WORLDWIDE PDB
PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 7, 2024 – 12:02 am GMT

PDB ID	:	6FTD
Title	:	Deinococcus radiodurans BphP PAS-GAF H290T mutant
Authors	:	Edlund, P.; Takala, H.; Westenhoff, S.; Ihalainen, J.A.
Deposited on	:	2018-02-21
Resolution	:	1.40 Å(reported)

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.40 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.
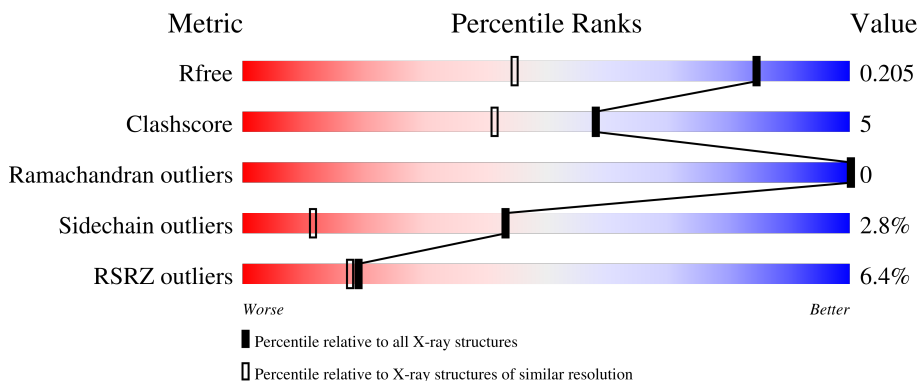
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1714 (1.40-1.40)
Clashscore	141614	1812 (1.40-1.40)
Ramachandran outliers	138981	1763 (1.40-1.40)
Sidechain outliers	138945	1762 (1.40-1.40)
RSRZ outliers	127900	1674 (1.40-1.40)

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 <=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	343	6% · 78% · 12% · 8%
1	B	343	6% · 76% · 13% · 8%

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	ACT	B	403	-	-	X	-

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 5741 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 Bacteriophytochrome.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	314	Total	C	N	O	S	0	19	0
			2526	1611	442	463	10			
1	B	314	Total	C	N	O	S	0	17	0
			2516	1608	436	461	11			

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	initiating methionine	UNP Q9RZA4
A	-12	ALA	-	expression tag	UNP Q9RZA4
A	-11	SER	-	expression tag	UNP Q9RZA4
A	-10	MET	-	expression tag	UNP Q9RZA4
A	-9	THR	-	expression tag	UNP Q9RZA4
A	-8	GLY	-	expression tag	UNP Q9RZA4
A	-7	GLY	-	expression tag	UNP Q9RZA4
A	-6	GLN	-	expression tag	UNP Q9RZA4
A	-5	GLN	-	expression tag	UNP Q9RZA4
A	-4	MET	-	expression tag	UNP Q9RZA4
A	-3	GLY	-	expression tag	UNP Q9RZA4
A	-2	ARG	-	expression tag	UNP Q9RZA4
A	-1	GLY	-	expression tag	UNP Q9RZA4
A	0	SER	-	expression tag	UNP Q9RZA4
A	290	THR	HIS	engineered mutation	UNP Q9RZA4
A	322	LEU	-	expression tag	UNP Q9RZA4
A	323	GLU	-	expression tag	UNP Q9RZA4
A	324	HIS	-	expression tag	UNP Q9RZA4
A	325	HIS	-	expression tag	UNP Q9RZA4
A	326	HIS	-	expression tag	UNP Q9RZA4
A	327	HIS	-	expression tag	UNP Q9RZA4
A	328	HIS	-	expression tag	UNP Q9RZA4
A	329	HIS	-	expression tag	UNP Q9RZA4
B	-13	MET	-	initiating methionine	UNP Q9RZA4
B	-12	ALA	-	expression tag	UNP Q9RZA4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-11	SER	-	expression tag	UNP Q9RZA4
B	-10	MET	-	expression tag	UNP Q9RZA4
B	-9	THR	-	expression tag	UNP Q9RZA4
B	-8	GLY	-	expression tag	UNP Q9RZA4
B	-7	GLY	-	expression tag	UNP Q9RZA4
B	-6	GLN	-	expression tag	UNP Q9RZA4
B	-5	GLN	-	expression tag	UNP Q9RZA4
B	-4	MET	-	expression tag	UNP Q9RZA4
B	-3	GLY	-	expression tag	UNP Q9RZA4
B	-2	ARG	-	expression tag	UNP Q9RZA4
B	-1	GLY	-	expression tag	UNP Q9RZA4
B	0	SER	-	expression tag	UNP Q9RZA4
B	290	THR	HIS	engineered mutation	UNP Q9RZA4
B	322	LEU	-	expression tag	UNP Q9RZA4
B	323	GLU	-	expression tag	UNP Q9RZA4
B	324	HIS	-	expression tag	UNP Q9RZA4
B	325	HIS	-	expression tag	UNP Q9RZA4
B	326	HIS	-	expression tag	UNP Q9RZA4
B	327	HIS	-	expression tag	UNP Q9RZA4
B	328	HIS	-	expression tag	UNP Q9RZA4
B	329	HIS	-	expression tag	UNP Q9RZA4

