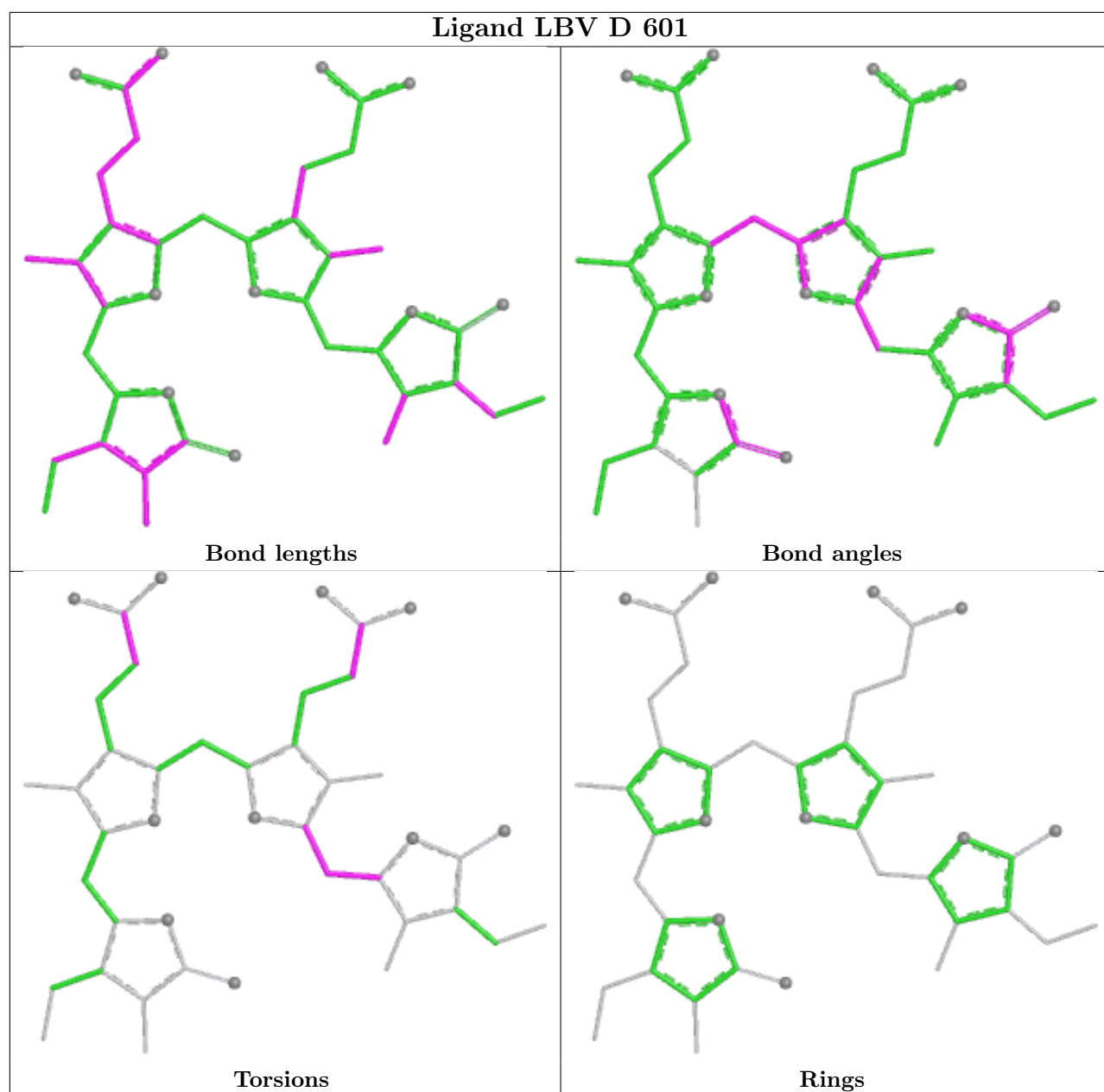
Bond angles



Torsions



Rings



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%)

The worst 5 of 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

5.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.3 Carbohydrates [i](#)

