



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:22 AM UTC

PDB ID : 2OOL / pdb_00002ool
Title : Crystal structure of the chromophore-binding domain of an unusual bacterio-
phytochrome RpBphP3 from *R. palustris*
Authors : Yang, X.; Stojkovic, E.A.; Kuk, J.; Moffat, K.
Deposited on : 2007-01-25
Resolution : 2.20 Å (reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

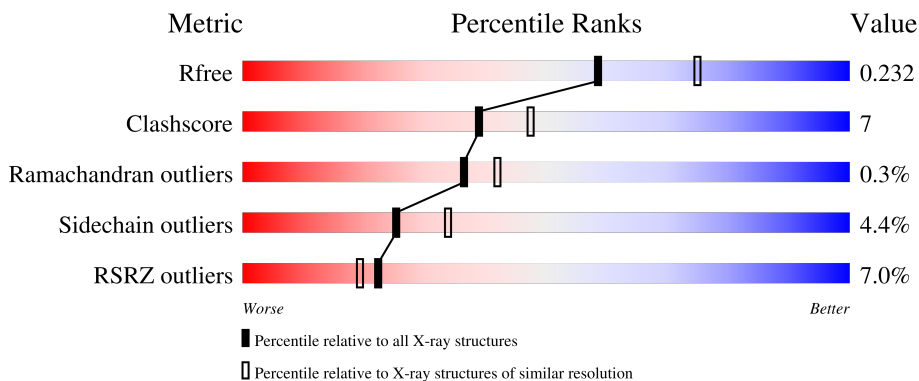
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	337	 5% 74% 15% 10%
1	B	337	 7% 72% 15% 12%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	LBV	A	400[A]	X	-	-	-
2	LBV	A	400[B]	X	-	-	-
2	LBV	B	400	X	-	-	-

2 Entry composition [i](#)

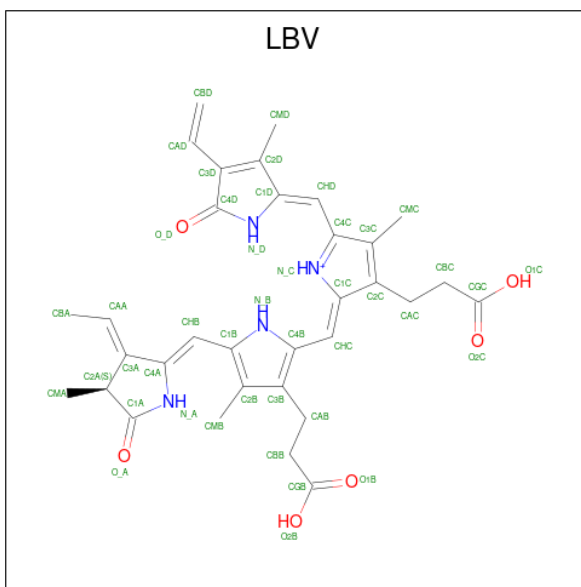
There are 3 unique types of molecules in this entry. The entry contains 5101 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Sensor protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	304	Total	C	N	O	S	15	5	0
			2431	1542	435	445	9			
1	B	298	Total	C	N	O	S	5	3	0
			2368	1501	428	430	9			

- Molecule 2 is 3-[2-[(Z)-[3-(2-carboxyethyl)-5-[(Z)-(4-ethenyl-3-methyl-5-oxidanylidene-pyrro- l-2-ylidene)methyl]-4-methyl-pyrrol-1-ium -2-ylidene]methyl]-5-[(Z)-[(3E)-3-ethylidene-4-me thyl-5-oxidanylidene-pyrrolidin-2-ylidene]methyl]-4-methyl-1H-pyrrol-3- yl]propanoic acid (CCD ID: LBV) (formula: C₃₃H₃₇N₄O₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	Total	C	N	O	0	1
			44	34	4	6		
2	B	1	Total	C	N	O	0	0
			43	33	4	6		

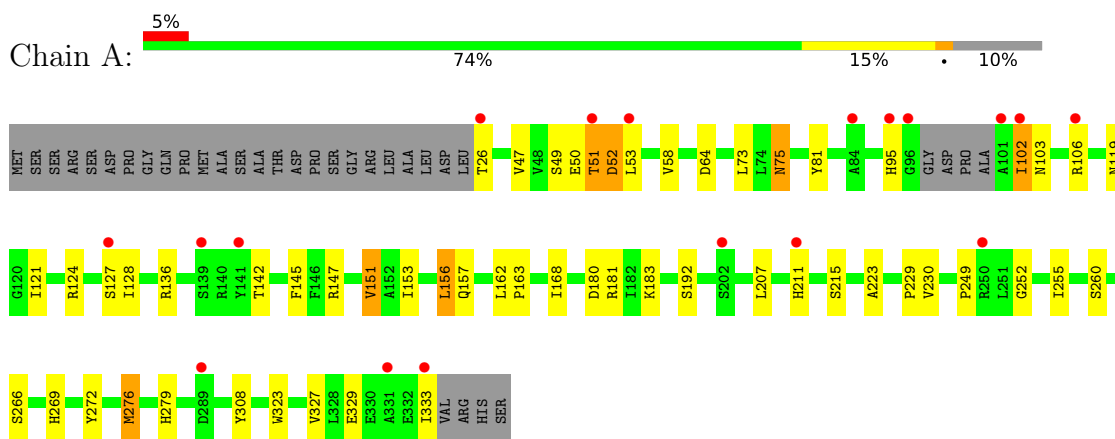
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	161	Total 161	O 161	0	0
3	B	54	Total 54	O 54	0	0