- Molecule 2 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).
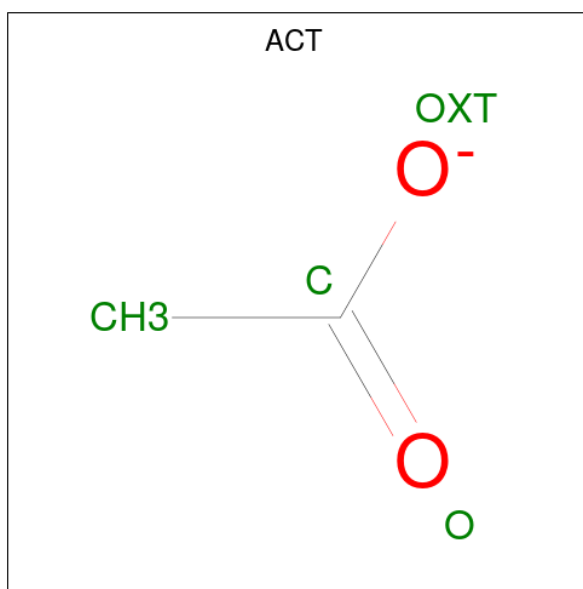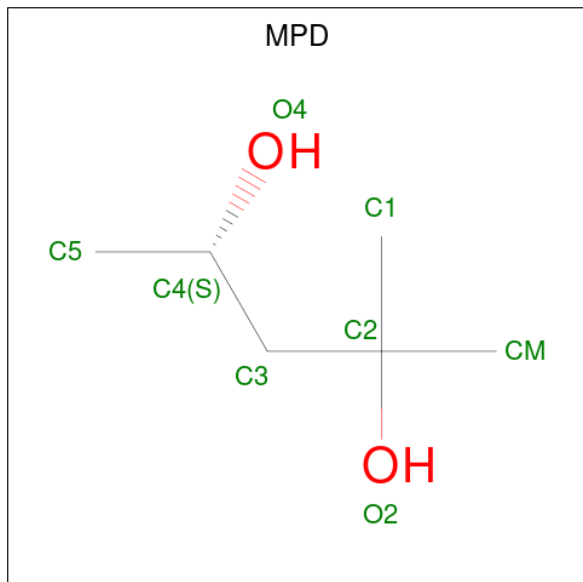

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 4	C 2	O 2	0	0
2	A	1	Total 4	C 2	O 2	0	0
2	B	1	Total 4	C 2	O 2	0	0
2	B	1	Total 4	C 2	O 2	0	0
2	B	1	Total 4	C 2	O 2	0	0

- Molecule 3 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 8	C 6	O 2	0	0
3	B	1	Total 8	C 6	O 2	0	0

- Molecule 4 is 3-[2-[(Z)-[3-(2-carboxyethyl)-5-[(Z)-(4-ethenyl-3-methyl-5-oxidanylidene-pyrrol-2-ylidene)methyl]-4-methyl-pyrrol-1-ium -2-ylidene]methyl]-5-[(Z)-[(3E)-3-ethylidene-4-methyl-5-oxidanylidene-pyrrolidin-2-ylidene]methyl]-4-methyl-1H-pyrrol-3- yl]propanoic acid (three-letter code: LBV) (formula: $C_{33}H_{37}N_4O_6$).

