



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 17, 2021 – 12:43 AM EDT

PDB ID : 1RO6  
Title : Crystal structure of PDE4B2B complexed with Rolipram (R & S)  
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Deposited on : 2003-12-01  
Resolution : 2.00 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 : 2.23.2  
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) : 2.23.2

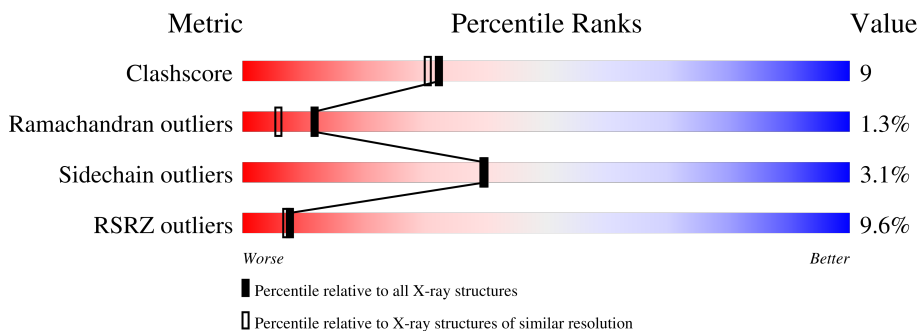
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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))
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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  $\geq 3$ , 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	378	
1	B	378	

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	ROL	A	601[B]	X	-	-	-
5	ROL	B	602[B]	X	-	-	-

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 6028 atoms, of which 84 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	344	2772	1748	469	536	19	0	0	0
1	B	344	2772	1748	469	536	19	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	151	MET	-	initiating methionine	UNP Q07343
A	487	ALA	SER	engineered mutation	UNP Q07343
A	489	ALA	SER	engineered mutation	UNP Q07343
B	151	MET	-	initiating methionine	UNP Q07343
B	487	ALA	SER	engineered mutation	UNP Q07343
B	489	ALA	SER	engineered mutation	UNP Q07343

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

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

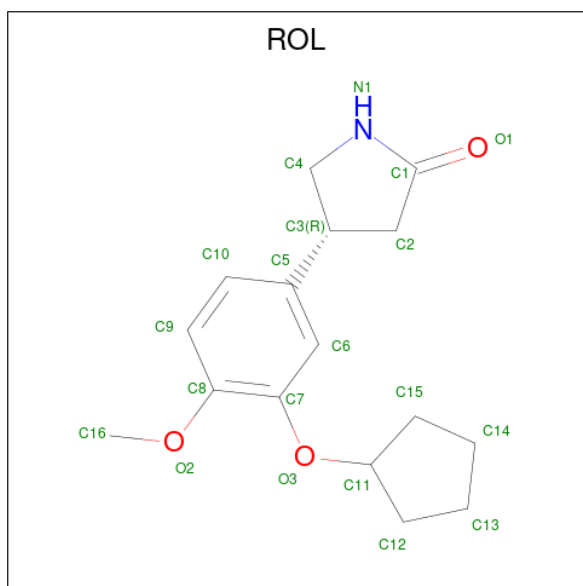
- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

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

- Molecule 4 is ARSENIC (three-letter code: ARS) (formula: As).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total As 1 1	0	0

- Molecule 5 is ROLIPRAM (three-letter code: ROL) (formula:  $C_{16}H_{21}NO_3$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	N	O		
5	A	1	Total 82	C 32	H 42	N 2	O 6	0	1
5	B	1	Total 82	C 32	H 42	N 2	O 6	0	1

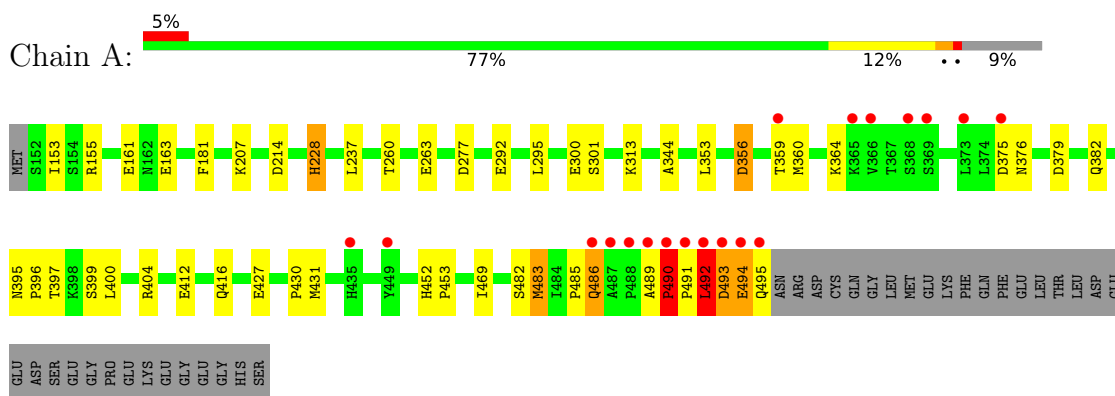
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	197	Total O 197 197	0	0
6	B	118	Total O 118 118	0	0