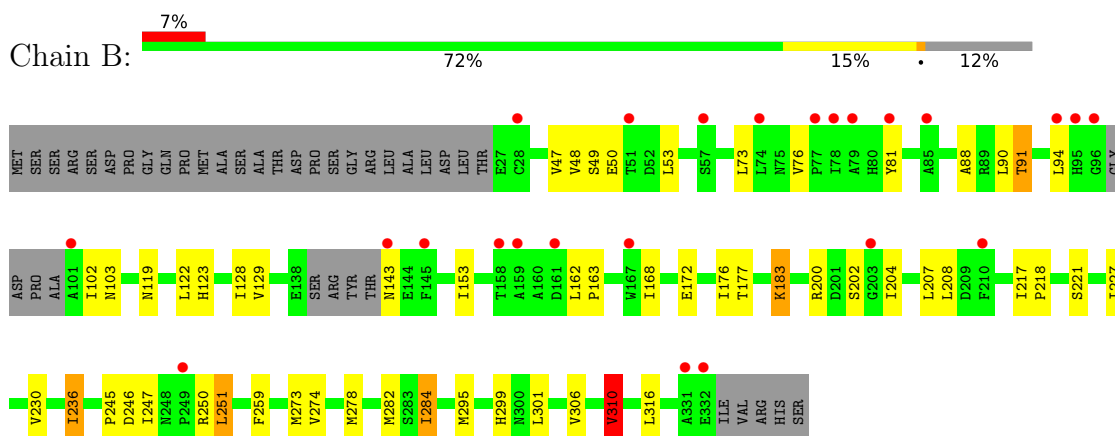
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Sensor protein



- Molecule 1: Sensor protein



4 Data and refinement statistics i

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, α , β , γ	151.87Å 151.87Å 76.00Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.75 – 2.20 49.75 – 2.20	Depositor EDS
% Data completeness (in resolution range)	93.3 (49.75-2.20) 92.5 (49.75-2.20)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.37 (at 2.10Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.188 , 0.231 0.191 , 0.232	Depositor DCC
R_{free} test set	4457 reflections (7.68%)	wwPDB-VP
Wilson B-factor (Å ²)	41.8	Xtrriage
Anisotropy	0.398	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 64.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.033 for -h,-k,l	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5101	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.26% 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: 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	1.03	2/2492 (0.1%)	1.01	5/3402 (0.1%)
1	B	0.78	1/2428 (0.0%)	0.88	1/3311 (0.0%)
All	All	0.91	3/4920 (0.1%)	0.95	6/6713 (0.1%)

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

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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	310	VAL	CA-CB	6.03	1.62	1.54
1	A	230	VAL	C-O	-5.79	1.18	1.24
1	A	223	ALA	CA-CB	5.14	1.61	1.53

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	252	GLY	N-CA-C	-6.30	103.48	112.81
1	B	236	ILE	CB-CA-C	-5.47	104.87	112.04
1	A	229	PRO	N-CA-C	5.39	121.08	114.35
1	A	180	ASP	N-CA-C	5.32	117.83	111.71
1	A	266	SER	CA-C-N	5.15	125.19	119.32
1	A	266	SER	C-N-CA	5.15	125.19	119.32

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	143	ASN	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	2431	0	2416	31	1
1	B	2368	0	2351	34	0
2	A	44	0	8	1	0
2	B	43	0	33	1	0
3	A	161	0	0	3	0
3	B	54	0	0	2	0
All	All	5101	0	4808	66	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 7.

All (66) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:73:LEU:O	1:B:76:VAL:HG12	1.63	0.98
1:A:51:THR:HG23	1:A:52:ASP:H	1.43	0.82
1:A:51:THR:HG23	1:A:52:ASP:OD1	1.88	0.72
1:B:236:ILE:HD11	1:B:278:MET:O	1.88	0.72
1:B:103:ASN:HD21	1:B:122:LEU:H	1.42	0.67
1:B:236:ILE:HD11	1:B:273:MET:HB3	1.75	0.66
1:B:204:ILE:HD12	1:B:301:LEU:HD21	1.77	0.65
1:B:123[A]:HIS:CD2	3:B:402:HOH:O	2.49	0.65
1:B:250:ARG:HB2	1:B:251:LEU:HD13	1.80	0.63
1:A:181:ARG:HE	1:A:183:LYS:HZ2	1.47	0.61
1:B:236:ILE:CD1	1:B:278:MET:O	2.48	0.61
1:A:215:SER:O	2:A:400[B]:LBV:HMA2	2.03	0.57
1:A:102:ILE:HG12	1:A:103:ASN:N	2.19	0.57
1:A:181:ARG:HE	1:A:183:LYS:NZ	2.04	0.56
1:B:204:ILE:HD12	1:B:301:LEU:CD2	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:123[A]:HIS:CE1	1:B:259:PHE:O	2.59	0.55
1:B:103:ASN:ND2	1:B:122:LEU:H	2.03	0.55
1:B:48:VAL:HG23	1:B:129:VAL:HB	1.88	0.55
1:B:245:PRO:HB2	1:B:247:ILE:HD12	1.89	0.54
1:A:121:ILE:HD12	1:A:308:TYR:CD1	2.44	0.53
1:B:177:THR:HG21	1:B:282:MET:HE1	1.91	0.53
1:A:26:THR:HG22	1:A:26:THR:O	2.11	0.51
1:A:156:LEU:HD13	1:A:168:ILE:CG2	2.40	0.51
1:B:123[A]:HIS:HD2	3:B:402:HOH:O	1.87	0.51
1:A:64:ASP:HB2	3:A:491:HOH:O	2.09	0.51
1:A:73:LEU:CD2	1:A:81:TYR:OH	2.61	0.49
1:B:183:LYS:HZ1	1:B:299:HIS:CE1	2.31	0.49
1:A:49:SER:O	1:A:53:LEU:HA	2.13	0.48
1:A:153:ILE:O	1:A:157:GLN:HG3	2.14	0.47
1:B:306:VAL:HB	1:B:310:VAL:HG21	1.95	0.47
1:A:142:THR:O	1:A:145:PHE:HB3	2.15	0.47
1:A:106:ARG:HG3	1:A:136:ARG:NH1	2.30	0.46
1:B:153:ILE:HD11	1:B:316:LEU:HG	1.96	0.46
1:A:50:GLU:OE1	1:A:124:ARG:NE	2.49	0.46
1:B:49:SER:O	1:B:53:LEU:HD23	2.15	0.46
1:A:49:SER:O	1:A:53:LEU:HD23	2.16	0.45
1:A:47:VAL:HG21	1:A:255:ILE:HD13	1.98	0.45
1:A:147:ARG:O	1:A:151:VAL:HG13	2.16	0.45
1:B:218:PRO:O	1:B:221:SER:HB2	2.16	0.45
1:B:88:ALA:O	1:B:91:THR:HG22	2.17	0.45
1:A:128:ILE:HG21	1:A:249:PRO:HD2	1.98	0.45
1:B:47:VAL:HG13	1:B:128:ILE:HD12	1.99	0.45
1:B:230:VAL:HG13	1:B:284:ILE:HD13	1.98	0.45
1:B:217:ILE:HD13	1:B:295:MET:HE2	1.99	0.44
1:A:192:SER:HB2	1:A:211[B]:HIS:CE1	2.53	0.43
1:A:121:ILE:HD12	1:A:308:TYR:CE1	2.53	0.43
1:A:75:ASN:HD22	1:A:75:ASN:HA	1.66	0.43
2:B:400:LBV:HBD1	2:B:400:LBV:O_D	2.18	0.43
1:B:306:VAL:HB	1:B:310:VAL:CG2	2.48	0.42
1:A:151:VAL:HG22	3:A:515:HOH:O	2.19	0.42
1:A:323:TRP:O	1:A:327:VAL:HG23	2.20	0.42
1:B:168:ILE:O	1:B:172:GLU:HG2	2.19	0.42
1:A:279:HIS:HE1	3:A:499:HOH:O	2.03	0.41
1:B:119:ASN:HD22	1:B:119:ASN:HA	1.67	0.41
1:B:162:LEU:HB3	1:B:163:PRO:HD3	2.01	0.41
1:B:200:ARG:NE	1:B:204:ILE:O	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:236:ILE:HG21	1:B:274:VAL:HG22	2.03	0.41
1:A:269:HIS:O	1:A:272:TYR:HB3	2.21	0.41
1:B:76:VAL:HG11	1:B:81:TYR:HE1	1.85	0.41
1:A:53:LEU:HA	1:A:53:LEU:HD23	1.85	0.41
1:A:156:LEU:HD13	1:A:168:ILE:HG22	2.03	0.41
1:A:162:LEU:HB3	1:A:163:PRO:HD3	2.02	0.41
1:B:172:GLU:O	1:B:176:ILE:HG23	2.20	0.41
1:B:246:ASP:C	1:B:247:ILE:HG13	2.46	0.41
1:A:207:LEU:HD11	1:A:276:MET:HE2	2.03	0.40
1:B:90:LEU:O	1:B:94:LEU:HD12	2.20	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:A:106:ARG:NH2	1:A:106:ARG:NH2[5_556]	1.99	0.21