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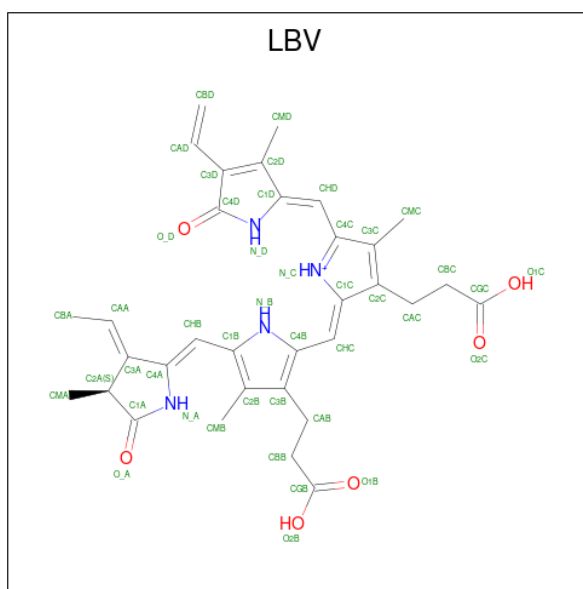
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total 43	C 33	N 4	O 6	0	0
4	B	1	Total 43	C 33	N 4	O 6	0	0

• Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	274	Total 274	O 274	0	0
5	B	299	Total 299	O 299	0	0

3 Residue-property plots ⓘ

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: Bacteriophytochrome
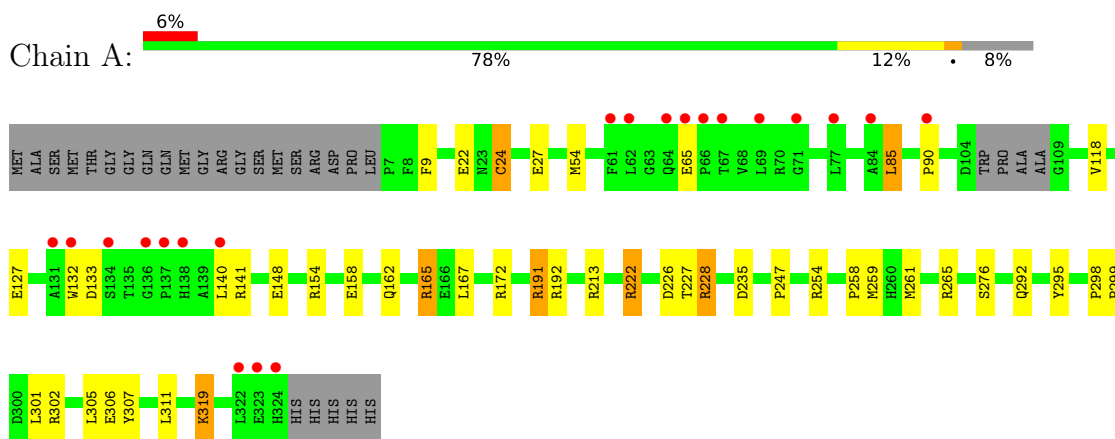
• Molecule 1: Bacteriophytochrome
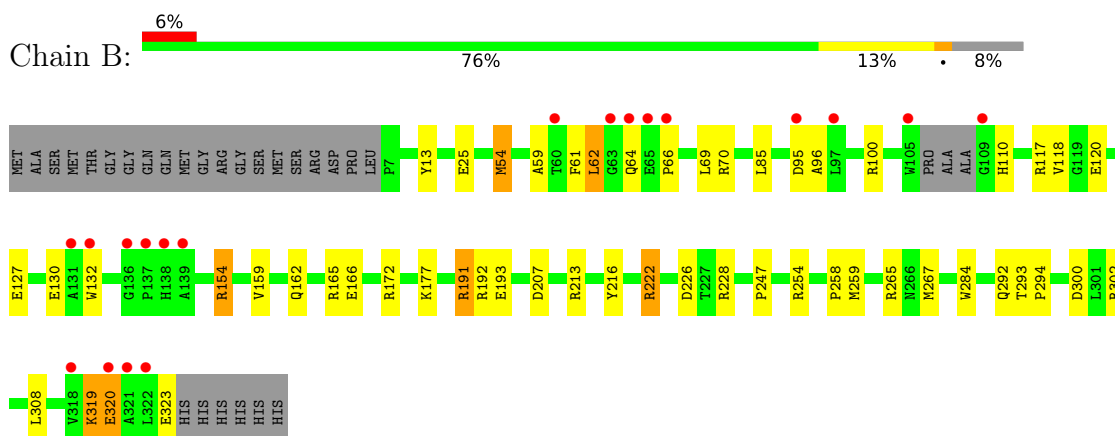
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	94.81Å 53.03Å 135.88Å 90.00° 93.30° 90.00°	Depositor
Resolution (Å)	47.33 – 1.40 47.33 – 1.40	Depositor EDS
% Data completeness (in resolution range)	99.8 (47.33-1.40) 99.7 (47.33-1.40)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.09 (at 1.40Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.148 , 0.198 0.157 , 0.205	Depositor DCC
R_{free} test set	6620 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å²)	16.6	Xtriage
Anisotropy	0.184	Xtriage
Bulk solvent k_{sol}(e/Å³), B_{sol}(Å²)	0.33 , 51.2	EDS
L-test for twinning [2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	5741	wwPDB-VP
Average B, all atoms (Å²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 32.73 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 8.9659e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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, MPD, ACT

