



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 10:52 pm BST

PDB ID : 6GGI  
Title : Crystal structure of CotB2 in complex with 2-fluoro-3,7,18-dolabellatriene  
Authors : Driller, R.; Janke, S.; Fuchs, M.; Warner, E.; Mhashal, A.R.; Major, D.T.; Christmann, M.; Brueck, T.; Loll, B.  
Deposited on : 2018-05-03  
Resolution : 1.80 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
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) : 2.11

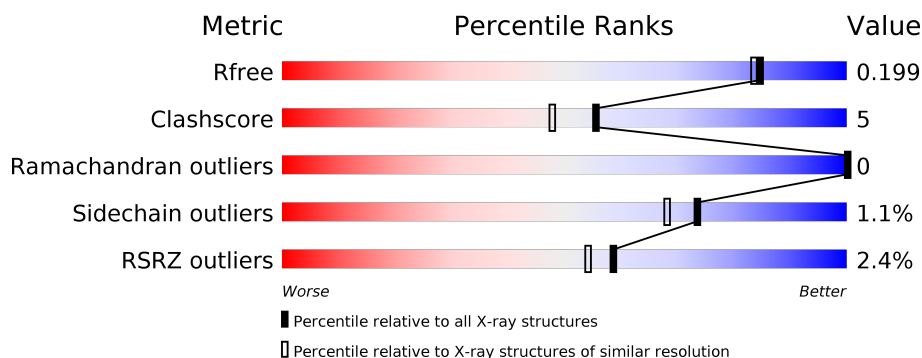
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	318	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, green 84%, yellow 9%, grey 8%);"></div> <div style="display: flex; justify-content: space-between; padding: 0 5px;"> <span>%</span> <span>84%</span> <span>9%</span> <span>8%</span> </div> </div>
1	B	318	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 3%, green 86%, yellow 7%, grey 6%);"></div> <div style="display: flex; justify-content: space-between; padding: 0 5px;"> <span>3%</span> <span>86%</span> <span>7%</span> <span>6%</span> </div> </div>

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
5	MPD	A	408	-	-	X	-
5	MPD	B	407	-	-	X	-
7	CCN	A	411	-	-	X	-

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 5313 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 Cyclooctat-9-en-7-ol synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	294	Total	C	N	O	S	0	6	0
			2439	1551	411	460	17			
1	B	300	Total	C	N	O	S	0	8	0
			2484	1579	420	468	17			

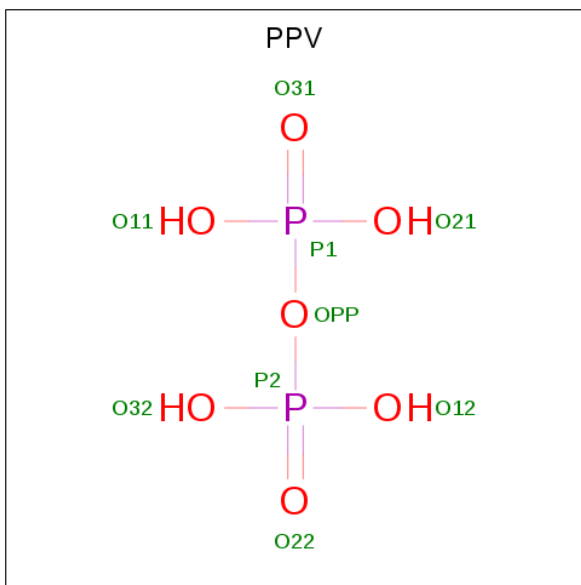
There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	308	ALA	-	expression tag	UNP C9K1X5
A	309	ALA	-	expression tag	UNP C9K1X5
A	310	ALA	-	expression tag	UNP C9K1X5
A	311	LEU	-	expression tag	UNP C9K1X5
A	312	GLU	-	expression tag	UNP C9K1X5
A	313	HIS	-	expression tag	UNP C9K1X5
A	314	HIS	-	expression tag	UNP C9K1X5
A	315	HIS	-	expression tag	UNP C9K1X5
A	316	HIS	-	expression tag	UNP C9K1X5
A	317	HIS	-	expression tag	UNP C9K1X5
A	318	HIS	-	expression tag	UNP C9K1X5
B	308	ALA	-	expression tag	UNP C9K1X5
B	309	ALA	-	expression tag	UNP C9K1X5
B	310	ALA	-	expression tag	UNP C9K1X5
B	311	LEU	-	expression tag	UNP C9K1X5
B	312	GLU	-	expression tag	UNP C9K1X5
B	313	HIS	-	expression tag	UNP C9K1X5
B	314	HIS	-	expression tag	UNP C9K1X5
B	315	HIS	-	expression tag	UNP C9K1X5
B	316	HIS	-	expression tag	UNP C9K1X5
B	317	HIS	-	expression tag	UNP C9K1X5
B	318	HIS	-	expression tag	UNP C9K1X5