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	305/337 (90%)	298 (98%)	5 (2%)	2 (1%)	18	19
1	B	295/337 (88%)	288 (98%)	7 (2%)	0	100	100
All	All	600/674 (89%)	586 (98%)	12 (2%)	2 (0%)	36	42

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	51	THR
1	A	95	HIS

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	267/288 (93%)	255 (96%)	12 (4%)	24	33
1	B	259/288 (90%)	248 (96%)	11 (4%)	26	36
All	All	526/576 (91%)	503 (96%)	23 (4%)	25	34

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	ASP
1	A	58	VAL
1	A	75	ASN
1	A	102	ILE
1	A	119	ASN
1	A	127	SER
1	A	151	VAL
1	A	156	LEU
1	A	260	SER
1	A	276	MET
1	A	329	GLU
1	A	333	ILE
1	B	50	GLU
1	B	91	THR
1	B	102	ILE
1	B	183	LYS
1	B	202	SER
1	B	207	LEU
1	B	208	LEU
1	B	227	ILE
1	B	251	LEU
1	B	284	ILE
1	B	310	VAL

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	75	ASN
1	A	119	ASN
1	A	125	HIS
1	B	75	ASN
1	B	103	ASN
1	B	119	ASN
1	B	157	GLN
1	B	312	GLN

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](#)

3 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	LBV	B	400	1	46,46,46	1.56	11 (23%)	58,67,67	1.83	15 (25%)
2	LBV	A	400[B]	-	46,46,46	1.70	13 (28%)	58,67,67	1.82	17 (29%)
2	LBV	A	400[A]	-	46,46,46	1.70	13 (28%)	58,67,67	1.82	17 (29%)

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	LBV	B	400	1	1/1/14/22	8/26/74/74	0/4/4/4
2	LBV	A	400[B]	-	1/1/14/22	8/26/74/74	0/4/4/4
2	LBV	A	400[A]	-	1/1/14/22	8/26/74/74	0/4/4/4

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	400[A]	LBV	CAD-C3D	-3.56	1.37	1.47
2	A	400[B]	LBV	CAD-C3D	-3.56	1.37	1.47
2	A	400[A]	LBV	CAA-C3A	3.28	1.41	1.33
2	A	400[B]	LBV	CAA-C3A	3.28	1.41	1.33
2	A	400[A]	LBV	C1D-N_D	-3.10	1.32	1.37
2	A	400[B]	LBV	C1D-N_D	-3.10	1.32	1.37
2	B	400	LBV	C1C-C2C	-3.07	1.40	1.45
2	B	400	LBV	CAD-C3D	-2.85	1.39	1.47
2	B	400	LBV	CAA-C3A	2.83	1.40	1.33
2	A	400[A]	LBV	CBC-CGC	2.68	1.56	1.50
2	A	400[B]	LBV	CBC-CGC	2.68	1.56	1.50
2	A	400[A]	LBV	C1C-C2C	-2.67	1.41	1.45
2	A	400[B]	LBV	C1C-C2C	-2.67	1.41	1.45
2	B	400	LBV	CBC-CGC	2.64	1.56	1.50
2	B	400	LBV	C1D-C2D	-2.50	1.40	1.45
2	B	400	LBV	C4C-C3C	-2.28	1.40	1.45
2	A	400[A]	LBV	C4C-C3C	-2.23	1.41	1.45
2	A	400[B]	LBV	C4C-C3C	-2.23	1.41	1.45
2	A	400[A]	LBV	O2B-CGB	-2.12	1.23	1.30
2	A	400[B]	LBV	O2B-CGB	-2.12	1.23	1.30
2	B	400	LBV	C3D-C4D	-2.10	1.38	1.47
2	B	400	LBV	C1D-N_D	-2.10	1.34	1.37
2	A	400[A]	LBV	C4A-N_A	-2.08	1.34	1.37
2	A	400[B]	LBV	C4A-N_A	-2.08	1.34	1.37
2	B	400	LBV	C1C-N_C	-2.06	1.34	1.38
2	A	400[A]	LBV	CMB-C2B	2.05	1.55	1.50
2	A	400[B]	LBV	CMB-C2B	2.05	1.55	1.50
2	B	400	LBV	O2B-CGB	-2.04	1.24	1.30
2	A	400[A]	LBV	CBA-CAA	2.04	1.57	1.49
2	A	400[B]	LBV	CBA-CAA	2.04	1.57	1.49
2	B	400	LBV	CBD-CAD	2.03	1.40	1.30
2	A	400[A]	LBV	CMD-C2D	2.01	1.54	1.50
2	A	400[B]	LBV	CMD-C2D	2.01	1.54	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	400[A]	LBV	C1D-C2D	-2.01	1.41	1.45
2	A	400[B]	LBV	C1D-C2D	-2.01	1.41	1.45
2	A	400[A]	LBV	CMC-C3C	2.00	1.54	1.50
2	A	400[B]	LBV	CMC-C3C	2.00	1.54	1.50