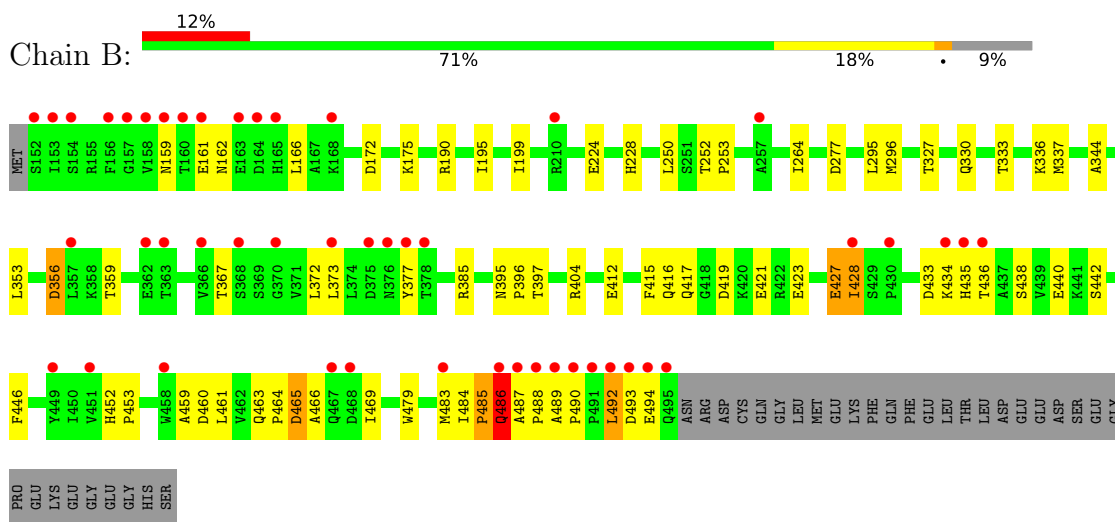
### 3 Residue-property plots [i](#)

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: cAMP-specific 3',5'-cyclic phosphodiesterase 4B



- Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4B



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	103.15Å 160.89Å 108.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00 19.89 – 1.99	Depositor EDS
% Data completeness (in resolution range)	90.5 (20.00-2.00) 89.9 (19.89-1.99)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.46 (at 1.99Å)	Xtrriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.217 , 0.245 0.214 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	28.7	Xtrriage
Anisotropy	0.383	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 52.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6028	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.73% of the height of the origin peak. No significant pseudotranslation is detected.*

<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: ROL, ARS, MN, ZN

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	0.33	0/2831	0.56	0/3843
1	B	0.31	0/2831	0.53	0/3843
All	All	0.32	0/5662	0.54	0/7686

There are no bond length outliers.

There are no bond angle outliers.

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	2772	0	2691	45	0
1	B	2772	0	2692	59	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	1	0	0	0	0
5	A	40	42	42	2	0
5	B	40	42	42	6	0
6	A	197	0	0	14	0
6	B	118	0	0	5	0
All	All	5944	84	5467	98	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 9.

