



# Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 11:27 pm BST

PDB ID : 1XLX  
Title : Catalytic Domain Of Human Phosphodiesterase 4B In Complex With Cilomilast  
Authors : Card, G.L.; England, B.P.; Suzuki, Y.; Fong, D.; Powell, B.; Lee, B.; Luu, C.; Tabrizizad, M.; Gillette, S.; Ibrahim, P.N.; Artis, D.R.; Bollag, G.; Milburn, M.V.; Kim, S.-H.; Schlessinger, J.; Zhang, K.Y.J.  
Deposited on : 2004-09-30  
Resolution : 2.19 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

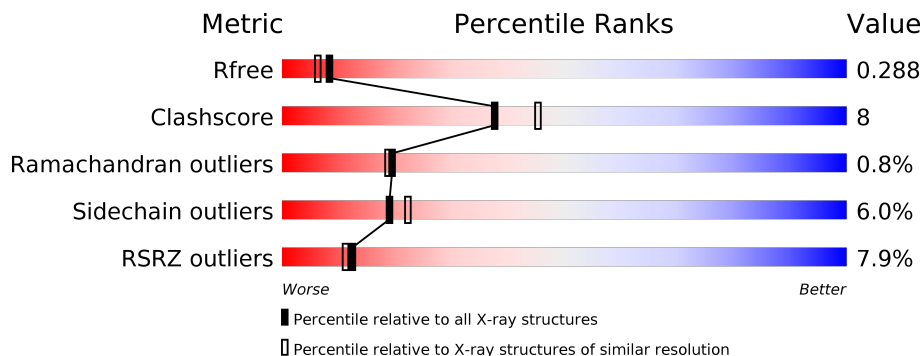
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.19 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (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 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	398	
1	B	398	

## 2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 5356 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 cAMP-specific 3',5'-cyclic phosphodiesterase 4B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	323	2617	1653	441	503	20	7	0	0
1	B	323	2612	1650	439	503	20	4	0	0

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	131	MET	-	CLONING ARTIFACT	UNP Q07343
A	132	GLY	-	CLONING ARTIFACT	UNP Q07343
A	133	SER	-	CLONING ARTIFACT	UNP Q07343
A	134	SER	-	CLONING ARTIFACT	UNP Q07343
A	135	HIS	-	CLONING ARTIFACT	UNP Q07343
A	136	HIS	-	CLONING ARTIFACT	UNP Q07343
A	137	HIS	-	CLONING ARTIFACT	UNP Q07343
A	138	HIS	-	CLONING ARTIFACT	UNP Q07343
A	139	HIS	-	CLONING ARTIFACT	UNP Q07343
A	140	HIS	-	CLONING ARTIFACT	UNP Q07343
A	141	SER	-	CLONING ARTIFACT	UNP Q07343
A	142	SER	-	CLONING ARTIFACT	UNP Q07343
A	143	GLY	-	CLONING ARTIFACT	UNP Q07343
A	144	LEU	-	CLONING ARTIFACT	UNP Q07343
A	145	VAL	-	CLONING ARTIFACT	UNP Q07343
A	146	PRO	-	CLONING ARTIFACT	UNP Q07343
A	147	ARG	-	CLONING ARTIFACT	UNP Q07343
A	148	GLY	-	CLONING ARTIFACT	UNP Q07343
A	149	SER	-	CLONING ARTIFACT	UNP Q07343
A	150	HIS	-	CLONING ARTIFACT	UNP Q07343
A	151	MET	-	CLONING ARTIFACT	UNP Q07343
A	194	CME	CYS	MODIFIED RESIDUE	UNP Q07343
B	131	MET	-	CLONING ARTIFACT	UNP Q07343
B	132	GLY	-	CLONING ARTIFACT	UNP Q07343
B	133	SER	-	CLONING ARTIFACT	UNP Q07343