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

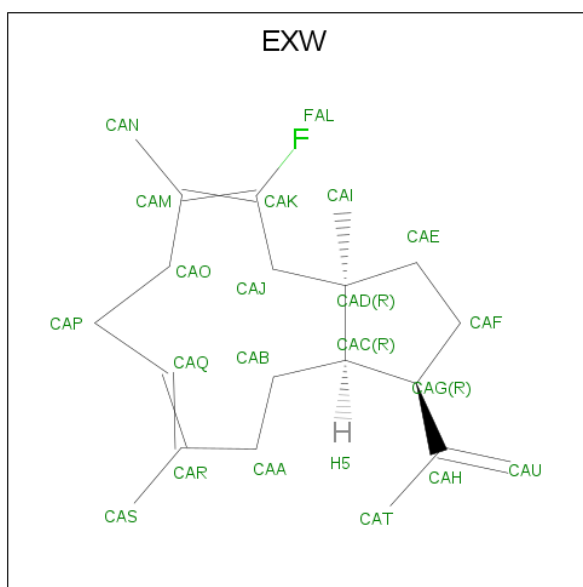
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	4	Total Mg 4 4	0	0
2	A	5	Total Mg 5 5	0	0

- Molecule 3 is PYROPHOSPHATE (three-letter code: PPV) (formula:  $\text{H}_4\text{O}_7\text{P}_2$ ).



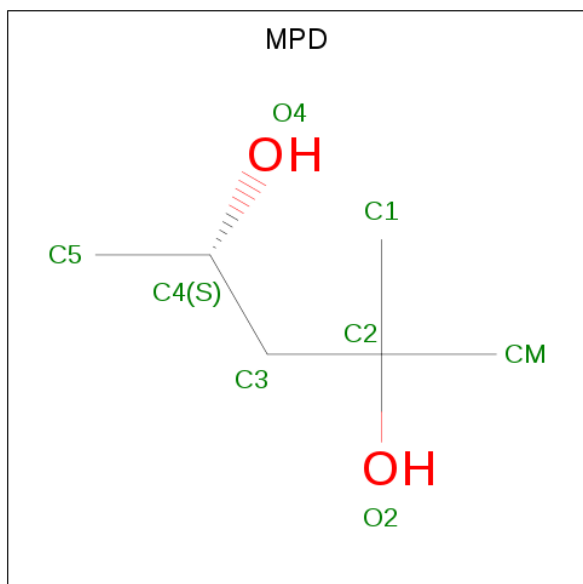
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O P 9 7 2	0	0
3	B	1	Total O P 9 7 2	0	0

- Molecule 4 is 2-fluoro-3,7,18-dolabellatriene (three-letter code: EXW) (formula:  $\text{C}_{20}\text{H}_{31}\text{F}$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	F	0	0
			21	20	1		
4	B	1	Total	C	F	0	0
			21	20	1		

- Molecule 5 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula:  $C_6H_{14}O_2$ ).



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

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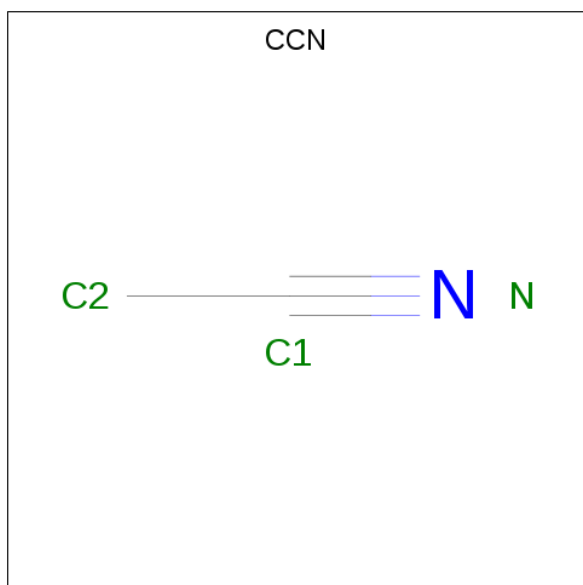
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			8	6	2		

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Cl	0	0
			1	1		
6	A	2	Total	Cl	0	0
			2	2		

- Molecule 7 is ACETONITRILE (three-letter code: CCN) (formula: C<sub>2</sub>H<sub>3</sub>N).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	N	0	0
			3	2	1		

- Molecule 8 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			7	4	3		
8	B	1	Total	C	O	0	0
			7	4	3		

- Molecule 9 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	B	1	Total	K	0	0
			1	1		
9	A	1	Total	K	0	0
			1	1		

- Molecule 10 is water.

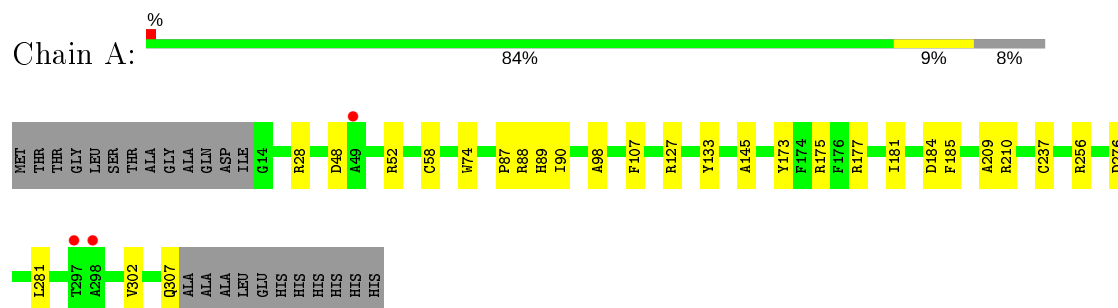
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	143	Total	O	0	3
			143	143		
10	B	140	Total	O	0	3
			140	140		



