



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:12 PM UTC

PDB ID : 1RO6 / pdb_00001ro6
Title : Crystal structure of PDE4B2B complexed with Rolipram (R & S)
Authors : Xu, R.X.; Rocque, W.J.; Lambert, M.H.; Vanderwall, D.E.; Nolte, R.T.
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

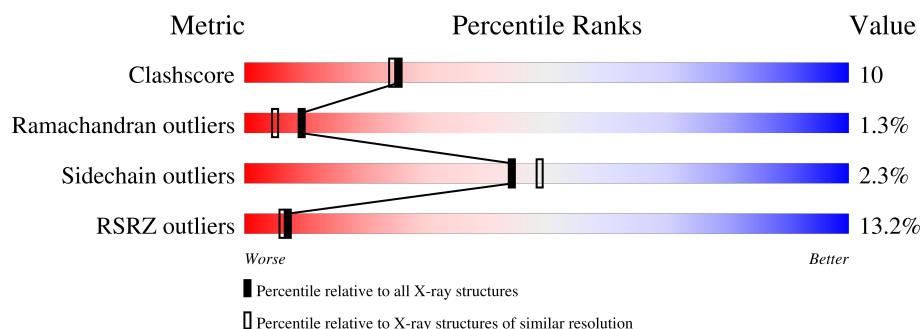
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (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 ≥ 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	 8% 75% 14% .. 9%
1	B	378	 16% 67% 22% • 9%

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

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
1	A	344	Total	C	N	O	S	0	0	0
			2772	1748	469	536	19			
1	B	344	Total	C	N	O	S	0	0	0
			2772	1748	469	536	19			

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 (CCD ID: ZN) (formula: Zn).

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

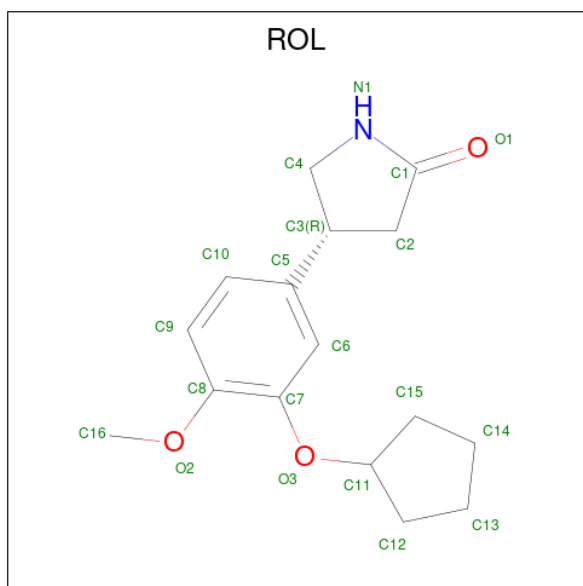
- Molecule 3 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

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

- Molecule 4 is ARSENIC (CCD ID: ARS) (formula: As).

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

- Molecule 5 is ROLIPRAM (CCD ID: ROL) (formula: $C_{16}H_{21}NO_3$).



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

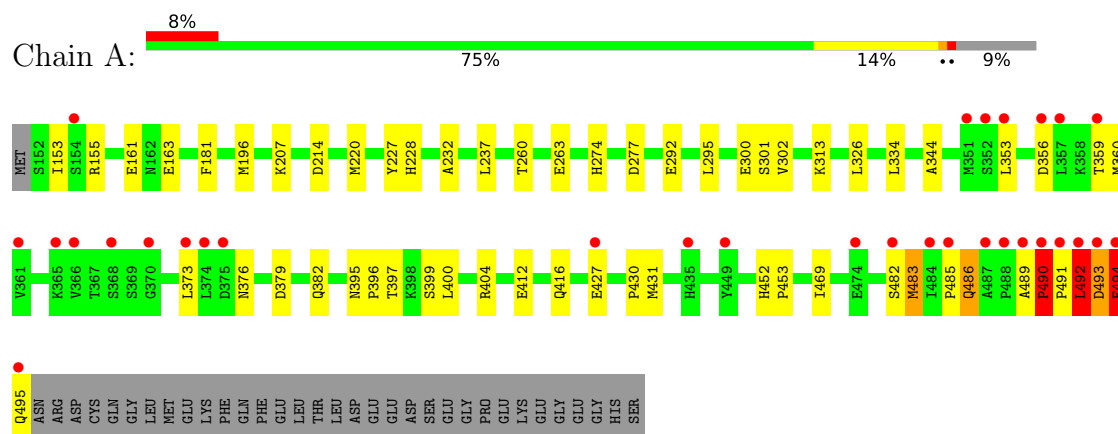
- Molecule 6 is water.