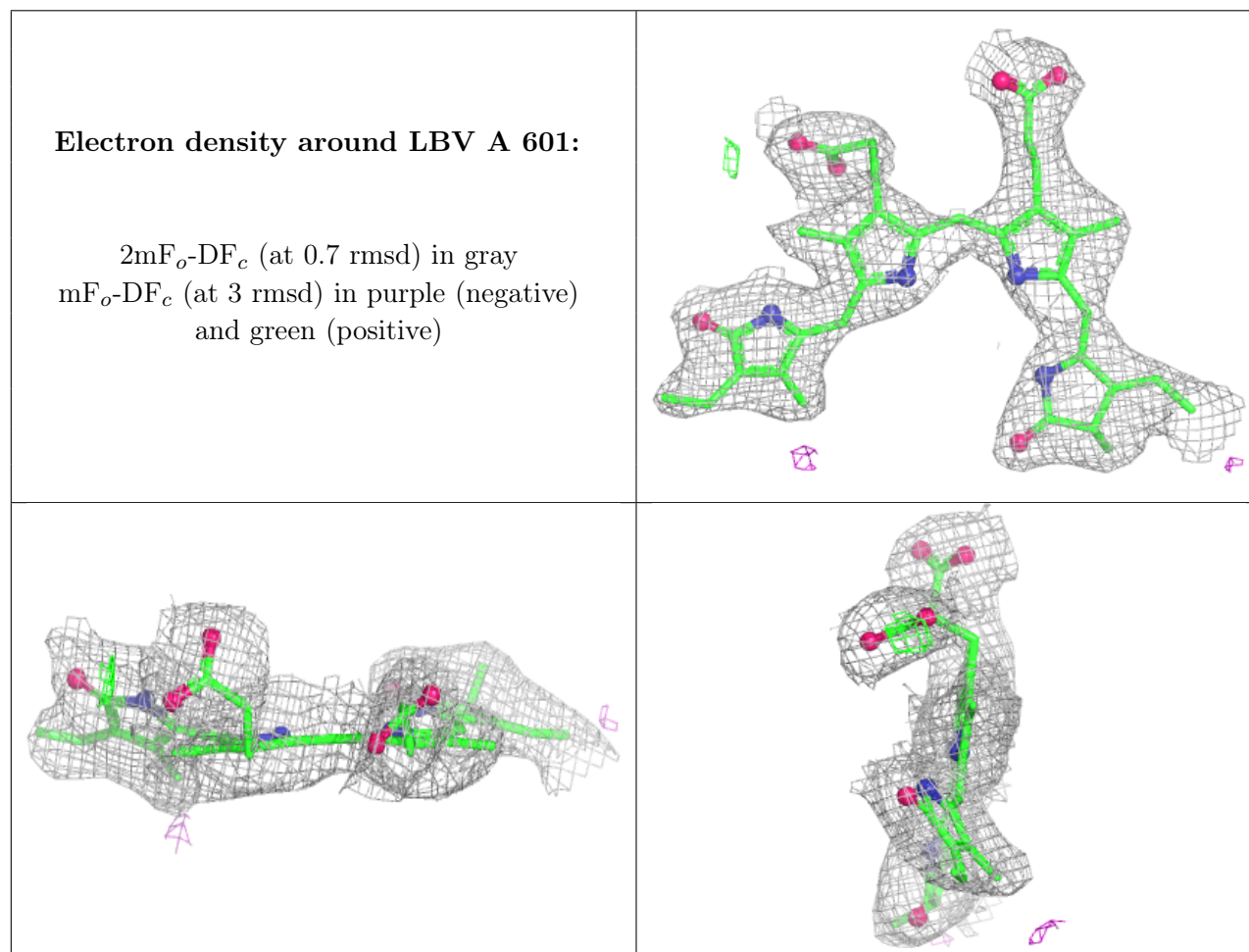
There are no oligosaccharides in this entry.