All (98) 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)
6:A:763:HOH:O	1:B:490:PRO:HB3	1.74	0.87
1:A:356:ASP:HB3	1:A:382:GLN:OE1	1.79	0.82
1:B:427:GLU:O	1:B:428:ILE:HG12	1.81	0.80
1:B:404:ARG:HD3	1:B:479:TRP:CH2	2.20	0.76
1:B:435:HIS:HB2	6:B:709:HOH:O	1.85	0.74
6:A:630:HOH:O	1:B:492:LEU:HD23	1.88	0.72
1:A:397:THR:HB	1:A:469:ILE:HG23	1.72	0.70
1:B:397:THR:HB	1:B:469:ILE:HG23	1.75	0.69
1:A:483:MET:HE1	1:B:485:PRO:HD3	1.75	0.68
1:B:436:THR:HG23	6:B:709:HOH:O	1.95	0.65
1:B:228:HIS:HE1	1:B:277:ASP:OD1	1.80	0.64
1:B:433:ASP:HB3	6:B:713:HOH:O	1.97	0.64
1:B:404:ARG:HD3	1:B:479:TRP:CZ3	2.32	0.64
1:A:295:LEU:HG	6:A:795:HOH:O	1.99	0.63
1:A:228:HIS:HE1	1:A:277:ASP:OD1	1.82	0.62
1:B:417:GLN:O	1:B:421:GLU:HG3	2.00	0.61
1:A:412:GLU:HG3	6:A:790:HOH:O	2.00	0.61
1:A:489:ALA:O	1:A:490:PRO:C	2.40	0.59
1:B:419:ASP:O	1:B:423:GLU:HG3	2.02	0.59
1:B:295:LEU:HG	6:B:705:HOH:O	2.02	0.59
1:B:395:ASN:HB2	1:B:396:PRO:HD3	1.84	0.59
1:A:494:GLU:CD	1:A:495:GLN:HG2	2.24	0.58
1:B:356:ASP:O	1:B:359:THR:HG22	2.03	0.58
1:A:483:MET:HE2	1:B:485:PRO:HB3	1.85	0.57
1:B:440:GLU:HG2	1:B:483:MET:CB	2.35	0.56
1:B:372:LEU:HD11	1:B:461:LEU:HG	1.87	0.56
1:B:460:ASP:O	1:B:463:GLN:HG3	2.06	0.56
1:A:492:LEU:HG	1:B:438:SER:OG	2.05	0.55
1:A:490:PRO:HB2	1:A:494:GLU:OE2	2.06	0.55
1:A:483:MET:CE	1:B:485:PRO:HB3	2.36	0.55
1:A:485:PRO:O	1:A:486:GLN:HB2	2.06	0.55
1:A:492:LEU:HD12	1:B:440:GLU:OE1	2.07	0.55
6:A:732:HOH:O	1:B:492:LEU:HD21	2.06	0.55
1:A:416:GLN:HG3	6:A:634:HOH:O	2.06	0.55
1:A:356:ASP:HA	1:A:359:THR:HG22	1.88	0.55
1:A:360:MET:HE1	1:A:379:ASP:HA	1.89	0.55
1:A:155:ARG:NH2	1:A:214:ASP:OD1	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:395:ASN:HB2	1:A:396:PRO:HD3	1.90	0.54
1:A:344:ALA:HB1	1:A:353:LEU:HD11	1.88	0.53
1:A:494:GLU:OE2	1:A:495:GLN:HG2	2.08	0.53
1:B:172:ASP:OD1	1:B:175:LYS:HD2	2.09	0.53
1:A:404:ARG:HD2	6:A:794:HOH:O	2.10	0.52
1:B:159:ASN:HB2	1:B:162:ASN:HD22	1.75	0.52
1:B:442:SER:HB3	5:B:602[B]:ROL:H131	1.92	0.52
1:A:228:HIS:HD2	6:A:607:HOH:O	1.93	0.51
1:B:195:ILE:O	1:B:199:ILE:HG13	2.10	0.51
1:A:313:LYS:HE2	6:A:703:HOH:O	2.10	0.50
1:A:482:SER:HB2	1:A:491:PRO:HA	1.93	0.50
5:A:601[A]:ROL:C1	6:A:778:HOH:O	2.59	0.50
1:B:446:PHE:HB2	5:B:602[B]:ROL:H121	1.93	0.50
1:B:253:PRO:HD2	1:B:465:ASP:OD2	2.11	0.49
1:B:492:LEU:HD13	1:B:493:ASP:CG	2.33	0.49
1:A:492:LEU:O	1:A:493:ASP:HB3	2.11	0.49
1:B:440:GLU:HG2	1:B:483:MET:HB3	1.94	0.49
1:B:442:SER:HB3	5:B:602[A]:ROL:C13	2.42	0.49
1:B:327:THR:OG1	1:B:330:GLN:HG3	2.13	0.49
1:B:367:THR:HG22	1:B:373:LEU:HD12	1.95	0.49
1:A:452:HIS:HB3	1:A:453:PRO:HD3	1.95	0.48
1:A:181:PHE:CD1	1:A:237:LEU:HD21	2.49	0.48
1:B:412:GLU:O	1:B:416:GLN:HG3	2.14	0.48
1:A:356:ASP:O	1:A:359:THR:HG22	2.14	0.47
1:B:344:ALA:HB1	1:B:353:LEU:HD11	1.96	0.47
1:B:190:ARG:HH11	1:B:224:GLU:HG2	1.78	0.47
1:B:415:PHE:CE1	1:B:434:LYS:HA	2.50	0.47
1:A:494:GLU:OE1	1:A:495:GLN:HG2	2.14	0.47
1:B:452:HIS:HB3	1:B:453:PRO:HD3	1.98	0.46
1:B:484:ILE:HA	1:B:485:PRO:HD2	1.75	0.46
1:A:400:LEU:HD23	1:B:483:MET:HG2	1.98	0.46
1:B:395:ASN:HD22	5:B:602[B]:ROL:H91	1.80	0.46
1:A:260:THR:OG1	1:A:263:GLU:HG3	2.15	0.46
1:B:250:LEU:HD13	1:B:264:ILE:HG23	1.98	0.46
1:A:376:ASN:OD1	1:A:379:ASP:HB2	2.16	0.45
1:B:442:SER:HB3	5:B:602[B]:ROL:C13	2.46	0.45
1:A:492:LEU:HB3	6:A:690:HOH:O	2.16	0.45
1:B:492:LEU:C	1:B:492:LEU:HD22	2.37	0.45
1:A:153:ILE:HG13	1:A:163:GLU:OE2	2.17	0.44
1:A:490:PRO:N	1:A:491:PRO:HD3	2.33	0.44
1:B:336:LYS:HE3	1:B:377:TYR:OH	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:395:ASN:HD22	5:A:601[B]:ROL:H91	1.83	0.43
1:B:440:GLU:HG2	1:B:483:MET:HB2	2.00	0.43
1:B:489:ALA:N	1:B:490:PRO:HD3	2.33	0.43
1:A:430:PRO:O	1:A:431:MET:HB2	2.19	0.42
1:B:353:LEU:HD21	1:B:385:ARG:CD	2.49	0.42
1:B:459:ALA:HA	1:B:466:ALA:HB3	2.02	0.42
1:B:485:PRO:O	1:B:486:GLN:O	2.38	0.42
1:B:296:MET:HE1	6:B:669:HOH:O	2.19	0.42
1:A:207:LYS:HE3	6:A:663:HOH:O	2.20	0.41
1:B:488:PRO:C	1:B:490:PRO:HD3	2.40	0.41
1:A:485:PRO:O	1:A:486:GLN:CB	2.68	0.41
1:B:442:SER:HB3	5:B:602[A]:ROL:H132	2.01	0.41
1:A:300:GLU:O	1:A:301:SER:C	2.59	0.41
1:A:364:LYS:HG3	1:A:364:LYS:O	2.21	0.41
1:B:333:THR:O	1:B:337:MET:HG3	2.19	0.41
1:A:491:PRO:O	1:A:492:LEU:HB2	2.21	0.41
1:A:412:GLU:CG	6:A:655:HOH:O	2.68	0.40
1:B:252:THR:O	1:B:252:THR:HG23	2.22	0.40
1:A:492:LEU:HD11	1:B:483:MET:O	2.22	0.40
6:A:732:HOH:O	1:B:492:LEU:HD11	2.21	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	342/378 (90%)	330 (96%)	8 (2%)	4 (1%)	13   7
1	B	342/378 (90%)	328 (96%)	9 (3%)	5 (2%)	10   4
All	All	684/756 (90%)	658 (96%)	17 (2%)	9 (1%)	12   6