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

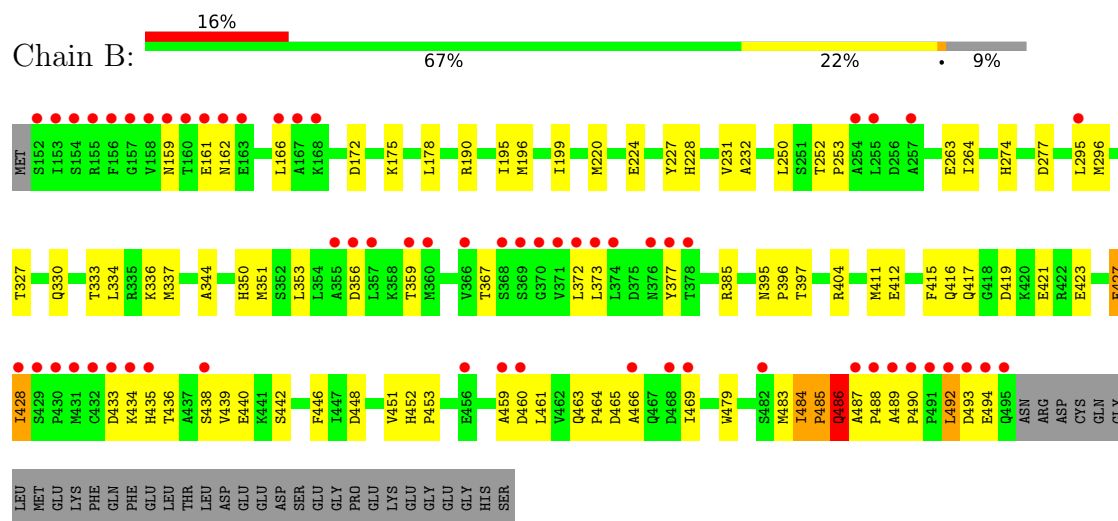
3 Residue-property plots [i](#)

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, α , β , γ	103.15Å 160.89Å 108.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00 20.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	90.5 (20.00-2.00) 90.2 (20.00-2.00)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.46 (at 1.99Å)	Xtriage
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 ²)	28.7	Xtriage
Anisotropy	0.383	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 40.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6028	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage'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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ARS, ROL, ZN, MN

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	0.43	0/2831	0.85	8/3843 (0.2%)
1	B	0.39	0/2831	0.85	8/3843 (0.2%)
All	All	0.41	0/5662	0.85	16/7686 (0.2%)

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	494	GLU	N-CA-C	7.63	117.26	108.49
1	B	484	ILE	CA-C-N	7.17	128.80	119.84
1	B	484	ILE	C-N-CA	7.17	128.80	119.84
1	A	274	HIS	N-CA-C	7.16	121.12	112.38
1	A	232	ALA	N-CA-C	6.78	118.67	111.28
1	B	274	HIS	N-CA-C	6.37	120.15	112.38
1	B	232	ALA	N-CA-C	6.09	118.70	111.33
1	B	451	VAL	N-CA-C	5.92	116.10	110.42
1	A	490	PRO	CA-C-N	5.73	127.00	119.84
1	A	490	PRO	C-N-CA	5.73	127.00	119.84
1	A	227	TYR	N-CA-C	-5.72	100.35	109.96
1	A	326	LEU	N-CA-C	-5.40	101.73	110.32
1	B	231	VAL	N-CA-C	-5.31	100.23	107.99
1	B	227	TYR	N-CA-C	-5.27	101.11	109.96
1	B	448	ASP	N-CA-C	5.26	117.02	111.28
1	A	302	VAL	N-CA-C	5.17	115.61	110.23

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	2772	0	2691	48	0
1	B	2772	0	2692	65	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	107	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 10.