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	400[A]	LBV	CMD-C2D-C1D	4.14	129.19	124.16
2	A	400[B]	LBV	CMD-C2D-C1D	4.14	129.19	124.16
2	A	400[A]	LBV	CHC-C4B-N_B	3.95	134.21	125.29
2	A	400[B]	LBV	CHC-C4B-N_B	3.95	134.21	125.29
2	B	400	LBV	O_A-C1A-C2A	-3.80	122.72	126.74
2	A	400[A]	LBV	CHB-C1B-N_B	3.64	133.51	125.29
2	A	400[B]	LBV	CHB-C1B-N_B	3.64	133.51	125.29
2	B	400	LBV	CHD-C1D-C2D	-3.59	119.82	126.97
2	A	400[A]	LBV	CAC-C2C-C1C	3.58	131.30	125.02
2	A	400[B]	LBV	CAC-C2C-C1C	3.58	131.30	125.02
2	B	400	LBV	CHB-C1B-N_B	3.51	133.21	125.29
2	B	400	LBV	CHD-C1D-N_D	3.36	133.22	126.06
2	A	400[A]	LBV	C1C-N_C-C4C	3.30	112.56	106.52
2	A	400[B]	LBV	C1C-N_C-C4C	3.30	112.56	106.52
2	B	400	LBV	C1C-N_C-C4C	3.24	112.47	106.52
2	A	400[A]	LBV	CHC-C4B-C3B	-3.23	120.29	127.22
2	A	400[B]	LBV	CHC-C4B-C3B	-3.23	120.29	127.22
2	B	400	LBV	CHC-C4B-N_B	3.20	132.52	125.29
2	B	400	LBV	CHC-C4B-C3B	-3.18	120.39	127.22
2	A	400[A]	LBV	CAC-C2C-C3C	-3.08	122.10	127.87
2	A	400[B]	LBV	CAC-C2C-C3C	-3.08	122.10	127.87
2	A	400[A]	LBV	CMC-C3C-C4C	3.06	129.85	125.10
2	A	400[B]	LBV	CMC-C3C-C4C	3.06	129.85	125.10
2	B	400	LBV	CHB-C4A-N_A	3.03	132.53	126.06
2	A	400[A]	LBV	CHB-C1B-C2B	-3.03	120.11	127.53
2	A	400[B]	LBV	CHB-C1B-C2B	-3.03	120.11	127.53
2	B	400	LBV	CHC-C1C-N_C	2.81	130.50	124.60
2	B	400	LBV	CMD-C2D-C1D	2.73	127.48	124.16
2	B	400	LBV	CAB-C3B-C4B	2.57	129.85	125.77
2	B	400	LBV	C3D-C4D-N_D	2.55	109.33	106.13
2	B	400	LBV	CHB-C1B-C2B	-2.53	121.32	127.53
2	A	400[A]	LBV	C2C-C1C-N_C	-2.48	106.53	110.04
2	A	400[B]	LBV	C2C-C1C-N_C	-2.48	106.53	110.04
2	A	400[A]	LBV	CHD-C1D-C2D	-2.41	122.17	126.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	400[B]	LBV	CHD-C1D-C2D	-2.41	122.17	126.97
2	A	400[A]	LBV	CHC-C1C-N_C	2.32	129.46	124.60
2	A	400[B]	LBV	CHC-C1C-N_C	2.32	129.46	124.60
2	A	400[A]	LBV	O_A-C1A-C2A	-2.24	124.37	126.74
2	A	400[B]	LBV	O_A-C1A-C2A	-2.24	124.37	126.74
2	A	400[A]	LBV	O1B-CGB-CBB	-2.20	116.12	123.09
2	A	400[B]	LBV	O1B-CGB-CBB	-2.20	116.12	123.09
2	A	400[A]	LBV	C4B-N_B-C1B	2.08	113.44	109.78
2	A	400[B]	LBV	C4B-N_B-C1B	2.08	113.44	109.78
2	A	400[A]	LBV	C3C-C4C-N_C	-2.06	106.09	110.58
2	A	400[B]	LBV	C3C-C4C-N_C	-2.06	106.09	110.58
2	A	400[A]	LBV	CAA-C3A-C4A	-2.01	123.93	126.36
2	A	400[B]	LBV	CAA-C3A-C4A	-2.01	123.93	126.36
2	B	400	LBV	C3C-C4C-N_C	-2.01	106.20	110.58
2	B	400	LBV	CAB-CBB-CGB	-2.01	108.35	113.67

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	400[A]	LBV	C2A
2	A	400[B]	LBV	C2A
2	B	400	LBV	C2A

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	400[A]	LBV	N_C-C4C-CHD-C1D
2	A	400[B]	LBV	N_C-C4C-CHD-C1D
2	B	400	LBV	N_C-C4C-CHD-C1D
2	A	400[A]	LBV	C3C-C4C-CHD-C1D
2	A	400[B]	LBV	C3C-C4C-CHD-C1D
2	B	400	LBV	C3C-C4C-CHD-C1D
2	B	400	LBV	N_D-C1D-CHD-C4C
2	A	400[A]	LBV	N_D-C1D-CHD-C4C
2	A	400[B]	LBV	N_D-C1D-CHD-C4C
2	B	400	LBV	CAB-CBB-CGB-O1B
2	B	400	LBV	CAC-CBC-CGC-O2C
2	B	400	LBV	CAC-CBC-CGC-O1C
2	A	400[A]	LBV	CAB-CBB-CGB-O2B
2	A	400[B]	LBV	CAB-CBB-CGB-O2B
2	B	400	LBV	CAB-CBB-CGB-O2B
2	A	400[A]	LBV	CAB-CBB-CGB-O1B