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Chain	Residue	Modelled	Actual	Comment	Reference
B	134	SER	-	CLONING ARTIFACT	UNP Q07343
B	135	HIS	-	CLONING ARTIFACT	UNP Q07343
B	136	HIS	-	CLONING ARTIFACT	UNP Q07343
B	137	HIS	-	CLONING ARTIFACT	UNP Q07343
B	138	HIS	-	CLONING ARTIFACT	UNP Q07343
B	139	HIS	-	CLONING ARTIFACT	UNP Q07343
B	140	HIS	-	CLONING ARTIFACT	UNP Q07343
B	141	SER	-	CLONING ARTIFACT	UNP Q07343
B	142	SER	-	CLONING ARTIFACT	UNP Q07343
B	143	GLY	-	CLONING ARTIFACT	UNP Q07343
B	144	LEU	-	CLONING ARTIFACT	UNP Q07343
B	145	VAL	-	CLONING ARTIFACT	UNP Q07343
B	146	PRO	-	CLONING ARTIFACT	UNP Q07343
B	147	ARG	-	CLONING ARTIFACT	UNP Q07343
B	148	GLY	-	CLONING ARTIFACT	UNP Q07343
B	149	SER	-	CLONING ARTIFACT	UNP Q07343
B	150	HIS	-	CLONING ARTIFACT	UNP Q07343
B	151	MET	-	CLONING ARTIFACT	UNP Q07343
B	194	CME	CYS	MODIFIED RESIDUE	UNP Q07343

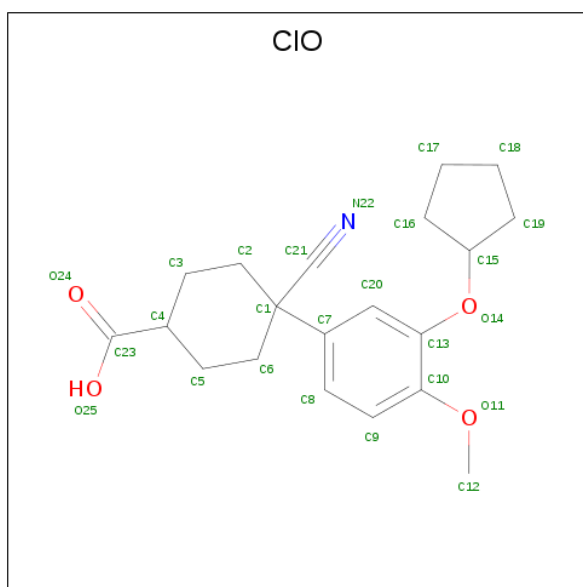
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Mg 1 1	0	0
3	A	1	Total Mg 1 1	0	0

- Molecule 4 is CILOMILAST (three-letter code: CIO) (formula: C<sub>20</sub>H<sub>25</sub>NO<sub>4</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	A	1	25	20	1	4	0	0
4	B	1	25	20	1	4	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	35	35	35	0	0
5	B	38	38	38	0	0



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	89.27Å 94.26Å 106.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	70.71 – 2.19 34.15 – 2.19	Depositor EDS
% Data completeness (in resolution range)	92.8 (70.71-2.19) 92.8 (34.15-2.19)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.06 (at 2.20Å)	Xtrriage
Refinement program	REFMAC 5.1.25	Depositor
R, $R_{free}$	0.232 , 0.282 0.239 , 0.288	Depositor DCC
$R_{free}$ test set	2198 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	41.2	Xtrriage
Anisotropy	0.667	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 50.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	5356	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 51.88 % 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 5.2661e-05. 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: MG, CIO, ZN, CME

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	0.89	0/2661	1.03	10/3608 (0.3%)
1	B	0.99	3/2655 (0.1%)	1.06	13/3600 (0.4%)
All	All	0.94	3/5316 (0.1%)	1.05	23/7208 (0.3%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	224	GLU	CD-OE1	7.27	1.33	1.25
1	B	227	TYR	CD1-CE1	-5.81	1.30	1.39
1	B	183	VAL	CB-CG2	-5.02	1.42	1.52