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	1.36	11/2603 (0.4%)	1.40	23/3560 (0.6%)
1	B	1.36	8/2594 (0.3%)	1.38	28/3548 (0.8%)
All	All	1.36	19/5197 (0.4%)	1.39	51/7108 (0.7%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	2
All	All	0	4

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	24	CYS	CB-SG	-8.25	1.68	1.82
1	B	132	TRP	CE3-CZ3	6.43	1.49	1.38
1	A	295	TYR	CD2-CE2	-6.34	1.29	1.39
1	B	13	TYR	CG-CD1	-6.08	1.31	1.39
1	B	120[A]	GLU	CD-OE1	6.04	1.32	1.25

The worst 5 of 51 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	213	ARG	NE-CZ-NH1	19.10	129.85	120.30
1	A	302	ARG	NE-CZ-NH2	-13.54	113.53	120.30
1	A	228[A]	ARG	NE-CZ-NH2	-12.43	114.09	120.30
1	A	228[B]	ARG	NE-CZ-NH2	-12.43	114.09	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	213	ARG	NE-CZ-NH2	-11.02	114.79	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	165	ARG	Sidechain
1	A	191	ARG	Sidechain
1	B	165	ARG	Sidechain
1	B	191	ARG	Sidechain

5.2 Too-close contacts ⓘ

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	2526	0	2545	20	0
1	B	2516	0	2531	29	0
2	A	12	0	9	1	0
2	B	12	0	9	2	0
3	A	8	0	14	0	0
3	B	8	0	14	0	0
4	A	43	0	33	2	0
4	B	43	0	34	0	0
5	A	274	0	0	7	0
5	B	299	0	0	8	0
All	All	5741	0	5189	50	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 50 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:162[A]:GLN:HE21	1:B:166[A]:GLU:HG3	1.32	0.94
1:B:54[B]:MET:HE1	1:B:69:LEU:HB2	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167[B]:LEU:HD23	1:A:305[B]:LEU:HD21	1.71	0.71
1:A:167[B]:LEU:HD23	1:A:305[B]:LEU:CD2	2.21	0.71
1:B:293[A]:THR:HG23	1:B:294:PRO:HD2	1.74	0.70

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	329/343 (96%)	324 (98%)	5 (2%)	0	100	100
1	B	327/343 (95%)	324 (99%)	3 (1%)	0	100	100
All	All	656/686 (96%)	648 (99%)	8 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	272/275 (99%)	265 (97%)	7 (3%)	46	13
1	B	270/275 (98%)	262 (97%)	8 (3%)	41	10
All	All	542/550 (98%)	527 (97%)	15 (3%)	43	11

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	54[A]	MET
1	B	222	ARG
1	B	54[B]	MET
1	B	319	LYS
1	B	110	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	86	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

10 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	ACT	B	402	-	3,3,3	1.39	1 (33%)	3,3,3	0.73	0
3	MPD	A	404	-	7,7,7	0.64	0	9,10,10	1.87	2 (22%)
2	ACT	A	402	-	3,3,3	0.94	0	3,3,3	1.24	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
4	LBV	A	405	1	42,46,46	2.25	16 (38%)	47,67,67	1.86	14 (29%)
2	ACT	A	403	-	3,3,3	0.99	0	3,3,3	1.94	2 (66%)
3	MPD	B	404	-	7,7,7	0.72	0	9,10,10	1.24	1 (11%)
2	ACT	B	401	-	3,3,3	0.74	0	3,3,3	0.90	0
2	ACT	A	401	-	3,3,3	0.55	0	3,3,3	1.50	0
4	LBV	B	405	1	42,46,46	2.55	13 (30%)	47,67,67	2.02	16 (34%)
2	ACT	B	403	-	3,3,3	0.89	0	3,3,3	1.09	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	LBV	A	405	1	-	6/26/74/74	0/4/4/4
3	MPD	A	404	-	-	1/5/5/5	-
3	MPD	B	404	-	-	3/5/5/5	-
4	LBV	B	405	1	-	7/26/74/74	0/4/4/4

The worst 5 of 30 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	405	LBV	CHC-C1C	10.90	1.44	1.35
4	A	405	LBV	CHC-C1C	7.35	1.41	1.35
4	B	405	LBV	C2A-C3A	-5.44	1.44	1.51
4	B	405	LBV	C2C-C3C	4.83	1.47	1.36
4	A	405	LBV	C2A-C3A	-4.02	1.46	1.51