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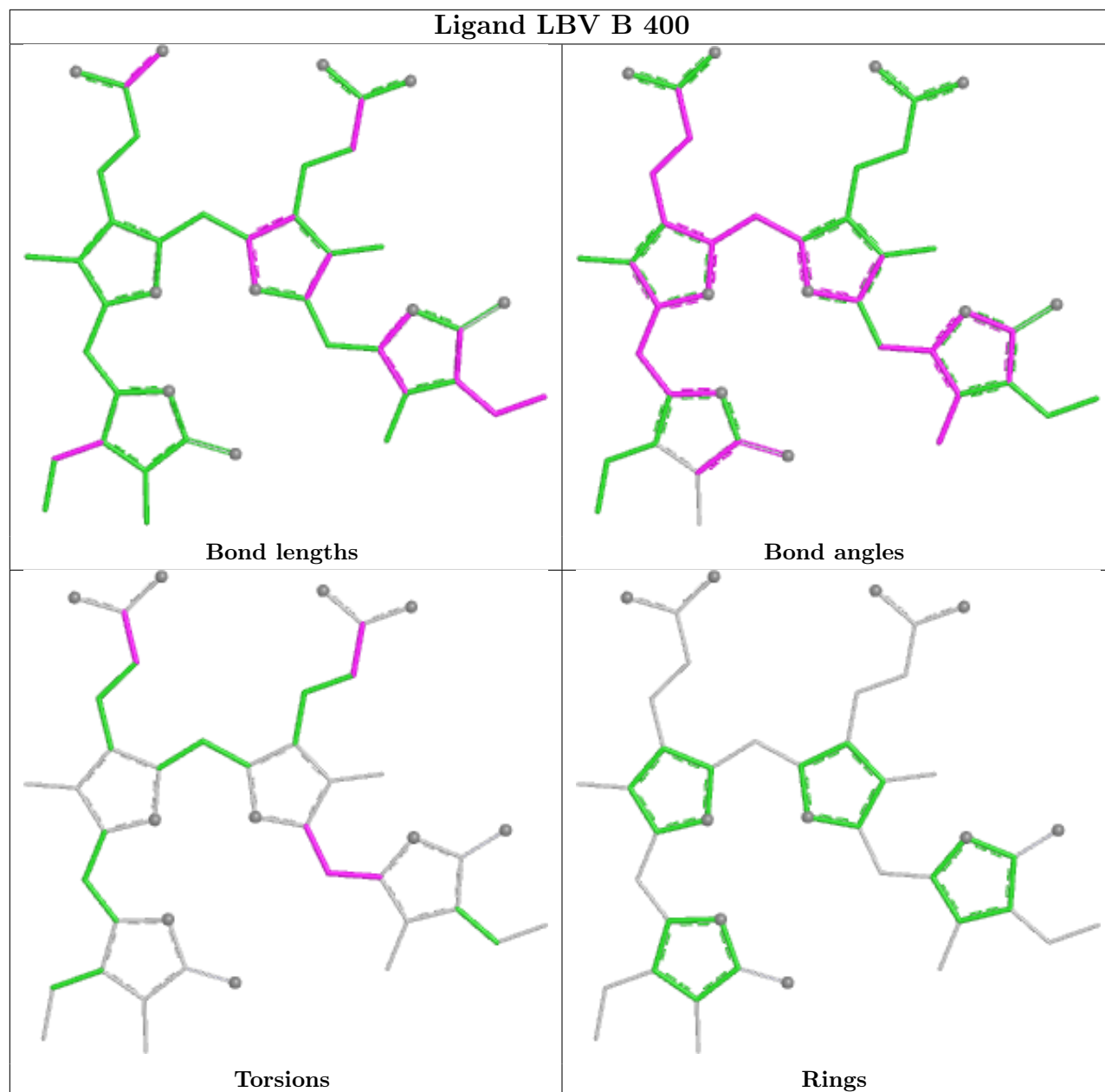
Mol	Chain	Res	Type	Atoms
2	A	400[B]	LBV	CAB-CBB-CGB-O1B
2	A	400[A]	LBV	CAC-CBC-CGC-O2C
2	A	400[B]	LBV	CAC-CBC-CGC-O2C
2	A	400[A]	LBV	CAC-CBC-CGC-O1C
2	A	400[B]	LBV	CAC-CBC-CGC-O1C
2	A	400[A]	LBV	C2D-C1D-CHD-C4C
2	A	400[B]	LBV	C2D-C1D-CHD-C4C
2	B	400	LBV	C2D-C1D-CHD-C4C