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	261	ASP	CB-CG-OD2	9.69	127.02	118.30
1	B	299	ASP	CB-CG-OD2	7.99	125.49	118.30
1	A	340	ASP	CB-CG-OD2	7.44	125.00	118.30
1	A	475	ASP	CB-CG-OD1	7.07	124.66	118.30
1	B	468	ASP	CB-CG-OD2	6.83	124.45	118.30
1	B	225	ASP	CB-CG-OD2	6.67	124.30	118.30
1	A	230	ASP	CB-CG-OD2	6.62	124.25	118.30
1	B	261	ASP	CB-CG-OD1	-6.58	112.38	118.30
1	A	468	ASP	CB-CG-OD2	6.45	124.10	118.30
1	B	340	ASP	CB-CG-OD2	6.38	124.04	118.30
1	A	214	ASP	CB-CG-OD2	5.96	123.66	118.30
1	B	256	ASP	CB-CG-OD2	5.81	123.53	118.30
1	A	460	ASP	CB-CG-OD1	5.68	123.42	118.30
1	A	379	ASP	CB-CG-OD2	5.45	123.21	118.30
1	B	221	MET	CG-SD-CE	5.43	108.88	100.20
1	A	321	ASP	CB-CG-OD2	5.39	123.15	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	375	ASP	CB-CG-OD2	5.38	123.14	118.30
1	B	277	ASP	CB-CG-OD2	5.22	123.00	118.30
1	A	484	ILE	CB-CA-C	-5.19	101.22	111.60
1	B	318	GLU	CA-CB-CG	-5.18	102.00	113.40
1	B	375	ASP	CB-CG-OD2	5.17	122.95	118.30
1	B	465	ASP	CB-CG-OD1	5.10	122.89	118.30
1	B	392	ASP	CB-CG-OD2	5.05	122.84	118.30

There are no chirality outliers.

There are no planarity outliers.

## 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	2617	0	2546	30	0
1	B	2612	0	2541	48	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	25	0	24	4	0
4	B	25	0	24	1	0
5	A	35	0	0	0	0
5	B	38	0	0	1	0
All	All	5356	0	5135	80	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 8.