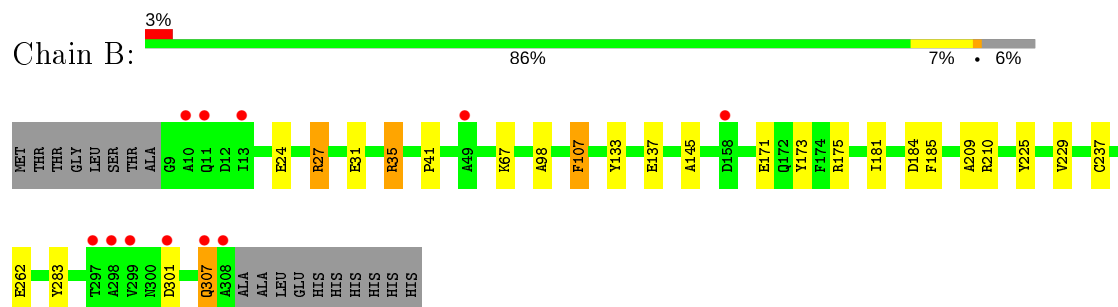
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: Cyclooctat-9-en-7-ol synthase



- Molecule 1: Cyclooctat-9-en-7-ol synthase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	62.88Å 98.72Å 105.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.74 – 1.80 47.42 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.5 (44.74-1.80) 92.2 (47.42-1.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.40 (at 1.81Å)	Xtriage
Refinement program	PHENIX (1.11.1 _2575: ???)	Depositor
R, $R_{free}$	0.170 , 0.200 0.169 , 0.199	Depositor DCC
$R_{free}$ test set	2100 reflections (3.43%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	19.0	Xtriage
Anisotropy	0.730	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 65.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	5313	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	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 65.02 % 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 7.5640e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: MPD, CL, K, MG, EXW, CCN, PPV, PEG

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	0.56	0/2515	0.65	2/3408 (0.1%)
1	B	0.56	0/2566	0.64	1/3480 (0.0%)
All	All	0.56	0/5081	0.65	3/6888 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	28	ARG	NE-CZ-NH2	-6.21	117.19	120.30
1	B	27	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	A	28	ARG	NE-CZ-NH1	5.18	122.89	120.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2439	0	2362	19	0
1	B	2484	0	2415	24	0
2	A	5	0	0	0	0
2	B	4	0	0	0	0
3	A	9	0	0	0	0
3	B	9	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	21	0	0	5	0
4	B	21	0	0	6	0
5	A	8	0	14	6	0
5	B	8	0	14	9	0
6	A	2	0	0	0	0
6	B	1	0	0	1	0
7	A	3	0	3	2	0
8	A	7	0	10	0	0
8	B	7	0	10	0	0
9	A	1	0	0	0	0
9	B	1	0	0	0	0
10	A	143	0	0	3	0
10	B	140	0	0	2	0
All	All	5313	0	4828	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.

All (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)
5:A:408:MPD:HM2	5:B:407:MPD:H11	1.44	0.97
5:A:408:MPD:H11	5:B:407:MPD:HM2	1.45	0.96
1:B:175:ARG:HE	5:B:407:MPD:H12	1.49	0.76
1:A:175:ARG:HE	5:A:408:MPD:H12	1.49	0.74
1:A:256:ARG:HH12	7:A:411:CCN:H22	1.54	0.72
1:A:48:ASP:O	1:A:52:ARG:HG2	1.92	0.69
1:A:276:ASP:OD1	10:A:501[B]:HOH:O	2.14	0.65
1:B:175:ARG:HH21	5:B:407:MPD:H52	1.63	0.64
1:B:175:ARG:HH21	5:B:407:MPD:C5	2.10	0.63
1:B:24:GLU:HG3	1:B:27:ARG:NH2	2.14	0.62
5:A:408:MPD:C1	5:B:407:MPD:HM2	2.28	0.58
1:B:262:GLU:OE1	10:B:501:HOH:O	2.16	0.58
4:A:407:EXW:CAM	4:A:407:EXW:CAB	2.84	0.56
1:A:88[B]:ARG:HD3	1:A:89:HIS:CE1	2.42	0.55
1:A:281:LEU:HD11	4:A:407:EXW:CAT	2.37	0.55
1:A:210:ARG:HB3	1:B:175:ARG:HG3	1.90	0.54
1:A:175:ARG:NE	5:A:408:MPD:H12	2.22	0.53
1:B:107:PHE:HZ	4:B:406:EXW:CAN	2.22	0.52
4:A:407:EXW:CAN	10:A:564:HOH:O	2.57	0.52
1:B:181:ILE:O	4:B:406:EXW:CAB	2.59	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:ARG:HG3	1:B:210:ARG:HB3	1.93	0.50
1:A:181:ILE:O	4:A:407:EXW:CAB	2.60	0.49
1:B:107:PHE:CZ	4:B:406:EXW:CAJ	2.95	0.49
4:B:406:EXW:CAM	4:B:406:EXW:CAB	2.91	0.48
1:A:87:PRO:HA	1:A:90:ILE:HD12	1.95	0.47
1:B:67:LYS:NZ	1:B:307:GLN:O	2.31	0.47
5:B:407:MPD:H52	5:B:407:MPD:H12	1.97	0.47
1:A:173:TYR:CE2	1:A:237:CYS:HB3	2.51	0.46
1:B:225:TYR:O	1:B:229[A]:VAL:HG22	2.15	0.46
4:A:407:EXW:CAU	4:A:407:EXW:CAB	2.94	0.46
1:B:137:GLU:HB2	6:B:408:CL:CL	2.53	0.46
1:B:181:ILE:O	4:B:406:EXW:CAC	2.65	0.45
1:A:98:ALA:HB2	1:A:133:TYR:CB	2.46	0.45
1:A:302:VAL:O	10:A:502:HOH:O	2.20	0.45
1:B:107:PHE:CZ	4:B:406:EXW:CAN	3.00	0.45
1:A:256:ARG:HH12	7:A:411:CCN:C2	2.26	0.44
1:B:31:GLU:HG2	1:B:35:ARG:HD2	1.98	0.44
1:B:301:ASP:OD1	1:B:301:ASP:N	2.41	0.44
1:B:171:GLU:OE1	10:B:502:HOH:O	2.20	0.43
1:B:98:ALA:HB2	1:B:133:TYR:CB	2.48	0.43
5:A:408:MPD:H11	5:B:407:MPD:CM	2.33	0.43
1:B:41:PRO:HD3	1:B:283:TYR:CD2	2.54	0.43
1:A:184:ASP:HA	1:A:209:ALA:HB2	2.01	0.42
1:A:58:CYS:HB3	1:A:74:TRP:CH2	2.55	0.42
1:A:127:ARG:HD3	1:A:127:ARG:HA	1.91	0.42
1:B:145:ALA:HB1	1:B:185:PHE:HA	2.02	0.42
1:B:184:ASP:HA	1:B:209:ALA:HB2	2.02	0.42
1:B:173:TYR:CE2	1:B:237:CYS:HB3	2.56	0.40
1:B:175:ARG:NE	5:B:407:MPD:H12	2.25	0.40
1:A:145:ALA:HB1	1:A:185:PHE:HA	2.03	0.40