All (107) 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:A:483:MET:HE2	1:B:485:PRO:HB3	1.49	0.91
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:B:350:HIS:HD2	1:B:351:MET:HE2	1.59	0.68
1:B:436:THR:HG23	6:B:709:HOH:O	1.95	0.65
1:A:489:ALA:O	1:A:490:PRO:C	2.40	0.64
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:494:GLU:CD	1:A:495:GLN:HG2	2.24	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:356:ASP:O	1:B:359:THR:HG22	2.03	0.58
1:A:360:MET:HE1	1:A:379:ASP:HA	1.86	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:485:PRO:O	1:A:486:GLN:HB2	2.06	0.55
1:B:411:MET:HE2	1:B:439:VAL:HG22	1.88	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:155:ARG:NH2	1:A:214:ASP:OD1	2.40	0.54
1:B:492:LEU:HD13	1:B:493:ASP:CG	2.33	0.54
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:A:196:MET:HG3	1:A:220:MET:HE2	1.90	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:B:263:GLU:HA	1:B:337:MET:HE1	1.92	0.50
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:492:LEU:C	1:B:492:LEU:HD22	2.37	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:296:MET:HE1	6:B:669:HOH:O	2.14	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:A:483:MET:HE2	1:B:485:PRO:CB	2.32	0.47
1:B:344:ALA:HB1	1:B:353:LEU:HD11	1.96	0.47
1:A:483:MET:HE1	1:A:492:LEU:HD22	1.97	0.47
1:B:190:ARG:HH11	1:B:224:GLU:HG2	1.78	0.47
1:B:488:PRO:C	1:B:490:PRO:HD3	2.40	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:300:GLU:O	1:A:301:SER:C	2.59	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:B:196:MET:HG3	1:B:220:MET:HE2	1.97	0.45
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: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
1:A:395:ASN:HD22	5:A:601[B]:ROL:H91	1.83	0.43
1:A:483:MET:CE	1:B:485:PRO:HB3	2.36	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:B:178:LEU:C	1:B:178:LEU:HD23	2.44	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:334:LEU:C	1:B:334:LEU:HD23	2.45	0.42
1:A:207:LYS:HE3	6:A:663:HOH:O	2.20	0.41
1:A:485:PRO:O	1:A:486:GLN:CB	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:442:SER:HB3	5:B:602[A]:ROL:H132	2.01	0.41
1:B:333:THR:O	1:B:337:MET:HG3	2.19	0.41
1:A:373:LEU:HD23	1:A:373:LEU:C	2.45	0.41
1:A:491:PRO:O	1:A:492:LEU:HB2	2.21	0.41
1:A:334:LEU:C	1:A:334:LEU:HD23	2.46	0.40
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

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	342/378 (90%)	330 (96%)	8 (2%)	4 (1%)	10	6
1	B	342/378 (90%)	328 (96%)	9 (3%)	5 (2%)	8	4
All	All	684/756 (90%)	658 (96%)	17 (2%)	9 (1%)	9	5

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 ⓘ

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%)	303 (97%)	8 (3%)	40	44
1	B	311/341 (91%)	305 (98%)	6 (2%)	50	56
All	All	622/682 (91%)	608 (98%)	14 (2%)	44	49

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	161	GLU
1	A	292	GLU
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	464	PRO
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 (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	189	ASN
1	A	228	HIS
1	A	332	GLN
1	A	463	GLN
1	A	476	ASN
1	A	486	GLN
1	B	162	ASN
1	B	188	HIS

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Mol	Chain	Res	Type
1	B	228	HIS
1	B	284	GLN
1	B	376	ASN
1	B	476	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	B	602[A]	-	22,22,22	1.17	3 (13%)	30,30,30	1.25	2 (6%)
5	ROL	A	601[B]	-	22,22,22	1.00	1 (4%)	30,30,30	1.04	2 (6%)
5	ROL	A	601[A]	-	22,22,22	1.09	2 (9%)	30,30,30	1.15	2 (6%)
5	ROL	B	602[B]	-	22,22,22	1.03	2 (9%)	30,30,30	1.18	4 (13%)

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

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	2.66	1.41	1.37
5	B	602[B]	ROL	O2-C8	2.51	1.41	1.37
5	A	601[A]	ROL	C6-C7	2.41	1.43	1.38
5	B	602[A]	ROL	C2-C1	2.40	1.54	1.51
5	B	602[A]	ROL	C6-C7	2.29	1.42	1.38
5	A	601[B]	ROL	C6-C7	2.18	1.42	1.38
5	A	601[A]	ROL	C2-C1	2.18	1.54	1.51
5	B	602[B]	ROL	C6-C7	2.12	1.42	1.38