The worst 5 of 35 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	405	LBV	O-A-C1A-N-A	-4.50	119.49	124.94
4	B	405	LBV	C2D-C1D-N-D	4.12	113.02	106.99
4	B	405	LBV	CAA-C3A-C4A	-4.08	121.44	126.36
4	A	405	LBV	CMD-C2D-C1D	4.06	129.24	124.17
4	B	405	LBV	CMC-C3C-C4C	3.96	131.16	125.06

There are no chirality outliers.
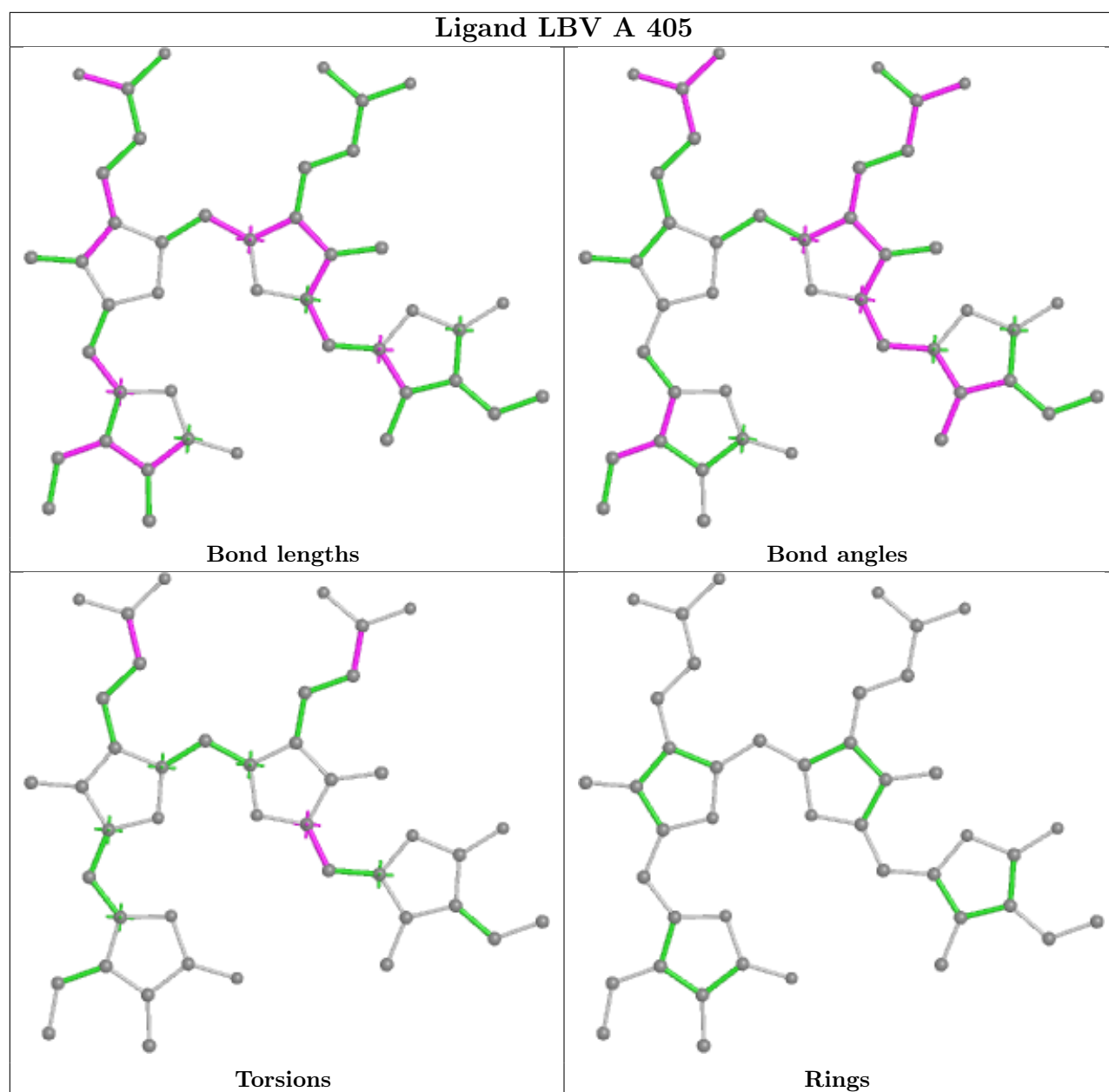
5 of 17 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	404	MPD	O2-C2-C3-C4
3	B	404	MPD	CM-C2-C3-C4
4	A	405	LBV	C3C-C4C-CHD-C1D
4	A	405	LBV	C-N-C4C-CHD-C1D
4	B	405	LBV	C3C-C4C-CHD-C1D