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	298/318 (94%)	293 (98%)	5 (2%)	0	100	100
1	B	306/318 (96%)	303 (99%)	3 (1%)	0	100	100
All	All	604/636 (95%)	596 (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	270/281 (96%)	267 (99%)	3 (1%)	73	68
1	B	275/281 (98%)	272 (99%)	3 (1%)	73	68
All	All	545/562 (97%)	539 (99%)	6 (1%)	73	68

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	107	PHE
1	A	177	ARG
1	A	307	GLN
1	B	35	ARG
1	B	107	PHE
1	B	307	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	307	GLN
1	B	307	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 23 ligands modelled in this entry, 14 are monoatomic - leaving 9 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$
3	PPV	A	406	2	6,8,8	0.88	0	13,13,13	1.20	1 (7%)
5	MPD	A	408	-	7,7,7	0.49	0	9,10,10	0.91	0
3	PPV	B	405	2	6,8,8	0.76	0	13,13,13	1.16	1 (7%)
4	EXW	B	406	-	21,22,22	5.29	9 (42%)	24,32,32	3.64	14 (58%)
8	PEG	A	412	-	6,6,6	0.44	0	5,5,5	0.50	0
7	CCN	A	411	-	2,2,2	0.85	0	1,1,1	0.51	0
5	MPD	B	407	-	7,7,7	0.45	0	9,10,10	0.79	0
4	EXW	A	407	-	21,22,22	5.11	9 (42%)	24,32,32	3.11	11 (45%)
8	PEG	B	409	-	6,6,6	0.52	0	5,5,5	0.33	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
3	PPV	A	406	2	-	0/6/6/6	-
5	MPD	A	408	-	-	1/5/5/5	-
3	PPV	B	405	2	-	0/6/6/6	-
4	EXW	B	406	-	-	9/20/40/40	1/2/2/2
8	PEG	A	412	-	-	4/4/4/4	-
5	MPD	B	407	-	-	2/5/5/5	-
4	EXW	A	407	-	-	11/20/40/40	1/2/2/2
8	PEG	B	409	-	-	2/4/4/4	-

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	406	EXW	CAM-CAK	16.23	1.52	1.32
4	A	407	EXW	CAM-CAK	15.15	1.51	1.32
4	A	407	EXW	CAF-CAG	-9.38	1.36	1.54
4	B	406	EXW	CAQ-CAR	9.20	1.55	1.33
4	B	406	EXW	CAF-CAG	-8.90	1.37	1.54
4	A	407	EXW	CAD-CAC	-8.28	1.35	1.55
4	B	406	EXW	CAD-CAC	-8.10	1.36	1.55
4	A	407	EXW	CAG-CAC	7.61	1.70	1.54
4	A	407	EXW	CAQ-CAR	6.64	1.48	1.33
4	B	406	EXW	CAG-CAC	6.61	1.68	1.54
4	A	407	EXW	CAU-CAH	5.32	1.55	1.34
4	A	407	EXW	CAE-CAD	3.63	1.64	1.54
4	B	406	EXW	CAI-CAD	-3.53	1.47	1.53
4	B	406	EXW	CAE-CAD	3.50	1.64	1.54
4	B	406	EXW	CAU-CAH	3.32	1.47	1.34
4	B	406	EXW	CAB-CAA	2.82	1.61	1.52
4	A	407	EXW	CAO-CAM	2.39	1.54	1.51
4	A	407	EXW	CAJ-CAD	2.10	1.57	1.55