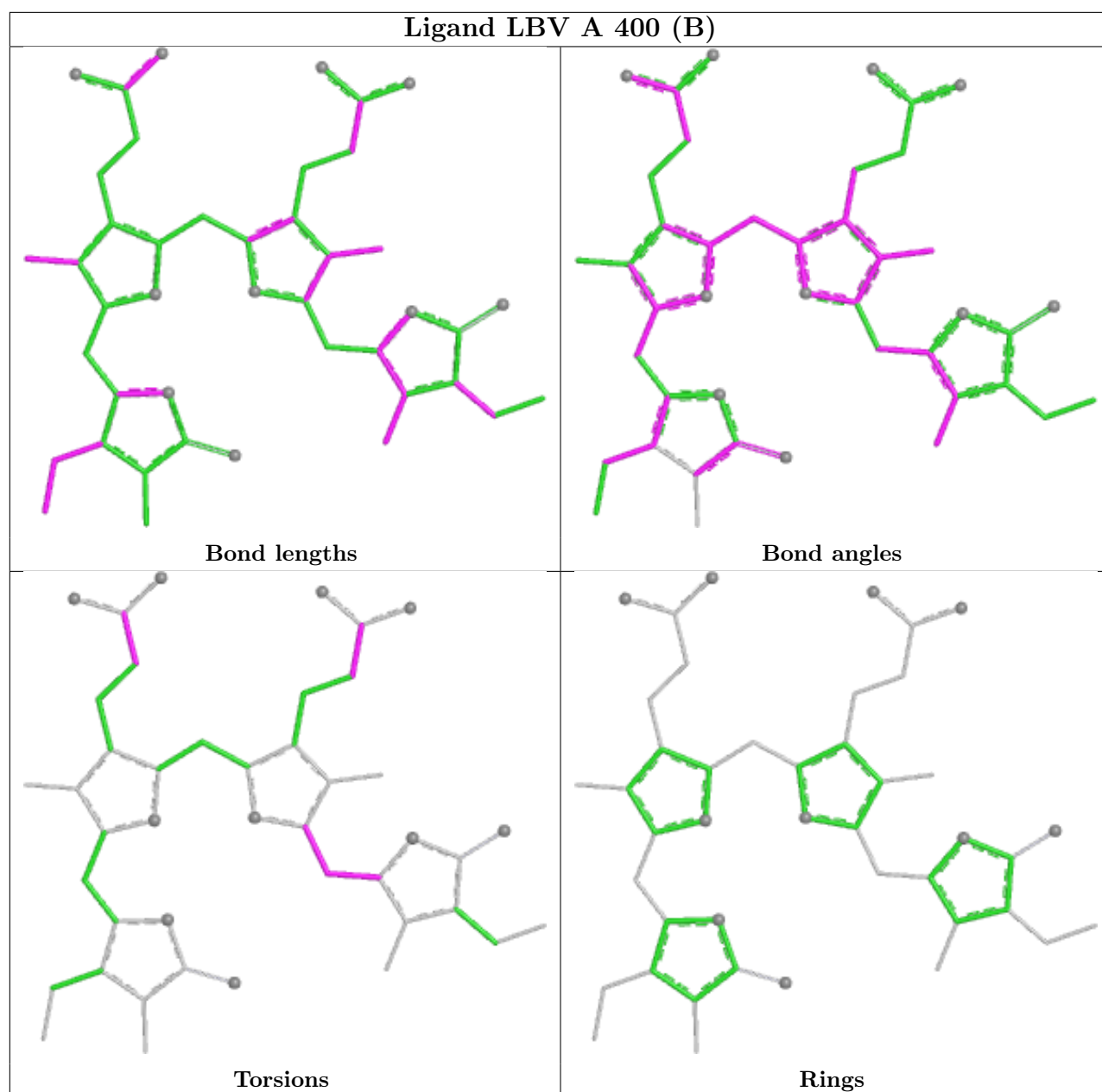
There are no ring outliers.

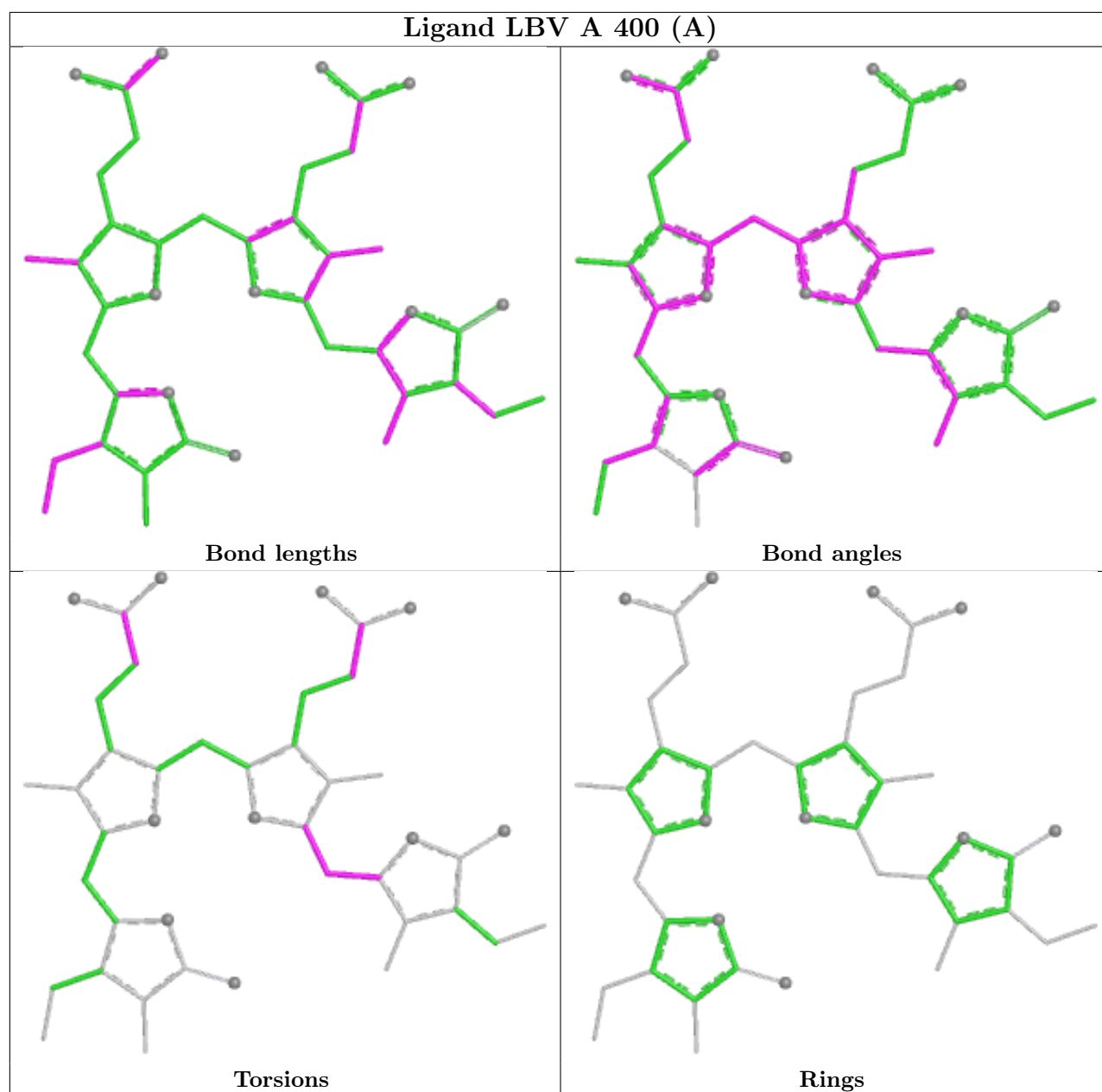
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	400	LBV	1	0
2	A	400[B]	LBV	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 [i](#)