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	490	PRO
1	A	492	LEU
1	B	427	GLU
1	B	486	GLN
1	A	486	GLN
1	A	493	ASP
1	B	428	ILE
1	B	485	PRO
1	B	487	ALA

### 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	311/341 (91%)	300 (96%)	11 (4%)	36	35
1	B	311/341 (91%)	303 (97%)	8 (3%)	46	48
All	All	622/682 (91%)	603 (97%)	19 (3%)	40	40

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	161	GLU
1	A	228	HIS
1	A	292	GLU
1	A	356	ASP
1	A	375	ASP
1	A	399	SER
1	A	427	GLU
1	A	483	MET
1	A	490	PRO
1	A	492	LEU
1	A	494	GLU
1	B	161	GLU
1	B	166	LEU
1	B	356	ASP
1	B	464	PRO

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Mol	Chain	Res	Type
1	B	465	ASP
1	B	486	GLN
1	B	492	LEU
1	B	494	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	228	HIS
1	A	395	ASN
1	A	463	GLN
1	A	486	GLN
1	B	162	ASN
1	B	228	HIS
1	B	395	ASN

### 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](#)

Of 9 ligands modelled in this entry, 5 are monoatomic - leaving 4 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
5	ROL	A	601[B]	-	22,22,22	0.99	1 (4%)	28,30,30	1.07	1 (3%)
5	ROL	B	602[B]	-	22,22,22	1.02	2 (9%)	28,30,30	1.15	2 (7%)
5	ROL	A	601[A]	-	22,22,22	1.07	2 (9%)	28,30,30	1.07	1 (3%)
5	ROL	B	602[A]	-	22,22,22	1.16	3 (13%)	28,30,30	1.09	1 (3%)

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
5	ROL	A	601[B]	-	1/1/4/4	0/10/26/26	0/3/3/3
5	ROL	B	602[B]	-	1/1/4/4	2/10/26/26	0/3/3/3
5	ROL	A	601[A]	-	-	0/10/26/26	0/3/3/3
5	ROL	B	602[A]	-	-	2/10/26/26	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	602[A]	ROL	O2-C8	2.72	1.41	1.37
5	B	602[B]	ROL	O2-C8	2.56	1.41	1.37
5	B	602[A]	ROL	C2-C1	2.49	1.54	1.51
5	A	601[A]	ROL	C6-C7	2.29	1.43	1.38
5	A	601[A]	ROL	C2-C1	2.26	1.54	1.51
5	B	602[A]	ROL	C6-C7	2.17	1.42	1.38
5	A	601[B]	ROL	C6-C7	2.08	1.42	1.38
5	B	602[B]	ROL	C6-C7	2.02	1.42	1.38

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	602[A]	ROL	C3-C4-N1	3.89	106.30	103.02
5	A	601[A]	ROL	C3-C4-N1	3.49	105.96	103.02
5	B	602[B]	ROL	C3-C4-N1	2.86	105.43	103.02
5	A	601[B]	ROL	C3-C4-N1	2.72	105.31	103.02
5	B	602[B]	ROL	O1-C1-C2	-2.09	123.63	126.39

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	601[B]	ROL	C3
5	B	602[B]	ROL	C3

All (4) torsion outliers are listed below:

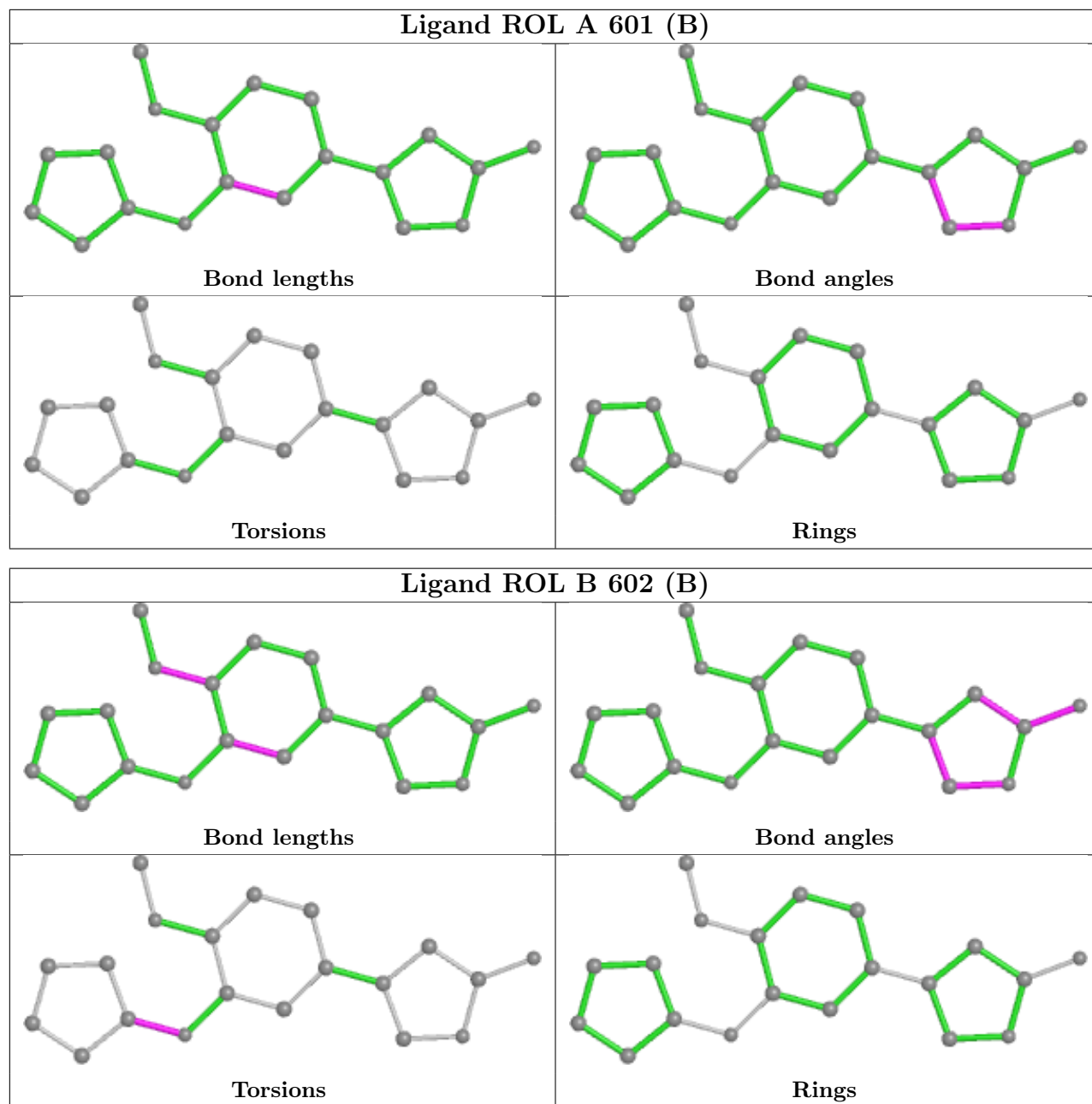
Mol	Chain	Res	Type	Atoms
5	B	602[B]	ROL	C12-C11-O3-C7
5	B	602[B]	ROL	C15-C11-O3-C7
5	B	602[A]	ROL	C15-C11-O3-C7
5	B	602[A]	ROL	C12-C11-O3-C7

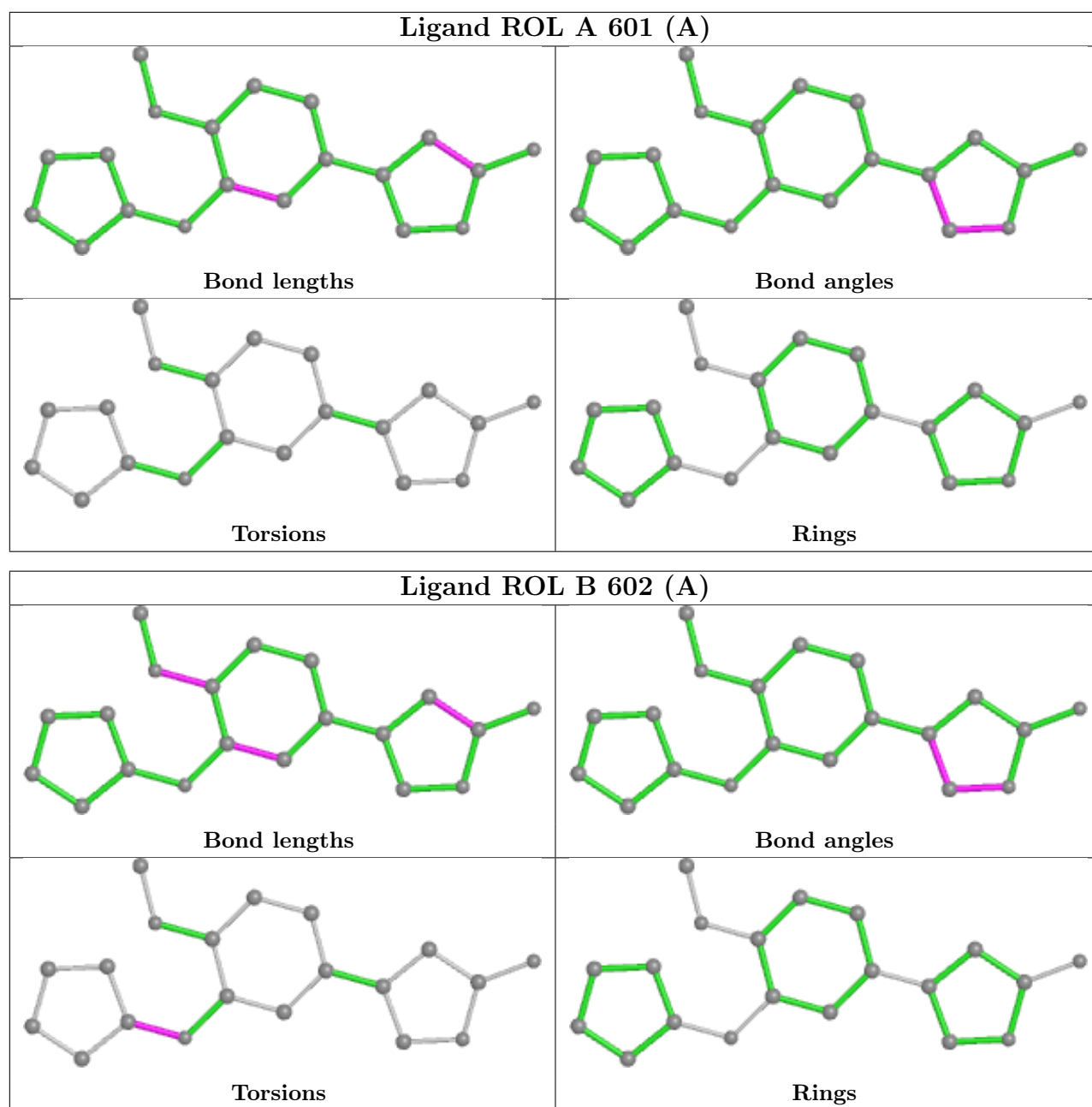
There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	601[B]	ROL	1	0
5	B	602[B]	ROL	4	0
5	A	601[A]	ROL	1	0
5	B	602[A]	ROL	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 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