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	406	EXW	CAT-CAH-CAU	-8.73	100.39	121.38
4	A	407	EXW	CAA-CAR-CAQ	-7.64	105.67	121.12
4	B	406	EXW	CAG-CAH-CAU	-6.07	104.49	121.12
4	A	407	EXW	CAS-CAR-CAQ	-5.78	108.84	123.68
4	A	407	EXW	CAA-CAB-CAC	-5.45	101.02	114.43
4	B	406	EXW	CAS-CAR-CAQ	-5.36	109.93	123.68
4	B	406	EXW	CAA-CAR-CAQ	-5.27	110.45	121.12
4	B	406	EXW	CAD-CAC-CAG	5.06	114.03	105.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	406	EXW	CAI-CAD-CAJ	-4.99	104.09	109.22
4	B	406	EXW	CAT-CAH-CAG	4.86	128.09	117.47
4	A	407	EXW	CAI-CAD-CAC	-4.70	102.35	113.55
4	A	407	EXW	CAN-CAM-CAO	-4.33	106.01	115.33
4	B	406	EXW	CAA-CAB-CAC	4.09	124.51	114.43
4	A	407	EXW	CAT-CAH-CAU	-3.58	112.78	121.38
4	B	406	EXW	CAE-CAF-CAG	3.56	111.80	106.09
4	B	406	EXW	CAC-CAG-CAH	3.13	121.69	115.56
3	B	405	PPV	P2-OPP-P1	-3.09	122.22	132.83
4	A	407	EXW	CAP-CAQ-CAR	-3.06	120.30	127.66
4	B	406	EXW	CAI-CAD-CAE	-2.94	101.83	110.47
4	A	407	EXW	CAI-CAD-CAE	-2.93	101.87	110.47
3	A	406	PPV	P2-OPP-P1	-2.85	123.06	132.83
4	A	407	EXW	CAG-CAH-CAU	2.78	128.74	121.12
4	B	406	EXW	CAP-CAQ-CAR	-2.71	121.14	127.66
4	B	406	EXW	CAF-CAG-CAH	-2.29	105.58	112.28
4	B	406	EXW	CAE-CAD-CAJ	2.26	114.34	109.57
4	A	407	EXW	CAP-CAO-CAM	-2.13	105.97	112.98
4	A	407	EXW	CAB-CAA-CAR	-2.06	109.05	113.85

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	407	MPD	C2-C3-C4-O4
4	B	406	EXW	CAD-CAJ-CAK-CAM
4	B	406	EXW	CAJ-CAK-CAM-CAN
4	B	406	EXW	CAP-CAQ-CAR-CAA
4	A	407	EXW	CAA-CAB-CAC-CAD
4	A	407	EXW	CAC-CAD-CAJ-CAK
4	A	407	EXW	CAE-CAD-CAJ-CAK
4	A	407	EXW	CAI-CAD-CAJ-CAK
4	A	407	EXW	CAD-CAJ-CAK-CAM
4	A	407	EXW	CAJ-CAK-CAM-CAN
4	A	407	EXW	CAP-CAQ-CAR-CAA
4	B	406	EXW	CAP-CAQ-CAR-CAS
4	A	407	EXW	CAP-CAQ-CAR-CAS
8	A	412	PEG	O2-C3-C4-O4
4	B	406	EXW	CAC-CAG-CAH-CAU
8	B	409	PEG	O1-C1-C2-O2
4	A	407	EXW	CAA-CAB-CAC-CAG
8	A	412	PEG	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
4	B	406	EXW	CAB-CAA-CAR-CAS
8	A	412	PEG	C4-C3-O2-C2
8	B	409	PEG	C4-C3-O2-C2
8	A	412	PEG	C1-C2-O2-C3
5	A	408	MPD	C2-C3-C4-O4
4	B	406	EXW	CAN-CAM-CAO-CAP
4	A	407	EXW	CAN-CAM-CAO-CAP
4	B	406	EXW	CAB-CAA-CAR-CAQ
5	B	407	MPD	O2-C2-C3-C4
4	A	407	EXW	CAB-CAA-CAR-CAQ
4	B	406	EXW	CAF-CAG-CAH-CAU