6.1 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	304/337 (90%)	0.75	18 (5%) 28 25	22, 55, 69, 78	5 (1%)
1	B	298/337 (88%)	0.97	24 (8%) 18 15	25, 59, 71, 87	3 (1%)
All	All	602/674 (89%)	0.86	42 (6%) 22 19	22, 57, 71, 87	8 (1%)

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	332	GLU	3.6
1	B	331	ALA	3.4
1	A	26	THR	3.3
1	B	79	ALA	3.2
1	A	331	ALA	3.2
1	A	333	ILE	3.2
1	B	203	GLY	3.1
1	B	210	PHE	3.0
1	A	289	ASP	3.0
1	A	84	ALA	2.9
1	B	28	CYS	2.9
1	A	211[A]	HIS	2.7
1	B	167	TRP	2.7
1	A	141	TYR	2.7
1	B	51	THR	2.7
1	B	74	LEU	2.7
1	A	101	ALA	2.6
1	A	95	HIS	2.6
1	B	94	LEU	2.6
1	B	81	TYR	2.6
1	B	101	ALA	2.5
1	B	57	SER	2.4
1	A	202	SER	2.4
1	B	77	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	250	ARG	2.3
1	B	95	HIS	2.3
1	A	96	GLY	2.2
1	B	96	GLY	2.2
1	A	51	THR	2.2
1	A	102	ILE	2.2
1	B	78	ILE	2.2
1	A	53	LEU	2.2
1	B	145	PHE	2.2
1	A	139	SER	2.2
1	B	159	ALA	2.2
1	B	143	ASN	2.1
1	B	161	ASP	2.1
1	A	127	SER	2.1
1	A	106	ARG	2.1
1	B	85	ALA	2.1
1	B	158	THR	2.1
1	B	249	PRO	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.

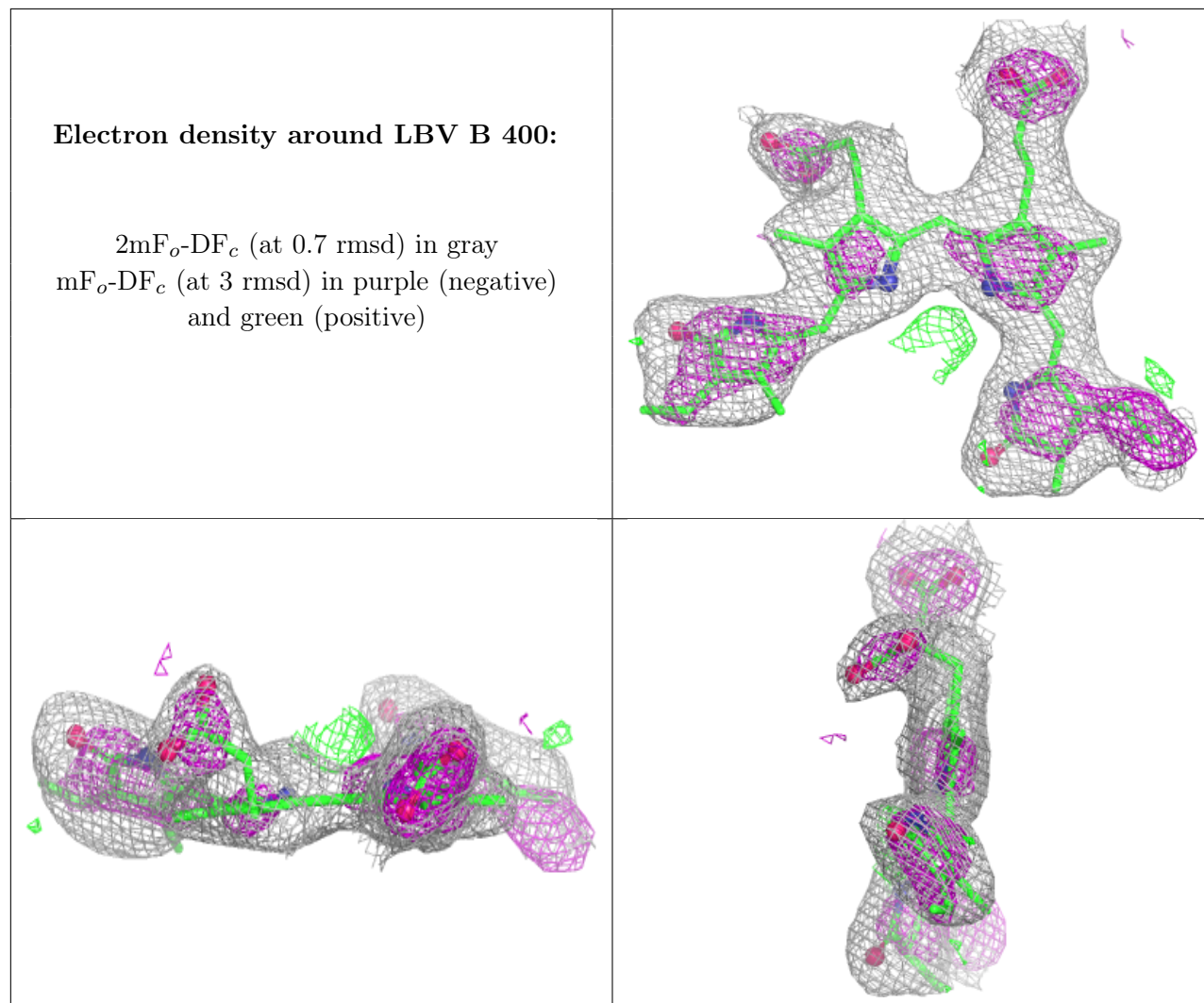
6.4 Ligands [i](#)

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(Å ²)	Q<0.9
2	LBV	B	400	43/43	0.87	0.18	61,75,81,82	0
2	LBV	A	400[B]	43/43	0.91	0.14	32,44,55,58	1
2	LBV	A	400[A]	43/43	0.91	0.14	32,44,55,58	1