### 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	344/378 (91%)	0.33	19 (5%) 25 24	17, 30, 71, 109	0
1	B	344/378 (91%)	0.82	47 (13%) 3 2	21, 41, 85, 110	0
All	All	688/756 (91%)	0.57	66 (9%) 8 7	17, 36, 75, 110	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	492	LEU	16.7
1	A	489	ALA	11.9
1	B	487	ALA	10.8
1	B	489	ALA	10.8
1	A	488	PRO	9.7
1	B	160	THR	9.4
1	B	493	ASP	9.2
1	A	495	GLN	9.1
1	A	490	PRO	8.8
1	B	490	PRO	8.8
1	A	487	ALA	8.7
1	B	491	PRO	8.6
1	A	494	GLU	8.3
1	B	495	GLN	7.8
1	A	492	LEU	7.8
1	A	491	PRO	7.5
1	B	488	PRO	7.4
1	B	152	SER	7.3
1	B	154	SER	5.6
1	B	159	ASN	5.6
1	B	494	GLU	5.4
1	B	428	ILE	5.3
1	B	157	GLY	4.9
1	B	158	VAL	4.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	435	HIS	4.1
1	A	435	HIS	4.1
1	B	486	GLN	4.0
1	B	257	ALA	4.0
1	A	368	SER	3.9
1	A	493	ASP	3.7
1	B	363	THR	3.6
1	A	375	ASP	3.5
1	B	370	GLY	3.3
1	A	365	LYS	3.3
1	B	373	LEU	3.3
1	A	369	SER	3.2
1	B	436	THR	3.2
1	B	153	ILE	3.2
1	B	430	PRO	3.1
1	A	366	VAL	3.1
1	B	366	VAL	3.0
1	B	163	GLU	3.0
1	A	486	GLN	3.0
1	A	449	TYR	2.9
1	B	378	THR	2.9
1	B	161	GLU	2.9
1	B	362	GLU	2.9
1	A	373	LEU	2.6
1	B	156	PHE	2.6
1	B	368	SER	2.6
1	B	357	LEU	2.6
1	B	468	ASP	2.5
1	B	377	TYR	2.5
1	B	376	ASN	2.5
1	B	165	HIS	2.4
1	B	375	ASP	2.4
1	A	359	THR	2.4
1	B	164	ASP	2.3
1	B	467	GLN	2.3
1	B	451	VAL	2.2
1	B	168	LYS	2.2
1	B	434	LYS	2.2
1	B	210	ARG	2.1
1	B	449	TYR	2.1
1	B	458	TRP	2.1
1	B	483	MET	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 monosaccharides in this entry.

## 6.4 Ligands [i](#)

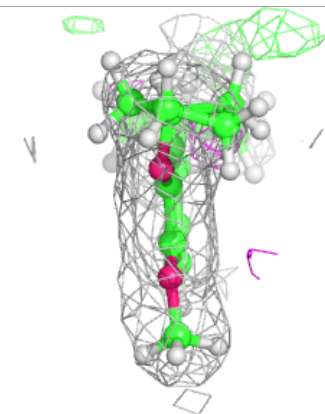
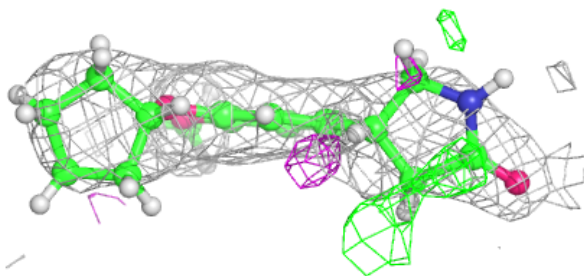
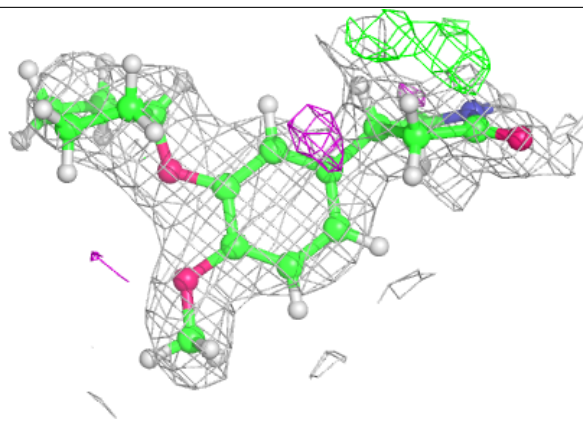
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
5	ROL	B	602[A]	20/20	0.86	0.22	41,42,43,43	41
5	ROL	B	602[B]	20/20	0.86	0.22	42,44,45,45	41
5	ROL	A	601[B]	20/20	0.88	0.20	38,39,39,40	41
3	MN	A	530	1/1	0.88	0.15	79,79,79,79	0
5	ROL	A	601[A]	20/20	0.88	0.20	34,36,37,38	41
3	MN	B	530	1/1	0.95	0.10	79,79,79,79	0
4	ARS	A	531	1/1	0.96	0.08	59,59,59,59	0
2	ZN	B	529	1/1	1.00	0.07	29,29,29,29	0
2	ZN	A	529	1/1	1.00	0.08	24,24,24,24	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.