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	602[A]	ROL	C3-C4-N1	3.85	106.30	103.09
5	B	602[A]	ROL	C4-N1-C1	-3.56	110.68	114.13
5	A	601[A]	ROL	C3-C4-N1	3.44	105.96	103.09
5	B	602[B]	ROL	C3-C4-N1	2.81	105.43	103.09
5	A	601[B]	ROL	C3-C4-N1	2.66	105.31	103.09
5	A	601[A]	ROL	C4-N1-C1	-2.59	111.62	114.13
5	B	602[B]	ROL	O1-C1-C2	-2.24	123.63	126.48
5	B	602[B]	ROL	O2-C8-C7	2.04	118.17	115.40
5	A	601[B]	ROL	O1-C1-C2	-2.00	123.93	126.48
5	B	602[B]	ROL	C4-N1-C1	-2.00	112.19	114.13

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

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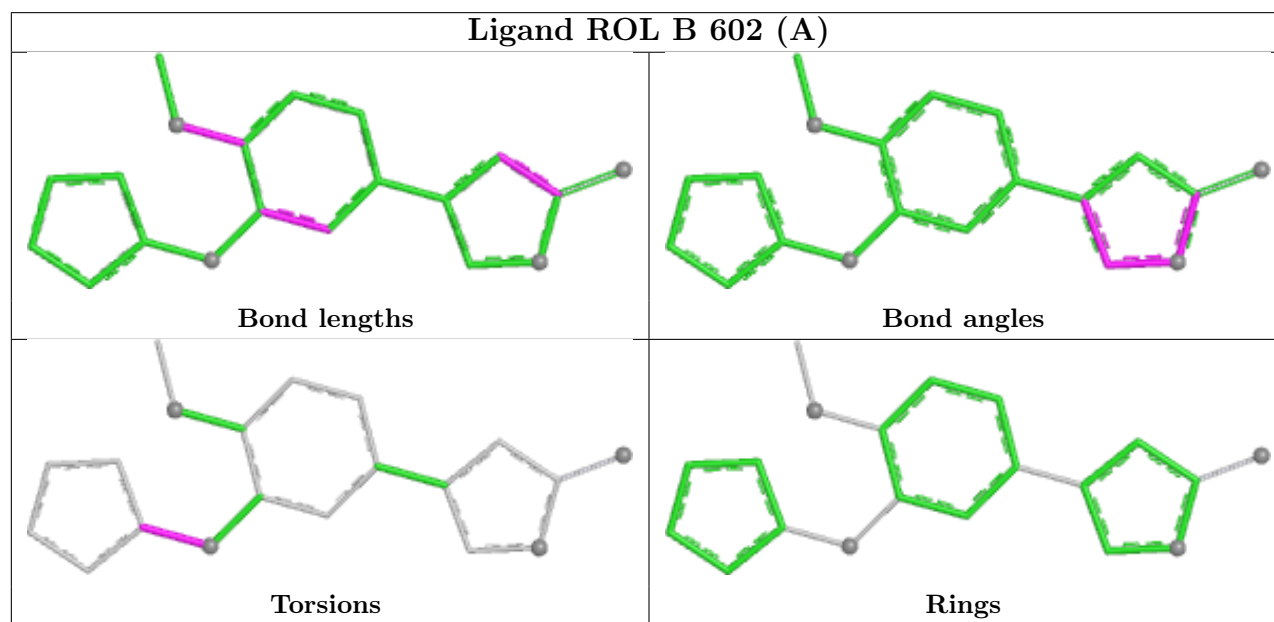
Mol	Chain	Res	Type	Atoms
5	B	602[A]	ROL	C15-C11-O3-C7
5	B	602[A]	ROL	C12-C11-O3-C7