All (80) 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:220:MET:CE	1:B:220:MET:SD	2.02	1.48
1:B:207:LYS:HB3	1:B:207:LYS:NZ	1.75	1.00
1:B:207:LYS:HB3	1:B:207:LYS:HZ3	1.32	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:HIS:ND1	1:A:413:GLU:OE2	2.17	0.77
1:A:340:ASP:OD1	1:A:385:ARG:HD3	1.87	0.75
1:B:376:ASN:CG	1:B:377:TYR:H	1.95	0.70
1:B:217:ILE:HG22	1:B:221:MET:CE	2.24	0.68
1:B:424:ARG:HB2	1:B:426:MET:HE3	1.76	0.67
1:A:367:THR:O	1:A:368:SER:CB	2.43	0.67
1:B:275:ASP:O	1:B:278:HIS:HB2	1.95	0.66
1:B:207:LYS:CB	1:B:207:LYS:NZ	2.52	0.66
1:B:207:LYS:HB3	1:B:207:LYS:HZ2	1.60	0.64
1:B:397:THR:HB	1:B:469:ILE:HG23	1.80	0.62
1:B:255:LEU:HD23	1:B:372:LEU:HD12	1.83	0.60
1:B:220:MET:CG	1:B:220:MET:CE	2.79	0.60
1:B:217:ILE:HG22	1:B:221:MET:HE2	1.83	0.60
1:B:286:LEU:HB3	1:B:291:SER:OG	2.03	0.58
1:A:234:HIS:HD1	1:A:413:GLU:CD	2.06	0.58
1:A:163:GLU:N	1:A:163:GLU:CD	2.57	0.57
1:A:421:GLU:HA	1:A:426:MET:HE2	1.86	0.57
1:B:340:ASP:OD1	1:B:385:ARG:HD3	2.05	0.56
1:B:331:ARG:HG3	1:B:331:ARG:HH11	1.70	0.56
1:A:397:THR:HB	1:A:469:ILE:HG23	1.89	0.55
1:B:237:LEU:HD23	1:B:409:ARG:NH1	2.20	0.55
1:B:337:MET:O	1:B:341:MET:HG3	2.07	0.54
1:B:250:LEU:HG	1:B:387:MET:HE3	1.88	0.53
1:B:424:ARG:HD2	1:B:426:MET:CE	2.39	0.53
1:A:411:MET:HG3	1:A:439:VAL:HG22	1.91	0.52
1:A:421:GLU:HA	1:A:426:MET:CE	2.39	0.52
1:A:367:THR:O	1:A:368:SER:HB3	2.09	0.51
1:A:411:MET:HE3	4:A:101:CIO:H181	1.92	0.51
1:A:381:ILE:O	1:A:385:ARG:HG3	2.11	0.51
1:B:244:GLN:O	1:B:247:HIS:HB3	2.12	0.50
1:A:197:TYR:CD1	1:A:217:ILE:HD11	2.45	0.50
1:A:411:MET:HE2	1:A:411:MET:HA	1.94	0.50
1:B:255:LEU:CD2	1:B:372:LEU:HD12	2.43	0.49
1:B:308:LEU:HG	1:B:342:VAL:HG11	1.93	0.49
1:A:356:ASP:HB3	1:A:382:GLN:NE2	2.27	0.49
1:A:242:VAL:HG12	1:A:271:ALA:HB1	1.96	0.48
1:B:331:ARG:NH1	1:B:331:ARG:HG3	2.28	0.48
1:B:207:LYS:CB	1:B:207:LYS:HZ2	2.20	0.48
1:B:258:VAL:HG11	1:B:374:LEU:HD12	1.97	0.47
1:A:411:MET:HE1	4:A:101:CIO:C18	2.45	0.47
1:A:258:VAL:HG11	1:A:374:LEU:HD12	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:HIS:HB3	1:A:186:TYR:CE2	2.49	0.46
1:B:416:GLN:O	1:B:417:GLN:C	2.52	0.46
1:B:390:CYS:HB3	1:B:455:TRP:CZ2	2.51	0.46
1:B:219:TYR:CD2	1:B:219:TYR:C	2.89	0.46
1:A:340:ASP:OD1	1:A:385:ARG:CD	2.61	0.45
1:A:323:PHE:HB3	1:A:326:LEU:HG	1.98	0.45
1:B:333:THR:O	1:B:337:MET:HG3	2.16	0.45
4:A:101:CIO:H20	4:A:101:CIO:H15	1.63	0.45
1:A:327:THR:HG22	1:A:330:GLN:H	1.80	0.45
1:B:395:ASN:HB2	1:B:396:PRO:HD3	1.98	0.44
1:A:300:GLU:O	1:A:301:SER:C	2.56	0.44
1:B:223:LEU:HD12	1:B:276:VAL:HG21	1.99	0.44
1:B:411:MET:HG3	1:B:439:VAL:HG13	2.00	0.44
1:B:250:LEU:CD2	1:B:387:MET:HE1	2.49	0.43
1:A:411:MET:CE	4:A:101:CIO:C18	2.96	0.42
1:B:213:SER:O	1:B:217:ILE:HG12	2.19	0.42
1:B:250:LEU:HD21	1:B:387:MET:HE1	2.00	0.42
1:B:278:HIS:CE1	1:B:303:LEU:HD13	2.54	0.42
1:B:274:HIS:O	1:B:307:HIS:CD2	2.72	0.42
1:B:336:LYS:HE2	1:B:336:LYS:HB3	1.93	0.42
1:B:289:THR:CG2	1:B:426:MET:HE1	2.50	0.42
1:A:165:HIS:HB3	1:A:186:TYR:CZ	2.54	0.42
1:B:203:ARG:NH2	1:B:247:HIS:O	2.50	0.42
1:A:269:PHE:CE2	1:A:273:ILE:HD13	2.55	0.41
1:B:376:ASN:CG	1:B:377:TYR:N	2.68	0.41
1:B:238:HIS:O	1:B:242:VAL:HG23	2.21	0.41
1:A:275:ASP:HA	1:A:307:HIS:CD2	2.56	0.41
4:B:102:CIO:H8	5:B:22:HOH:O	2.20	0.41
1:B:313:LYS:NZ	1:B:316:GLN:OE1	2.54	0.41
1:A:209:PHE:CD2	1:A:265:LEU:HD22	2.56	0.41
1:B:327:THR:HG22	1:B:329:LYS:H	1.86	0.41
1:A:209:PHE:CE2	1:A:265:LEU:HD22	2.57	0.40
1:B:421:GLU:OE1	1:B:428:ILE:HA	2.21	0.40
1:B:196:MET:HE1	1:B:268:ILE:HG22	2.04	0.40
1:B:242:VAL:HG21	1:B:274:HIS:CE1	2.57	0.40
1:A:275:ASP:O	1:A:278:HIS:HB2	2.22	0.40

There are no symmetry-related clashes.