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	405	LBV	2	0
2	A	403	ACT	1	0
2	B	403	ACT	2	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 then 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 A 405

Bond lengths

Bond angles

Torsions

Rings

Ligand LBV B 405

Bond lengths

Bond angles

Torsions

Rings
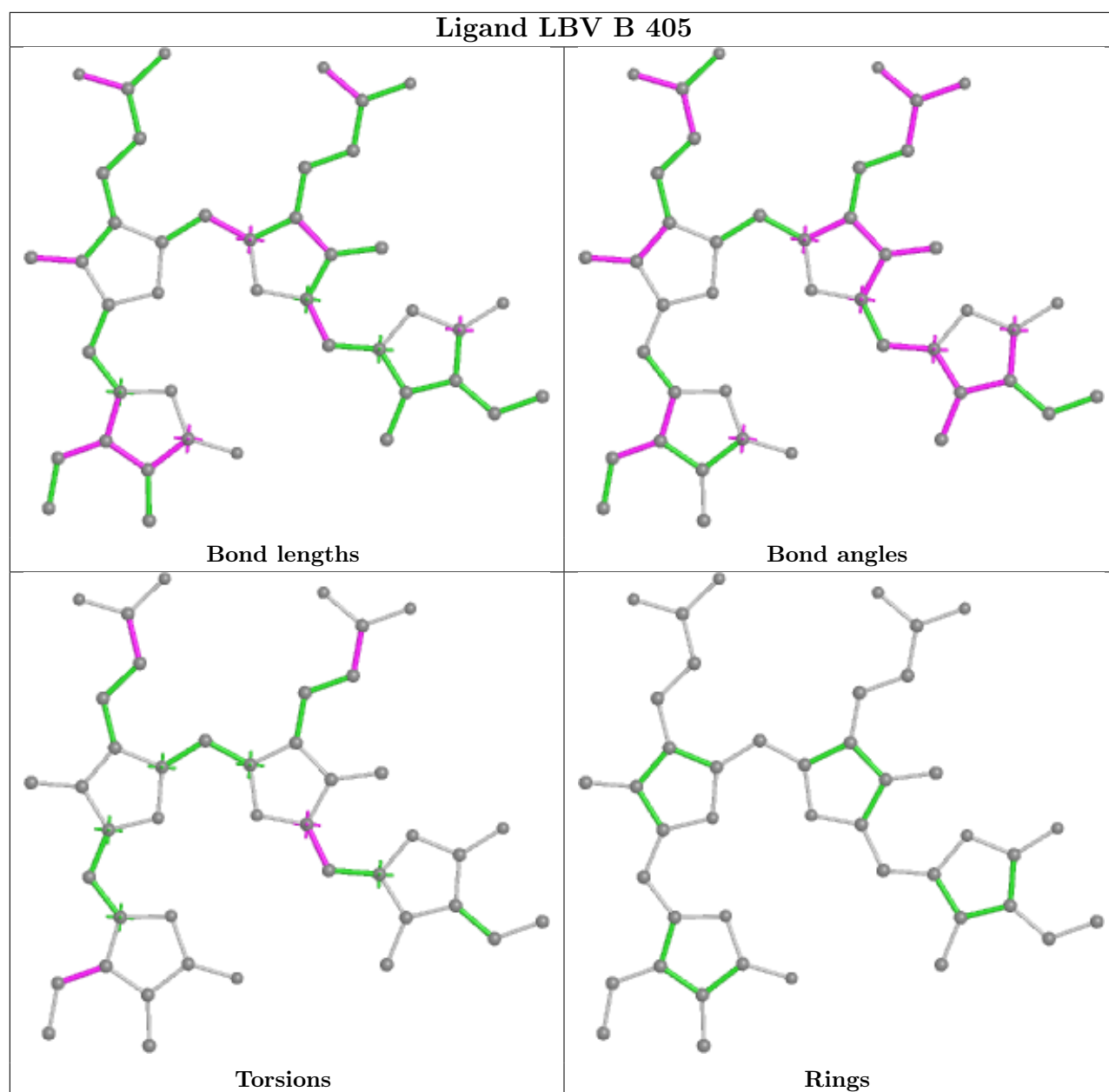
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	314/343 (91%)	0.10	21 (6%)	17	16	11, 20, 57, 105	0
1	B	314/343 (91%)	0.14	19 (6%)	21	19	10, 17, 55, 88	0
All	All	628/686 (91%)	0.12	40 (6%)	19	18	10, 18, 55, 105	0