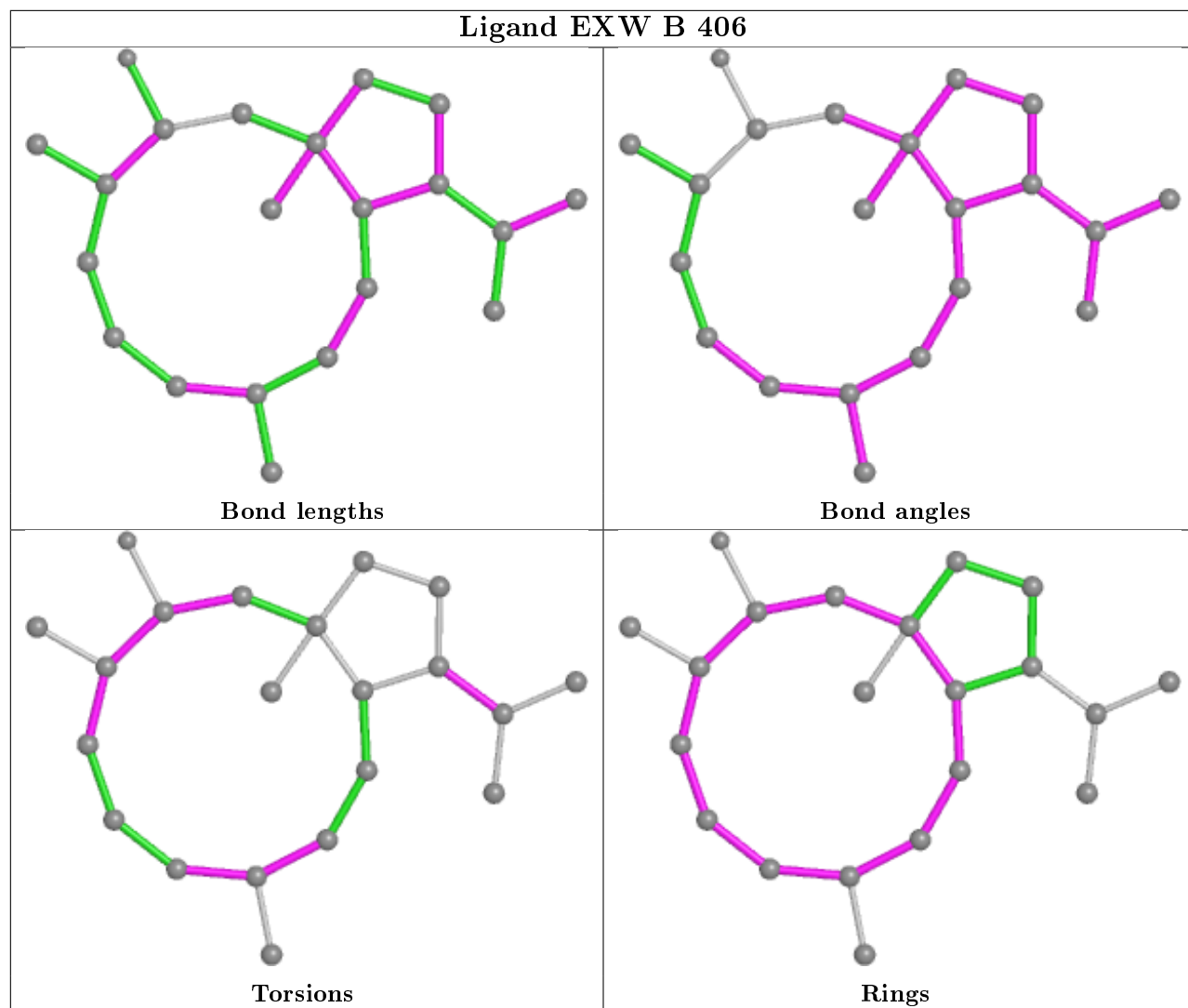
All (2) ring outliers are listed below:

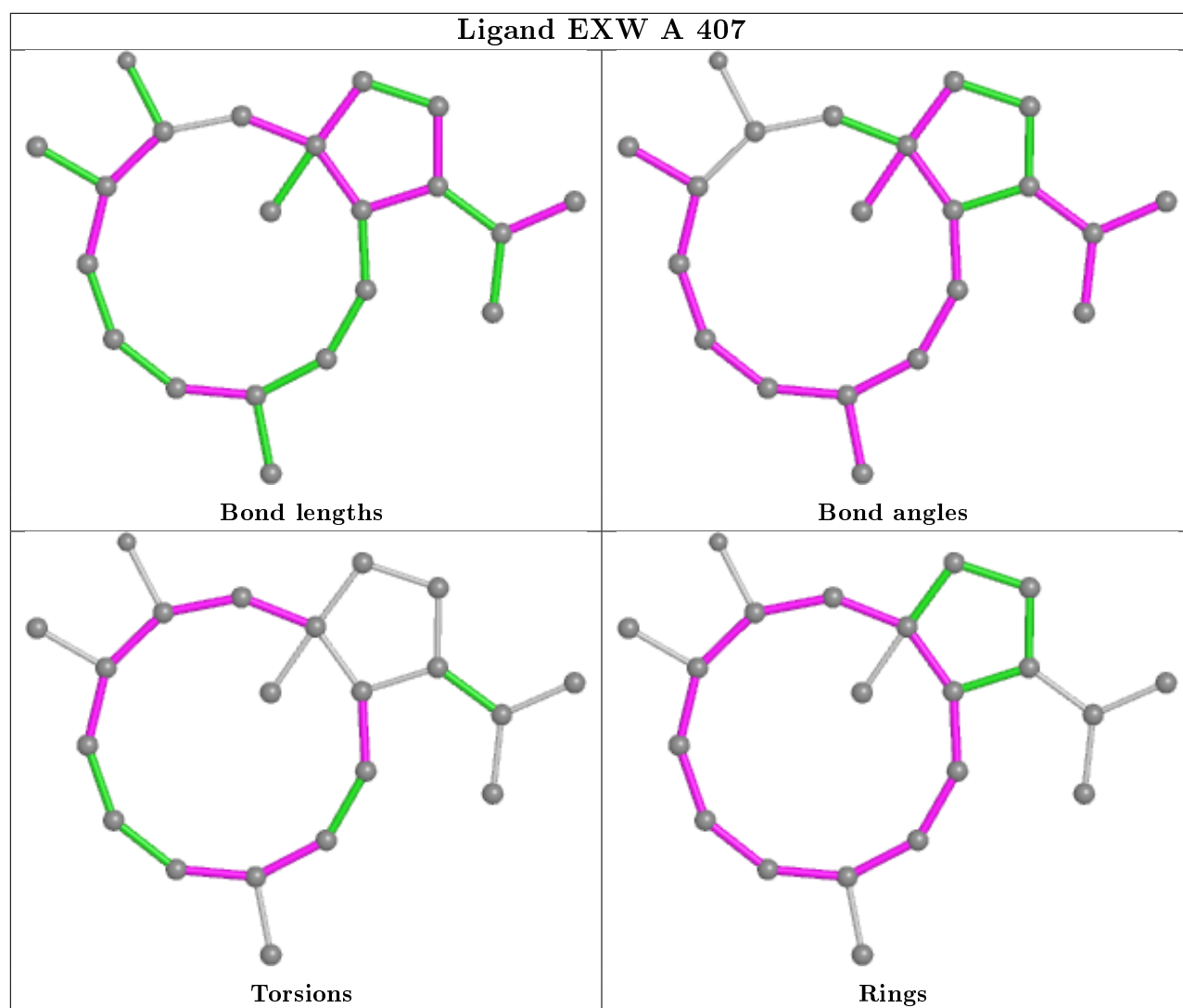
Mol	Chain	Res	Type	Atoms
4	B	406	EXW	CAA-CAB-CAC-CAD-CAJ-CAK-CAM-CAO-CAP-CAQ-CAR
4	A	407	EXW	CAA-CAB-CAC-CAD-CAJ-CAK-CAM-CAO-CAP-CAQ-CAR