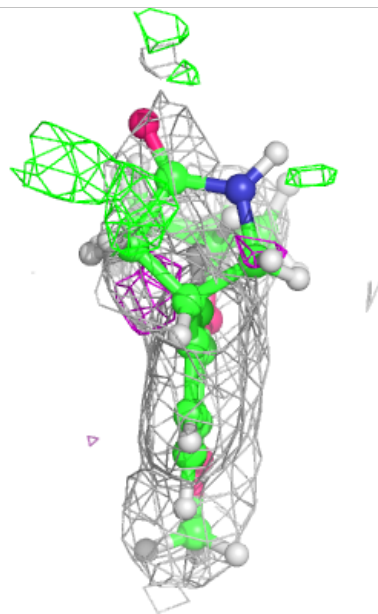
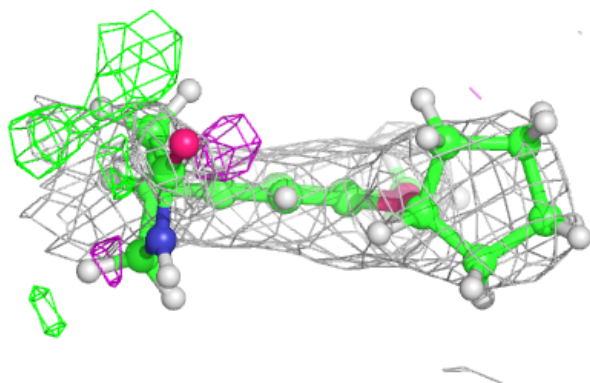
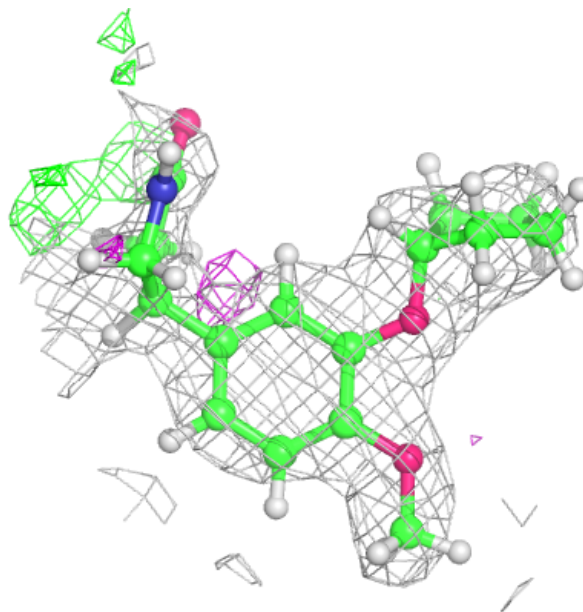
**Electron density around ROL B 602 (A):**

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



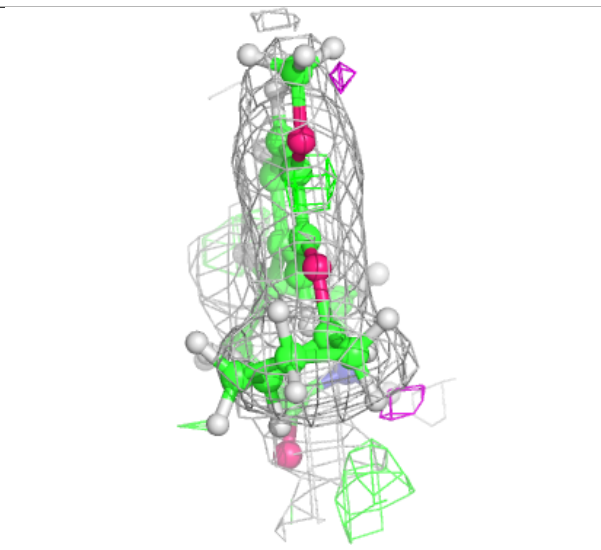
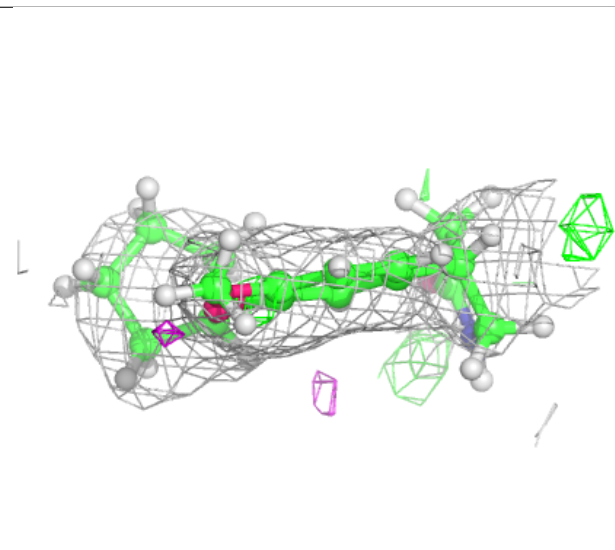
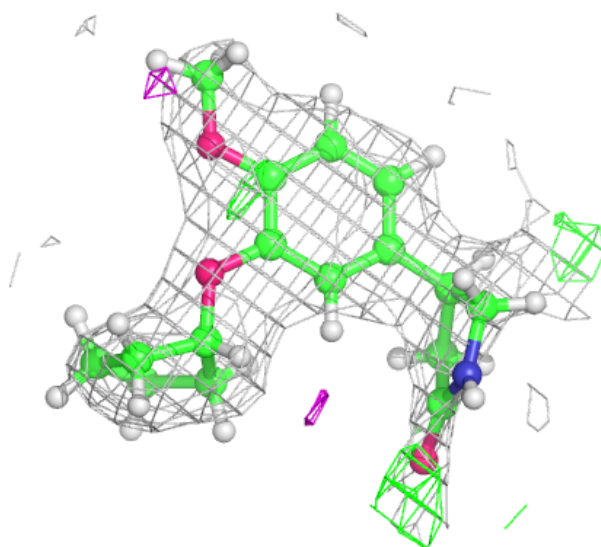
**Electron density around ROL B 602 (B):**