## 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	320/398 (80%)	306 (96%)	10 (3%)	4 (1%)	12	9
1	B	320/398 (80%)	306 (96%)	13 (4%)	1 (0%)	41	46
All	All	640/796 (80%)	612 (96%)	23 (4%)	5 (1%)	19	19

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	376	ASN
1	A	256	ASP
1	A	368	SER
1	B	375	ASP
1	A	318	GLU

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	292/359 (81%)	278 (95%)	14 (5%)	25	32
1	B	291/359 (81%)	270 (93%)	21 (7%)	14	15
All	All	583/718 (81%)	548 (94%)	35 (6%)	19	22

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	163	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	178	LEU
1	A	189	ASN
1	A	204	ASP
1	A	210	ARG
1	A	213	SER
1	A	295	LEU
1	A	313	LYS
1	A	326	LEU
1	A	327	THR
1	A	331	ARG
1	A	352	SER
1	A	442	SER
1	A	470	LEU
1	B	168	LYS
1	B	189	ASN
1	B	204	ASP
1	B	207	LYS
1	B	212	SER
1	B	213	SER
1	B	317	GLU
1	B	319	HIS
1	B	324	MET
1	B	329	LYS
1	B	352	SER
1	B	356	ASP
1	B	373	LEU
1	B	375	ASP
1	B	385	ARG
1	B	408	ASP
1	B	423	GLU
1	B	429	SER
1	B	436	THR
1	B	441	LYS
1	B	477	ARG

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

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	382	GLN
1	A	481	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](#)

2 non-standard protein/DNA/RNA residues 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
1	CME	A	194	1	8,9,10	1.50	1 (12%)	5,9,11	2.03	3 (60%)
1	CME	B	194	1	8,9,10	1.65	1 (12%)	5,9,11	0.98	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
1	CME	A	194	1	-	1/5/8/10	-
1	CME	B	194	1	-	1/5/8/10	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	194	CME	OH-CZ	-3.70	1.23	1.42
1	A	194	CME	OH-CZ	-3.63	1.23	1.42

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	194	CME	CB-SG-SD	2.57	110.47	103.82
1	A	194	CME	CE-SD-SG	2.43	114.66	103.45
1	A	194	CME	CA-CB-SG	-2.25	104.91	114.55

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	194	CME	CE-SD-SG-CB
1	B	194	CME	CE-SD-SG-CB

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 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	CIO	A	101	-	22,27,27	0.95	1 (4%)	26,38,38	1.57	4 (15%)
4	CIO	B	102	-	22,27,27	0.97	1 (4%)	26,38,38	1.48	4 (15%)

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	CIO	A	101	-	-	2/12/38/38	0/3/3/3
4	CIO	B	102	-	-	2/12/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	102	CIO	C20-C7	2.59	1.43	1.39
4	A	101	CIO	O11-C10	2.09	1.40	1.37

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	101	CIO	C2-C3-C4	-4.48	107.12	111.37
4	B	102	CIO	C12-O11-C10	4.01	123.58	117.53
4	B	102	CIO	C5-C4-C23	-2.93	105.67	111.88
4	A	101	CIO	C8-C7-C1	2.87	123.91	121.07
4	B	102	CIO	O11-C10-C9	-2.84	119.50	124.37
4	A	101	CIO	O11-C10-C13	2.83	119.35	115.41
4	A	101	CIO	C12-O11-C10	2.72	121.63	117.53
4	B	102	CIO	O11-C10-C13	2.30	118.61	115.41

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	101	CIO	C16-C15-O14-C13
4	A	101	CIO	C19-C15-O14-C13
4	B	102	CIO	C16-C15-O14-C13
4	B	102	CIO	C19-C15-O14-C13

There are no ring outliers.