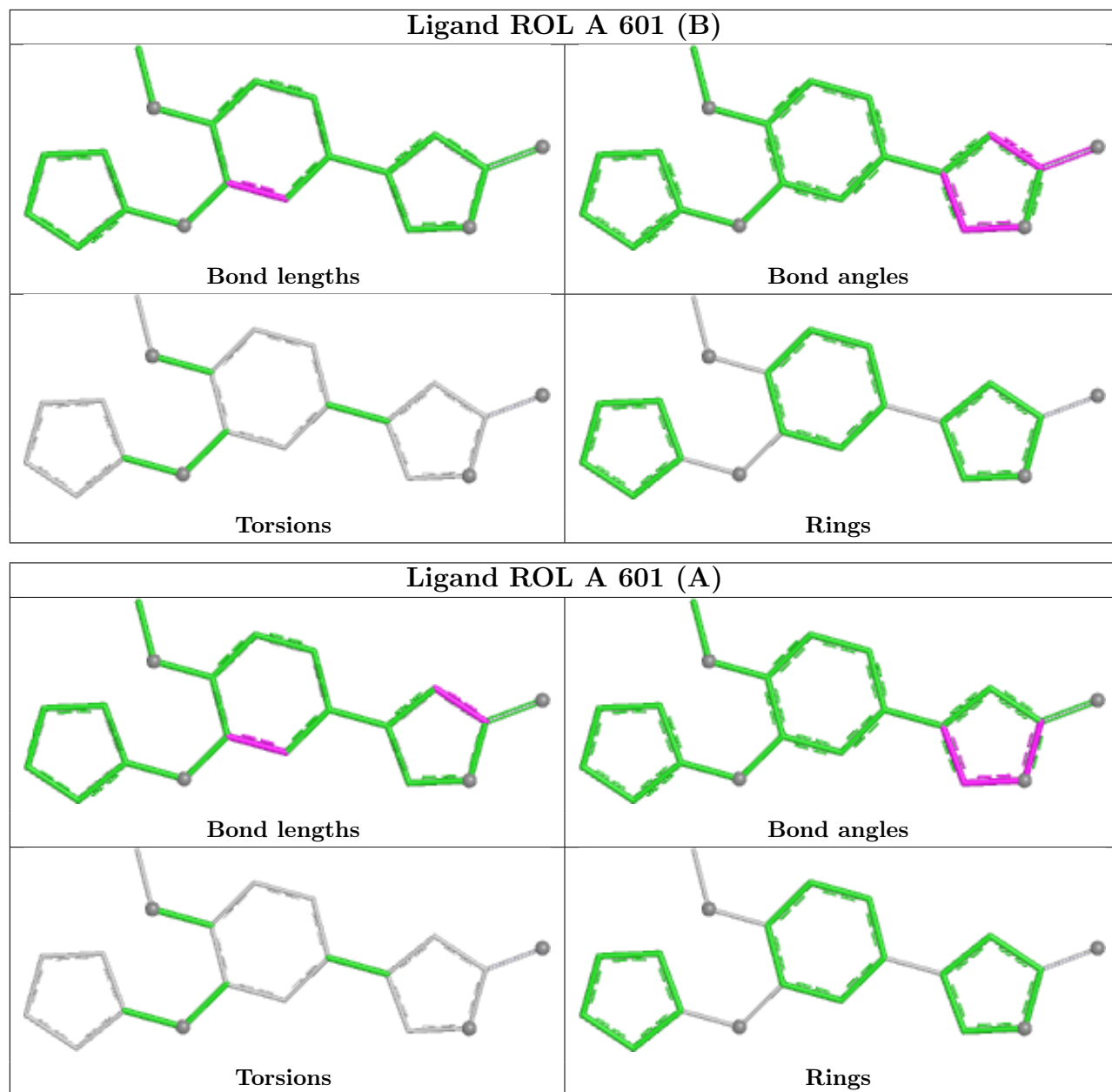
There are no ring outliers.