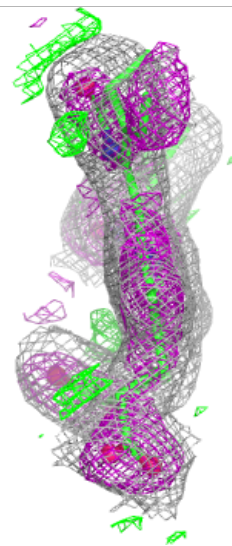
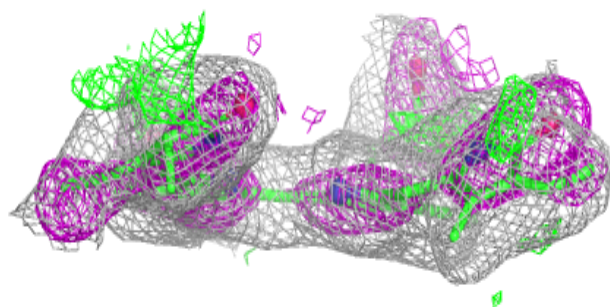
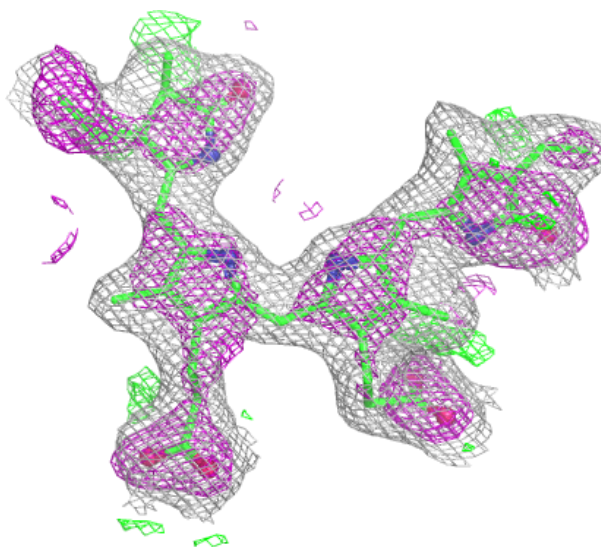
The following is a graphical depiction of the model fit to experimental electron density of all

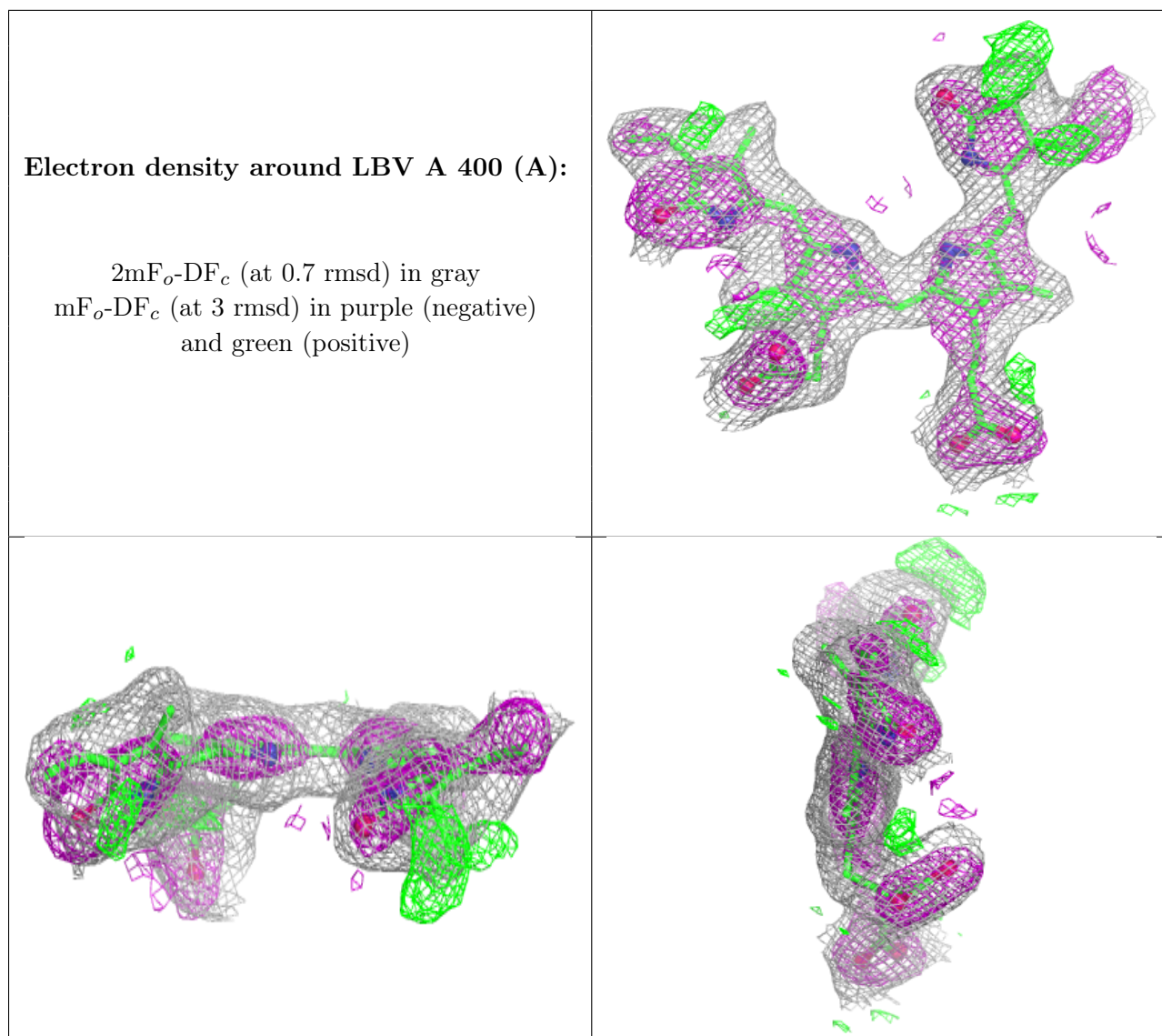
instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



Electron density around LBV A 400 (B):

$2mF_o-DF_c$ (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.