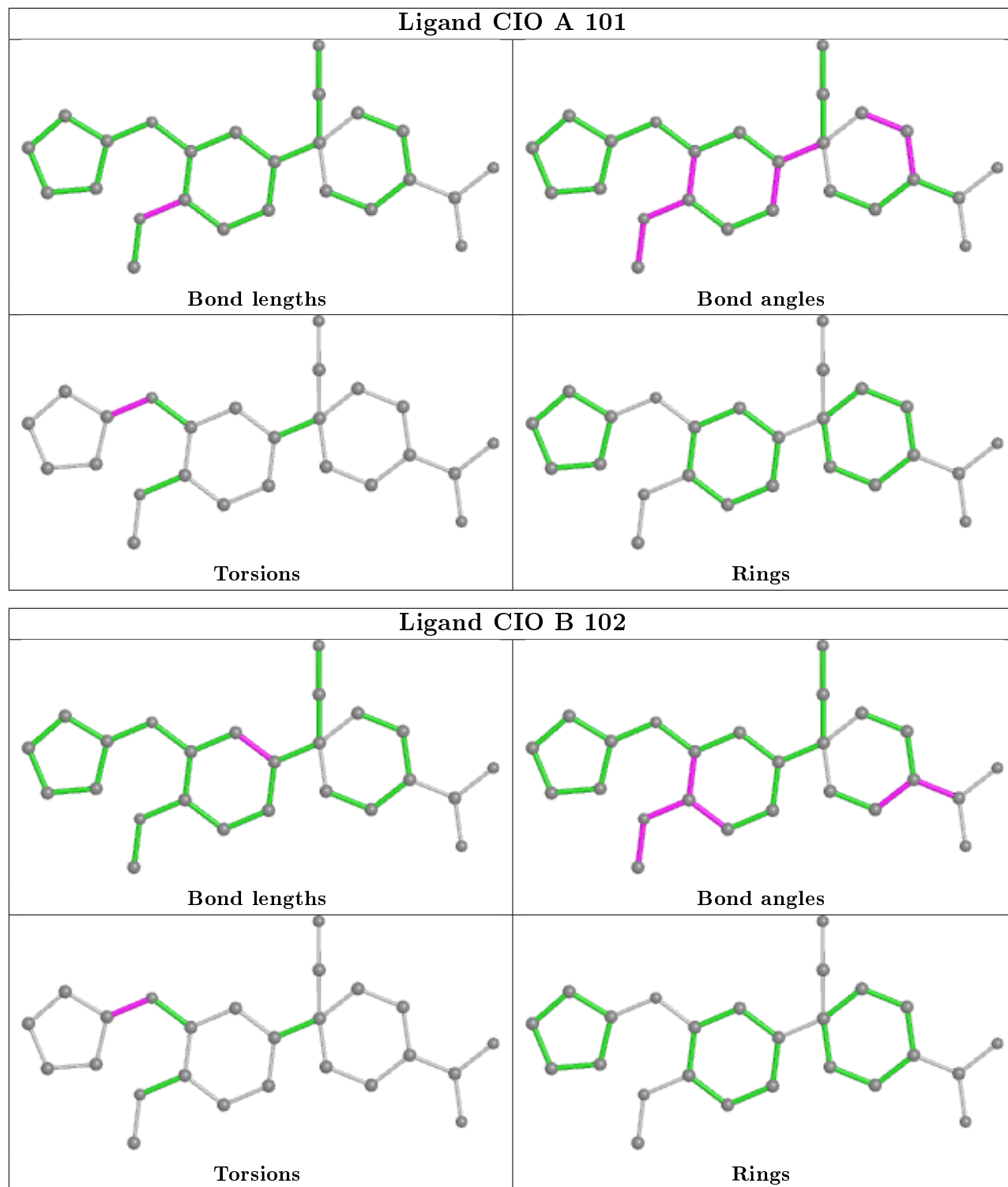
2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	101	CIO	4	0
4	B	102	CIO	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

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, 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	322/398 (80%)	0.59	25 (7%) <b>13</b> <b>11</b>	16, 24, 31, 43	2 (0%)
1	B	322/398 (80%)	0.55	26 (8%) <b>12</b> <b>10</b>	14, 24, 30, 38	1 (0%)
All	All	644/796 (80%)	0.57	51 (7%) <b>12</b> <b>11</b>	14, 24, 31, 43	3 (0%)