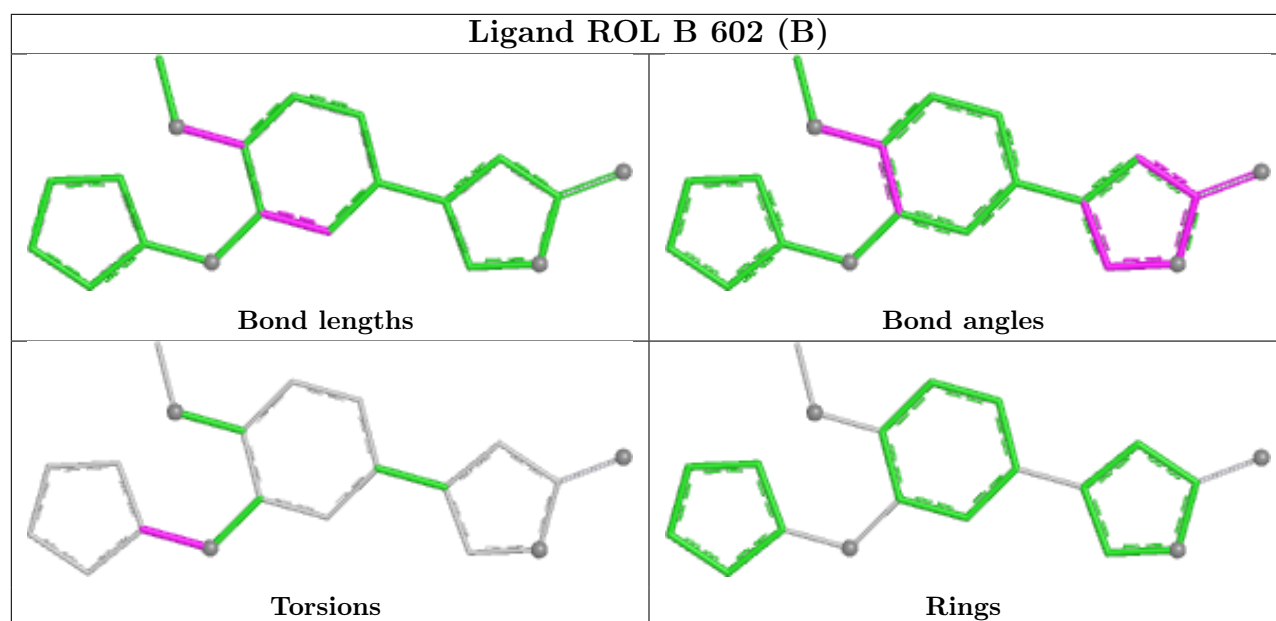
4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	602[A]	ROL	2	0
5	A	601[B]	ROL	1	0
5	A	601[A]	ROL	1	0
5	B	602[B]	ROL	4	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, 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	344/378 (91%)	0.46	31 (9%) 15 14	17, 30, 71, 109	0
1	B	344/378 (91%)	1.08	60 (17%) 4 3	21, 41, 85, 110	0
All	All	688/756 (91%)	0.77	91 (13%) 7 6	17, 36, 75, 110	0

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	492	LEU	9.8
1	B	489	ALA	8.7
1	B	491	PRO	8.5
1	B	487	ALA	6.8
1	B	156	PHE	5.9
1	A	489	ALA	5.9
1	B	157	GLY	5.8
1	B	492	LEU	5.6
1	B	160	THR	5.5
1	B	490	PRO	5.3
1	A	487	ALA	5.1
1	A	490	PRO	5.0
1	B	153	ILE	4.7
1	B	430	PRO	4.6
1	B	368	SER	4.4
1	B	488	PRO	4.4
1	B	370	GLY	4.3
1	B	154	SER	4.3
1	A	491	PRO	4.3
1	B	493	ASP	4.2
1	B	428	ILE	4.2
1	B	372	LEU	4.0
1	B	158	VAL	3.9
1	A	488	PRO	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	482	SER	3.8
1	B	152	SER	3.7
1	B	369	SER	3.7
1	A	373	LEU	3.7
1	A	493	ASP	3.6
1	A	494	GLU	3.6
1	B	435	HIS	3.5
1	A	359	THR	3.3
1	B	166	LEU	3.2
1	B	495	GLN	3.2
1	A	484	ILE	3.1
1	B	371	VAL	3.1
1	A	357	LEU	3.1
1	B	374	LEU	3.1
1	B	431	MET	3.1
1	A	495	GLN	3.0
1	B	494	GLU	3.0
1	B	460	ASP	3.0
1	B	359	THR	3.0
1	A	485	PRO	2.9
1	B	257	ALA	2.9
1	B	378	THR	2.9
1	B	373	LEU	2.8
1	B	433	ASP	2.8
1	B	468	ASP	2.8
1	A	427	GLU	2.8
1	B	466	ALA	2.7
1	B	429	SER	2.7
1	A	352	SER	2.7
1	B	432	CYS	2.7
1	A	375	ASP	2.6
1	A	435	HIS	2.6
1	B	459	ALA	2.5
1	B	254	ALA	2.5
1	B	162	ASN	2.5
1	B	366	VAL	2.4
1	A	154	SER	2.4
1	A	353	LEU	2.4
1	B	155	ARG	2.4
1	B	376	ASN	2.4
1	B	356	ASP	2.4
1	B	434	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	355	ALA	2.4
1	A	365	LYS	2.3
1	B	482	SER	2.3
1	B	159	ASN	2.3
1	A	351	MET	2.3
1	B	438	SER	2.3
1	B	255	LEU	2.3
1	B	377	TYR	2.3
1	B	168	LYS	2.2
1	B	469	ILE	2.2
1	B	167	ALA	2.2
1	A	356	ASP	2.2
1	B	360	MET	2.2
1	A	361	VAL	2.2
1	A	368	SER	2.2
1	A	474	GLU	2.1
1	B	163	GLU	2.1
1	B	161	GLU	2.1
1	A	370	GLY	2.1
1	A	374	LEU	2.1
1	B	357	LEU	2.1
1	B	456	GLU	2.1
1	A	366	VAL	2.1
1	B	295	LEU	2.0
1	A	449	TYR	2.0