5 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	408	MPD	6	0
4	B	406	EXW	6	0
7	A	411	CCN	2	0
5	B	407	MPD	9	0
4	A	407	EXW	5	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	294/318 (92%)	-0.43	3 (1%) 82 80	13, 23, 37, 52	0
1	B	300/318 (94%)	-0.29	11 (3%) 41 36	13, 24, 43, 61	0
All	All	594/636 (93%)	-0.36	14 (2%) 59 54	13, 23, 41, 61	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	11	GLN	4.7
1	B	49	ALA	4.4
1	B	10	ALA	4.2
1	B	298	ALA	4.1
1	B	297	THR	3.9
1	B	299	VAL	3.8
1	A	49	ALA	3.5
1	B	301	ASP	3.2
1	B	13	ILE	3.0
1	B	158	ASP	3.0
1	A	297	THR	3.0
1	B	307	GLN	2.3
1	B	308	ALA	2.2
1	A	298	ALA	2.1

### 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 carbohydrates in this entry.

## 6.4 Ligands ⓘ

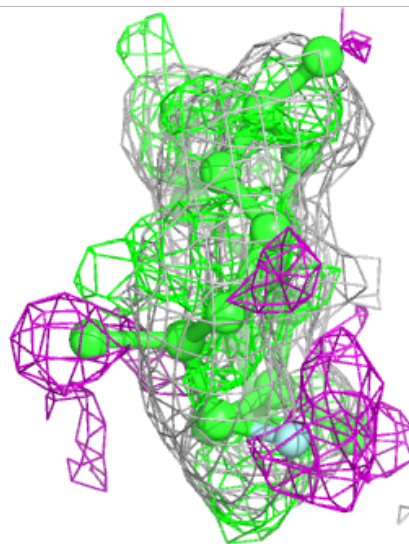
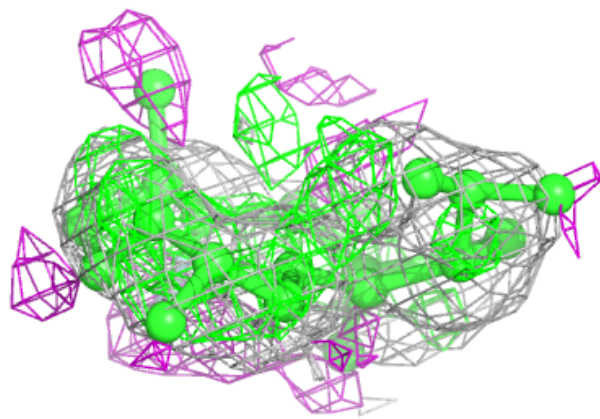
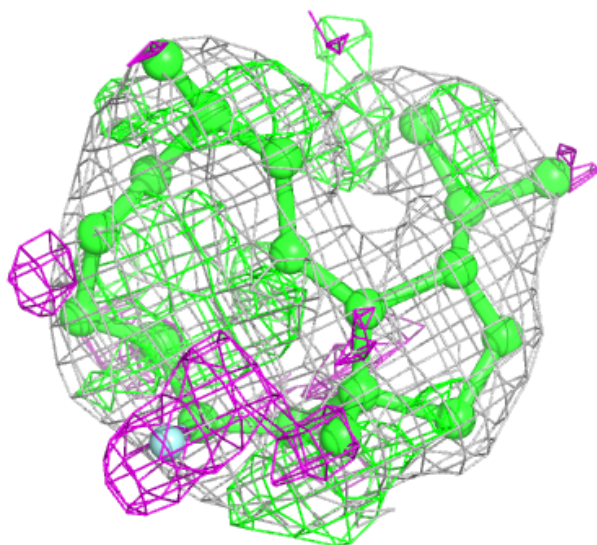
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