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	319	HIS	5.7
1	A	318	GLU	4.8
1	B	430	PRO	4.6
1	B	425	GLY	4.6
1	B	428	ILE	3.9
1	B	482	SER	3.8
1	A	425	GLY	3.8
1	A	186	TYR	3.5
1	B	391	ALA	3.3
1	A	369	SER	3.3
1	A	426	MET	3.2
1	B	423	GLU	3.2
1	A	393	LEU	3.2
1	B	319	HIS	3.2
1	A	423	GLU	3.1
1	B	243	ALA	3.0
1	A	249	LEU	2.9
1	A	242	VAL	2.9
1	B	422	ARG	2.9
1	B	390	CYS	2.8
1	B	375	ASP	2.7
1	A	427	GLU	2.7
1	B	481	GLN	2.6
1	A	167	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	273	ILE	2.5
1	B	272	ALA	2.5
1	B	171	GLU	2.5
1	B	366	VAL	2.4
1	B	273	ILE	2.4
1	A	207	LYS	2.4
1	A	271	ALA	2.4
1	B	345	THR	2.4
1	B	338	VAL	2.3
1	B	394	SER	2.3
1	A	317	GLU	2.3
1	A	316	GLN	2.3
1	B	388	VAL	2.3
1	B	242	VAL	2.3
1	B	377	TYR	2.2
1	A	329	LYS	2.2
1	B	239	ALA	2.2
1	A	377	TYR	2.2
1	B	274	HIS	2.2
1	A	396	PRO	2.2
1	A	257	ALA	2.1
1	A	267	ALA	2.1
1	A	428	ILE	2.1
1	A	164	ASP	2.0
1	A	166	LEU	2.0
1	B	246	THR	2.0
1	B	185	GLY	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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, 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
1	CME	B	194	10/11	0.86	0.17	33,36,55,57	0
1	CME	A	194	10/11	0.94	0.16	32,36,59,64	0

### 6.3 Carbohydrates [i](#)

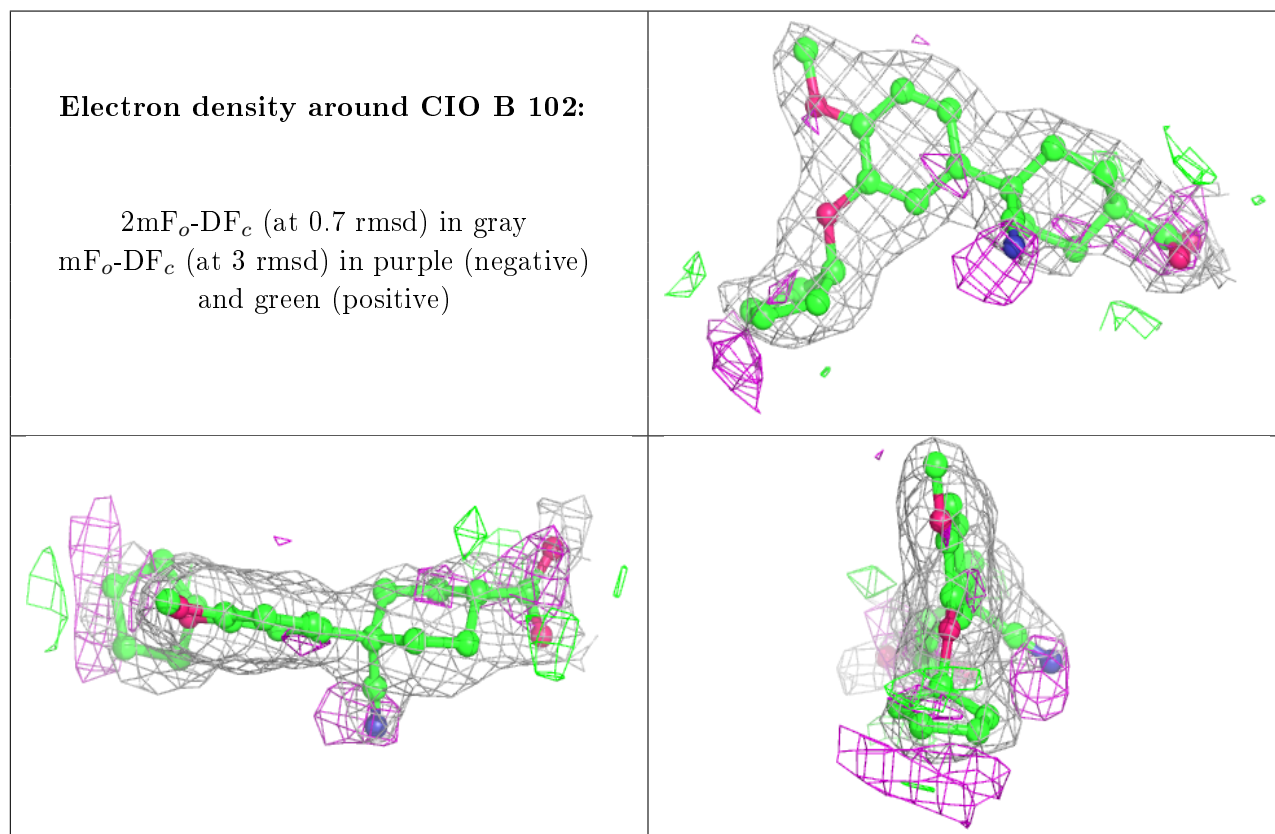
There are no carbohydrates in this entry.