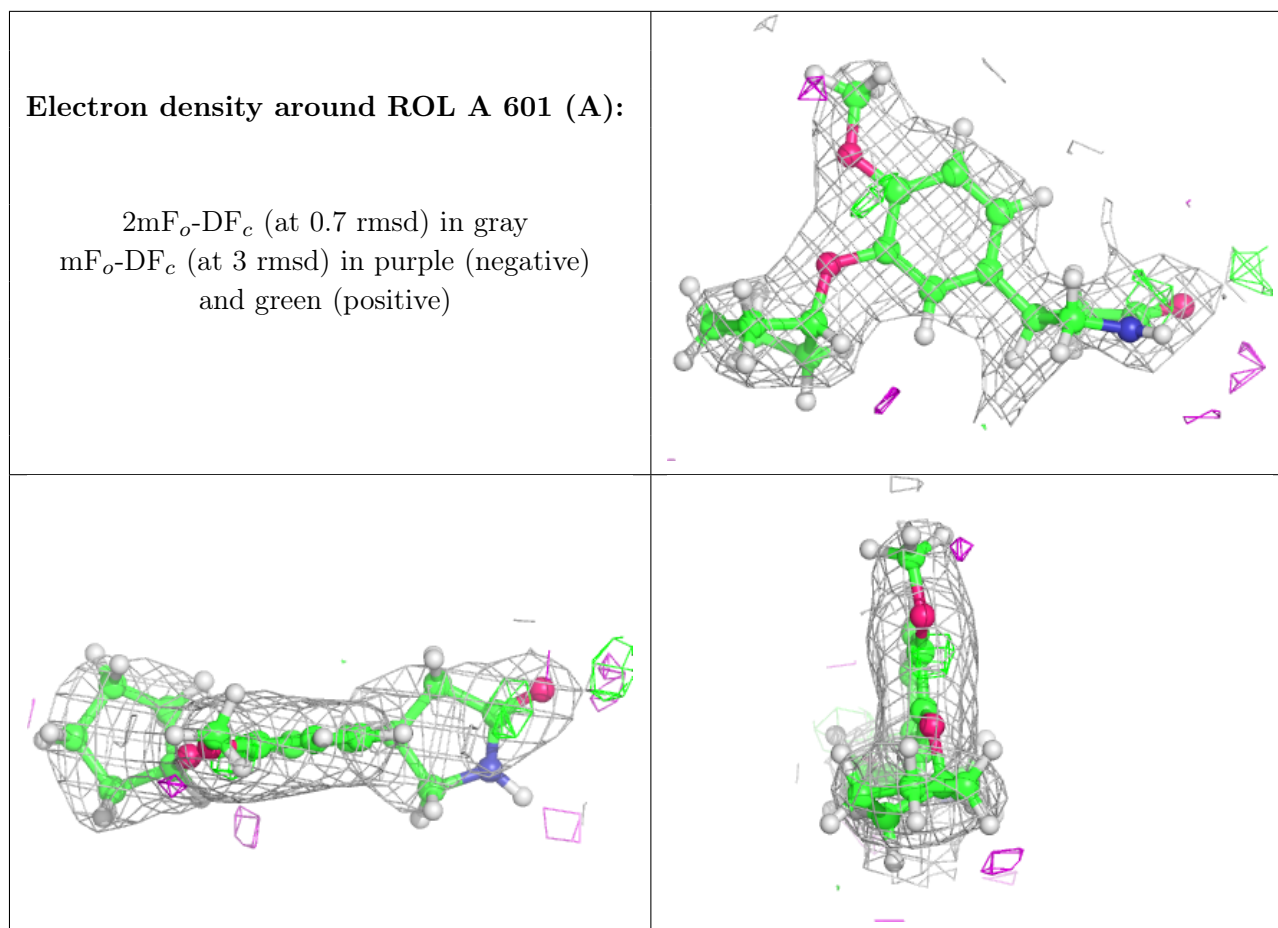
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around ROL A 601 (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.