The worst 5 of 40 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	132	TRP	16.2
1	B	105	TRP	10.2
1	A	132	TRP	9.7
1	B	322	LEU	7.9
1	B	318	VAL	6.6

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

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

6.3 Carbohydrates ⓘ
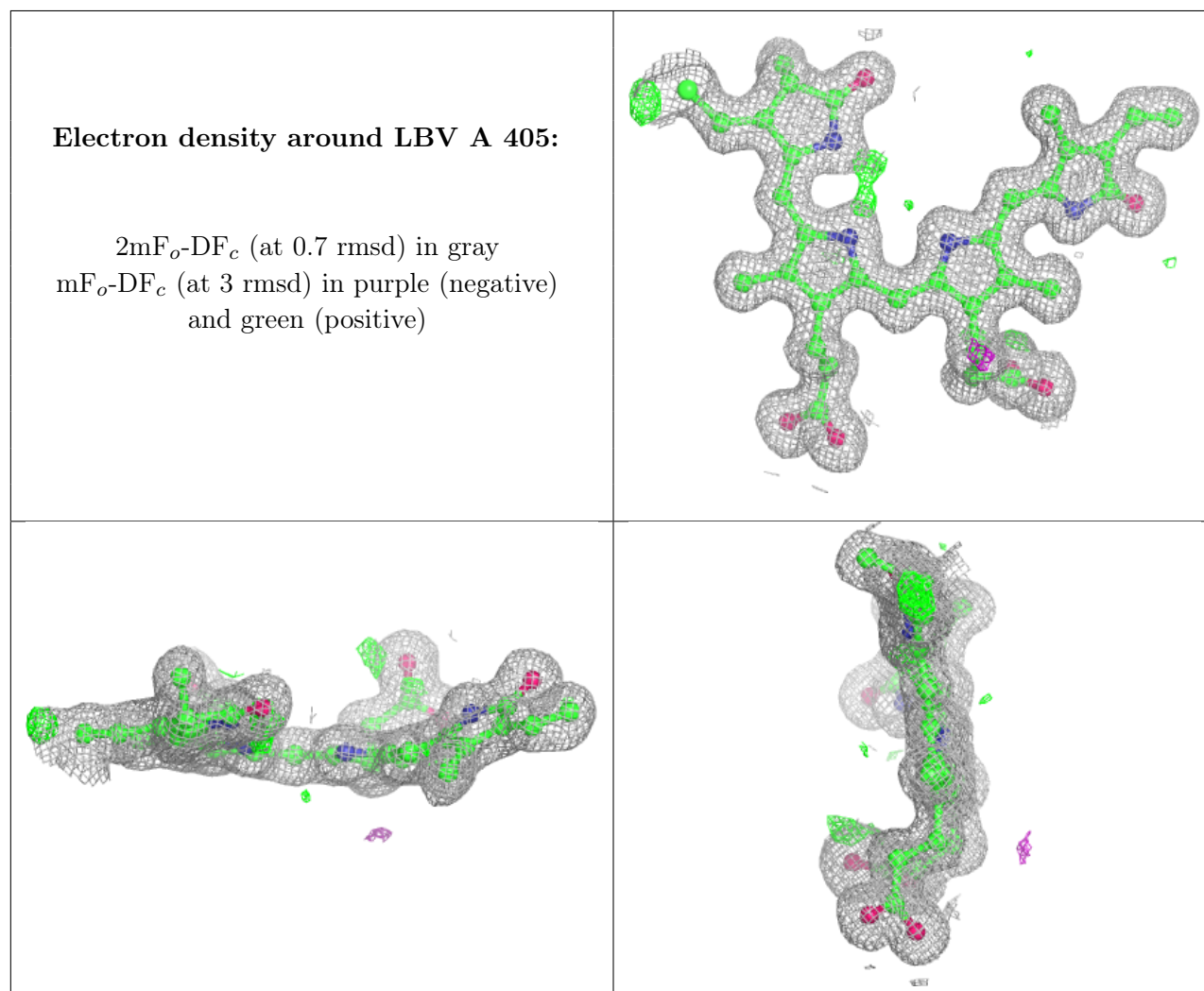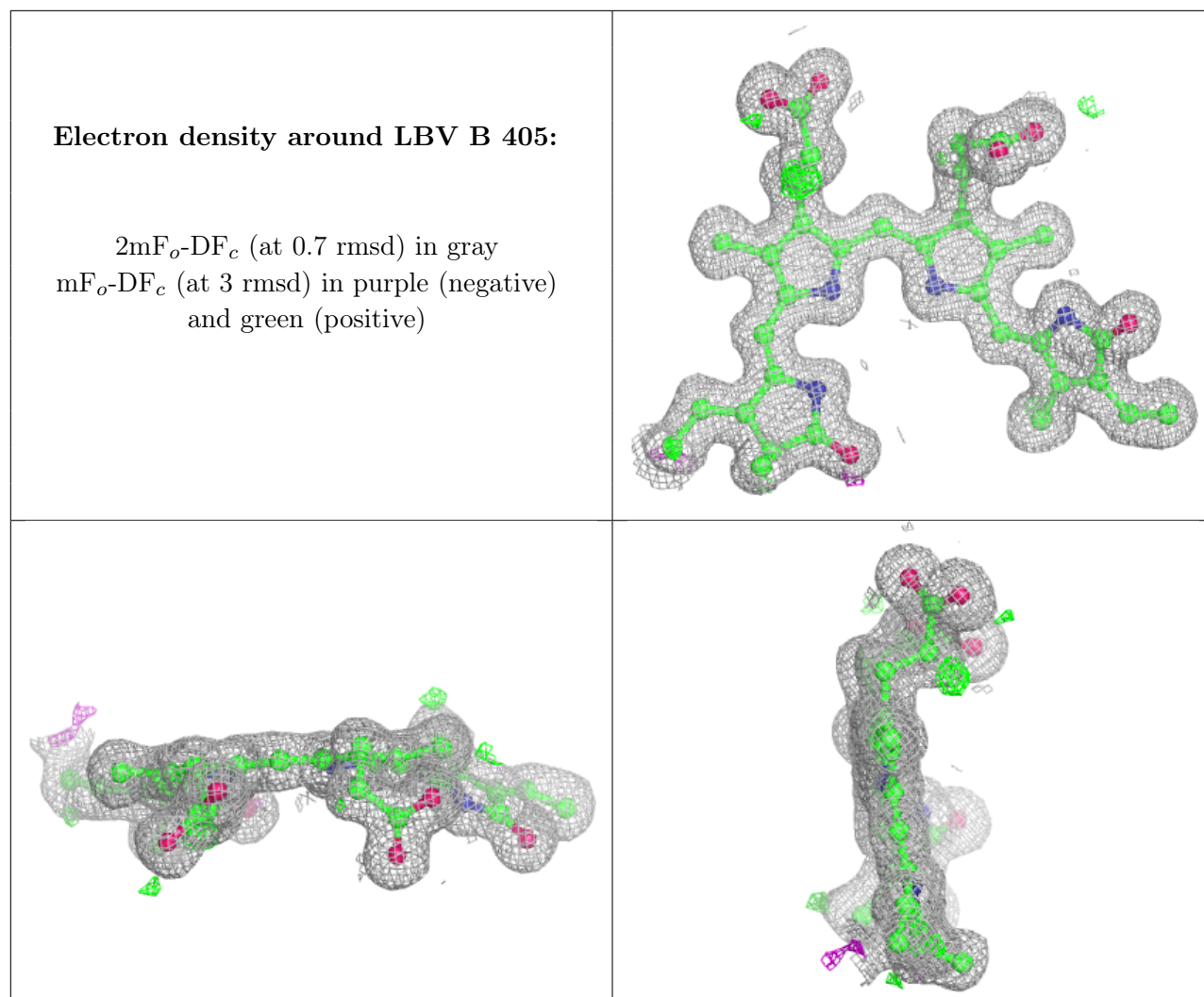
There are no monosaccharides in this entry.

6.4 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	ACT	A	401	4/4	0.84	0.16	41,44,45,54	0
2	ACT	B	403	4/4	0.88	0.10	25,26,26,30	0
2	ACT	A	402	4/4	0.90	0.08	28,45,49,49	0
2	ACT	B	401	4/4	0.91	0.12	61,63,64,75	0
3	MPD	A	404	8/8	0.91	0.12	22,25,31,32	8
3	MPD	B	404	8/8	0.93	0.10	17,24,28,31	8
2	ACT	A	403	4/4	0.94	0.10	31,36,43,49	0
2	ACT	B	402	4/4	0.96	0.06	27,36,39,60	0
4	LBV	A	405	43/43	0.96	0.08	9,11,19,31	0
4	LBV	B	405	43/43	0.97	0.08	8,10,18,24	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 405:

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

Electron density around LBV B 405:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray

$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

6.5 Other polymers ⓘ

There are no such residues in this entry.