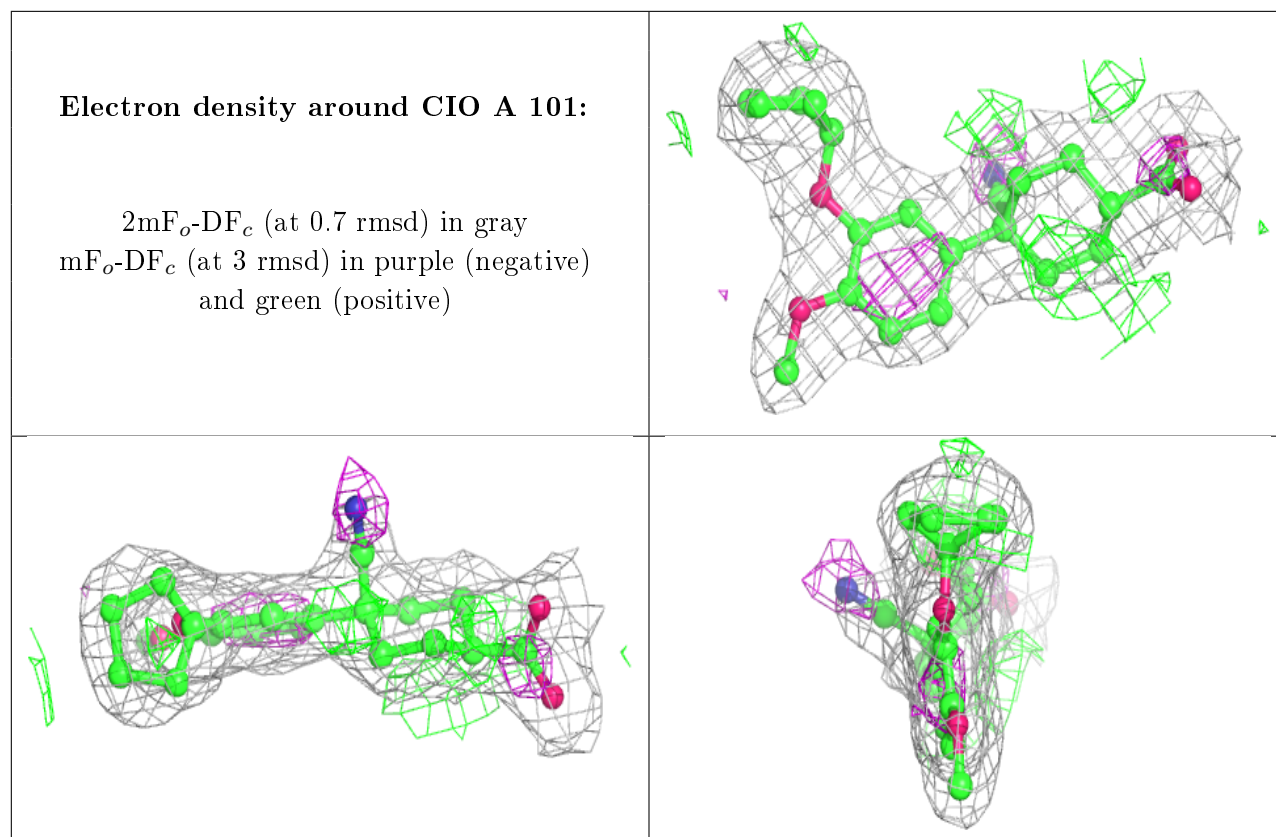
### 6.4 Ligands [i](#)

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, 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( $\text{\AA}^2$ )	Q<0.9
4	CIO	B	102	25/25	0.88	0.19	39,51,56,62	0
4	CIO	A	101	25/25	0.90	0.16	45,48,52,57	0
3	MG	A	1002	1/1	0.97	0.13	29,29,29,29	0
3	MG	B	1002	1/1	0.98	0.14	30,30,30,30	0
2	ZN	B	1001	1/1	0.99	0.05	39,39,39,39	0
2	ZN	A	1001	1/1	0.99	0.04	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.





## 6.5 Other polymers [i](#)

There are no such residues in this entry.