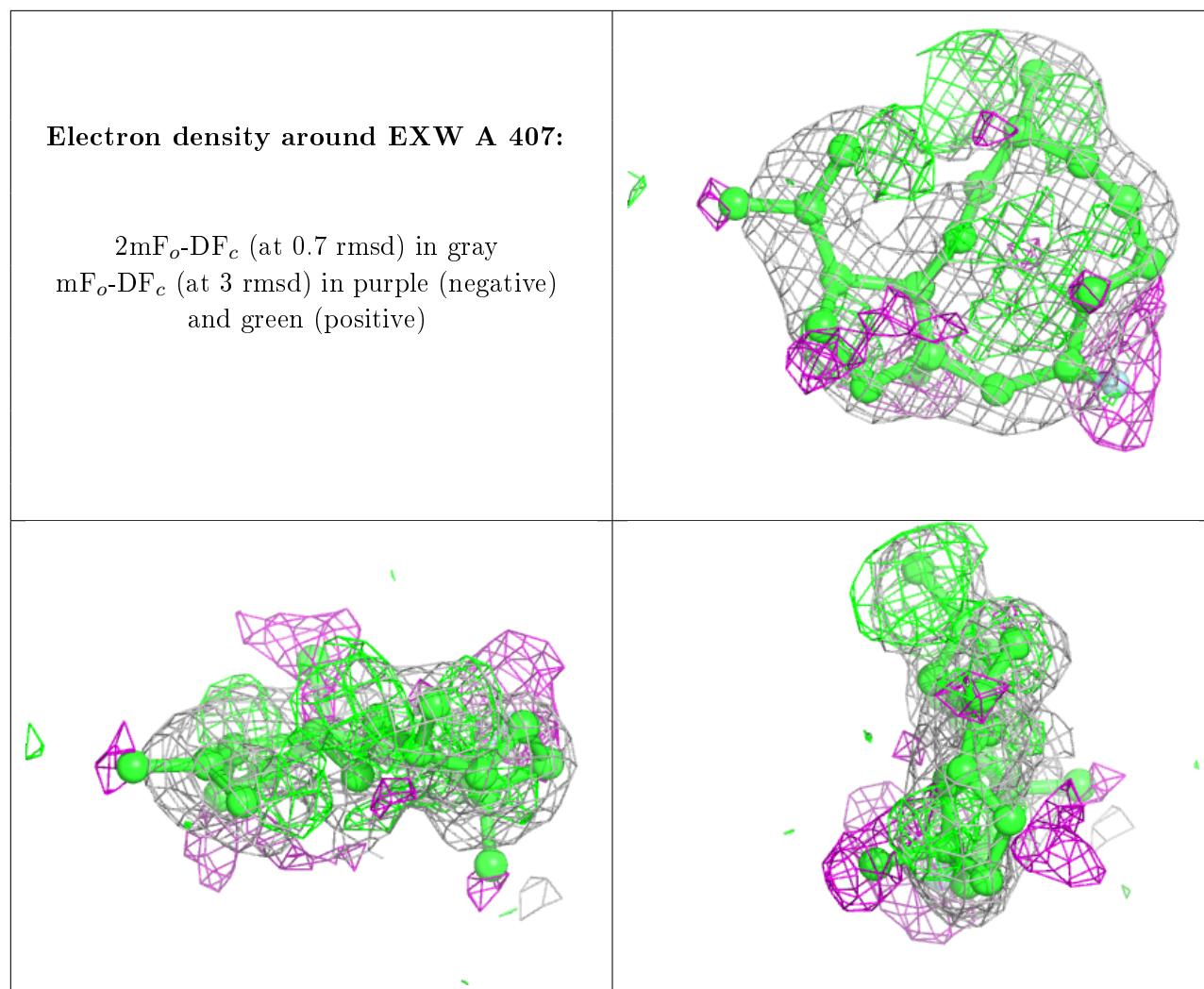
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	MPD	B	407	8/8	0.76	0.21	24,29,41,42	0
8	PEG	A	412	7/7	0.84	0.18	37,41,49,51	0
5	MPD	A	408	8/8	0.84	0.15	23,31,41,41	0
4	EXW	B	406	21/21	0.84	0.27	7,27,33,44	0
4	EXW	A	407	21/21	0.85	0.29	3,26,42,46	0
7	CCN	A	411	3/3	0.90	0.10	19,19,29,38	0
8	PEG	B	409	7/7	0.91	0.15	36,38,49,50	0
6	CL	B	408	1/1	0.92	0.06	48,48,48,48	0
2	MG	A	405	1/1	0.92	0.11	35,35,35,35	0
9	K	A	413	1/1	0.95	0.31	52,52,52,52	0
2	MG	A	404	1/1	0.95	0.26	37,37,37,37	0
2	MG	B	404	1/1	0.96	0.05	32,32,32,32	0
9	K	B	410	1/1	0.97	0.39	52,52,52,52	0
2	MG	A	401	1/1	0.97	0.06	21,21,21,21	0
2	MG	A	402	1/1	0.98	0.05	16,16,16,16	0
2	MG	B	401	1/1	0.98	0.04	19,19,19,19	0
2	MG	A	403	1/1	0.98	0.07	19,19,19,19	0
6	CL	A	409	1/1	0.98	0.04	29,29,29,29	0
2	MG	B	402	1/1	0.99	0.06	17,17,17,17	0
3	PPV	B	405	9/9	0.99	0.06	14,16,19,20	0
3	PPV	A	406	9/9	0.99	0.07	15,18,19,20	0
2	MG	B	403	1/1	1.00	0.03	16,16,16,16	0
6	CL	A	410	1/1	1.00	0.08	20,20,20,20	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 EXW B 406:**

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





## 6.5 Other polymers ⓘ

There are no such residues in this entry.