5.4 Ligands [i](#)

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

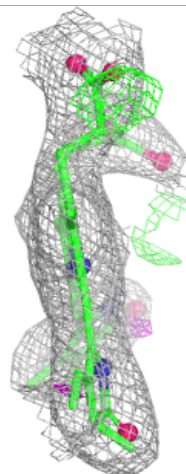
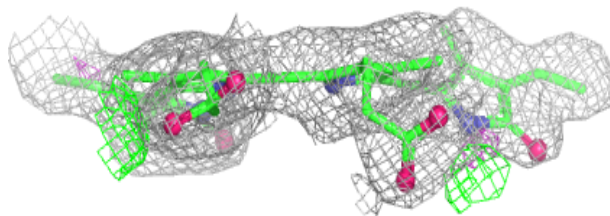
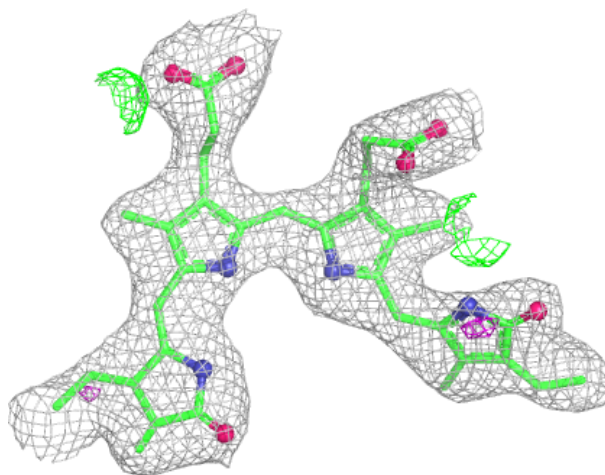
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	LBV	A	601	43/43	0.94	0.09	44,56,65,69	0
2	LBV	C	601	43/43	0.94	0.09	38,50,56,68	0
3	CL	A	603	1/1	0.94	0.15	90,90,90,90	0
2	LBV	D	601	43/43	0.95	0.08	33,39,50,56	0
2	LBV	B	601	43/43	0.96	0.06	33,40,45,53	0
3	CL	C	603	1/1	0.96	0.11	80,80,80,80	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.



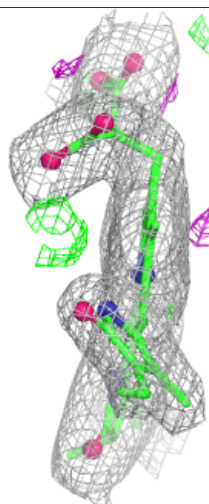
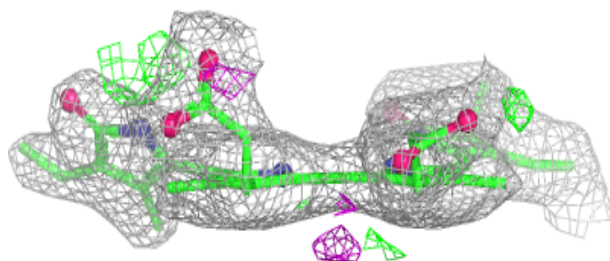
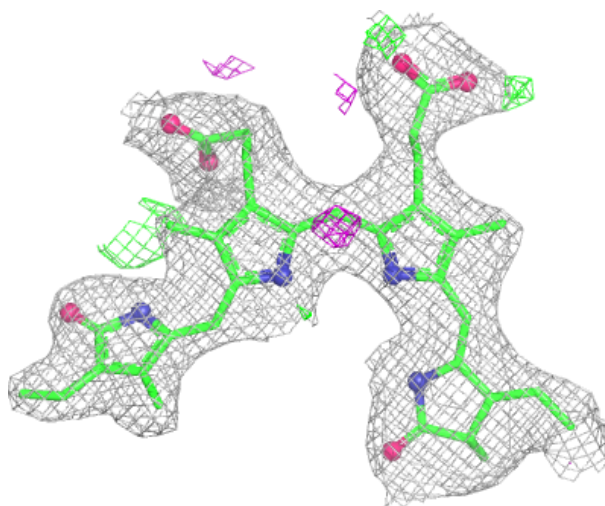
Electron density around LBV C 601:

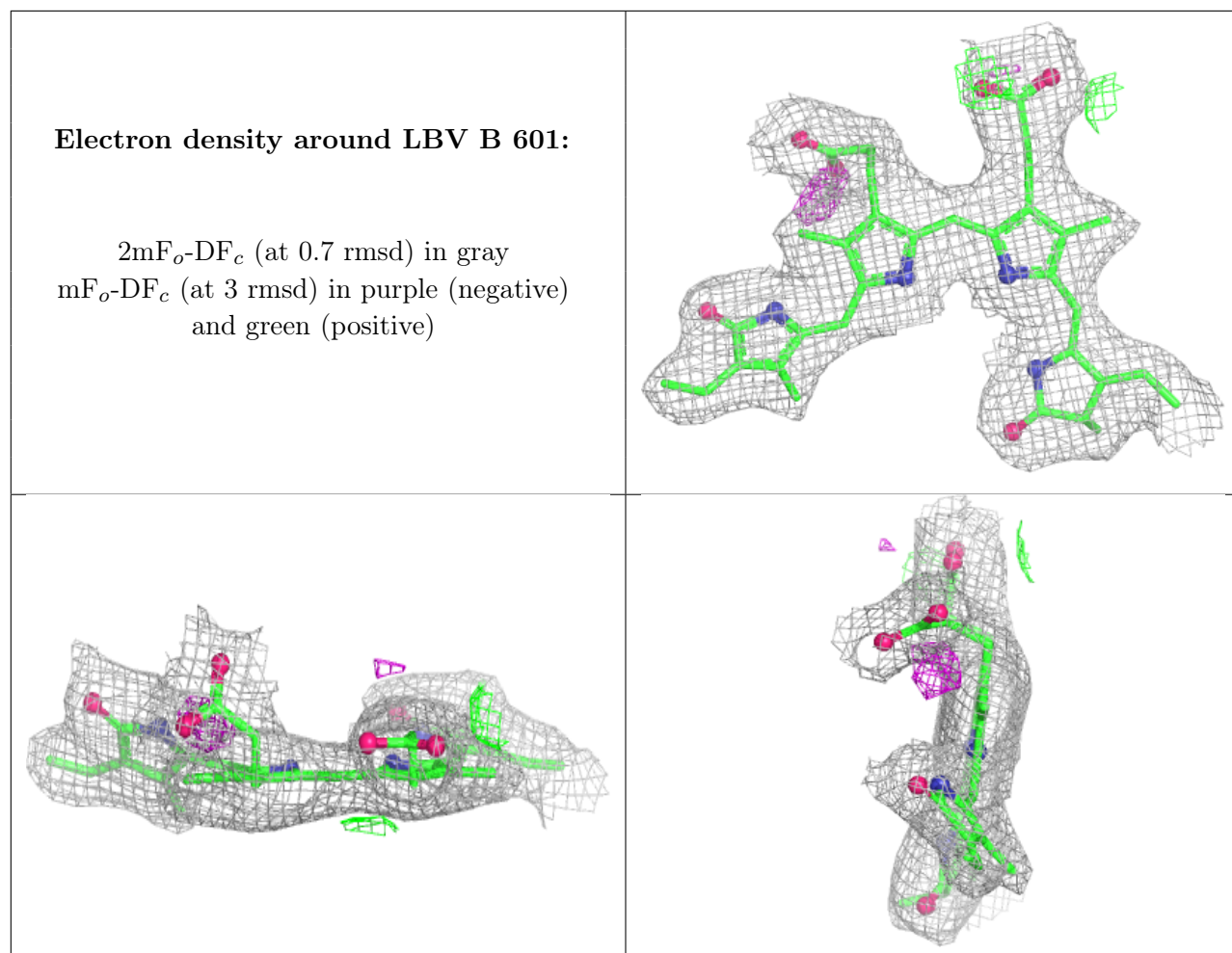
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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.