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 oligosaccharides in this entry.

6.4 Ligands ⓘ

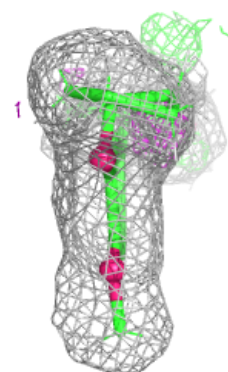
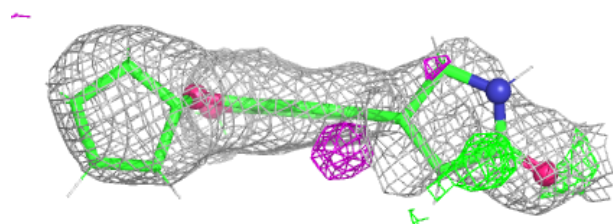
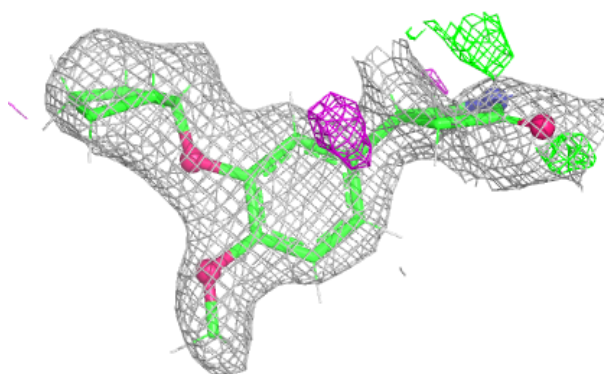
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	ROL	B	602[A]	20/20	0.75	0.15	41,42,43,43	41
5	ROL	B	602[B]	20/20	0.75	0.15	42,44,45,45	41
5	ROL	A	601[A]	20/20	0.80	0.13	34,36,37,38	41
5	ROL	A	601[B]	20/20	0.80	0.13	38,39,39,40	41
3	MN	A	530	1/1	0.88	0.22	79,79,79,79	0
3	MN	B	530	1/1	0.94	0.15	79,79,79,79	0
4	ARS	A	531	1/1	0.96	0.09	59,59,59,59	0
2	ZN	B	529	1/1	1.00	0.02	29,29,29,29	0
2	ZN	A	529	1/1	1.00	0.04	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.

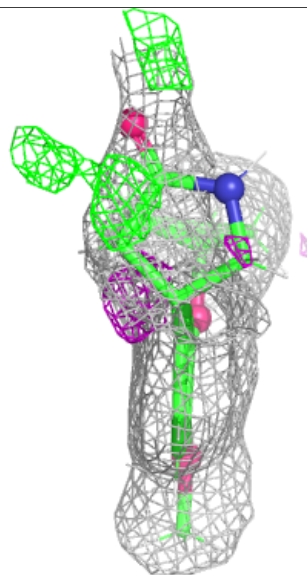
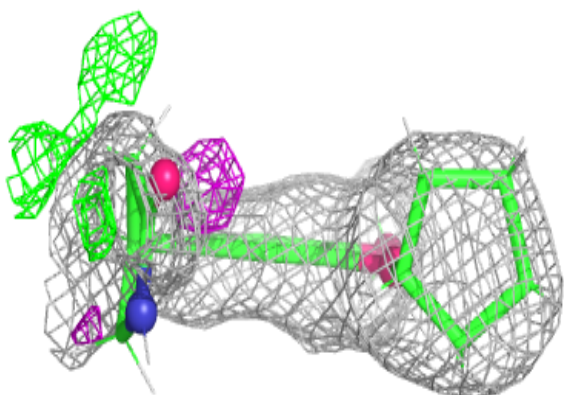
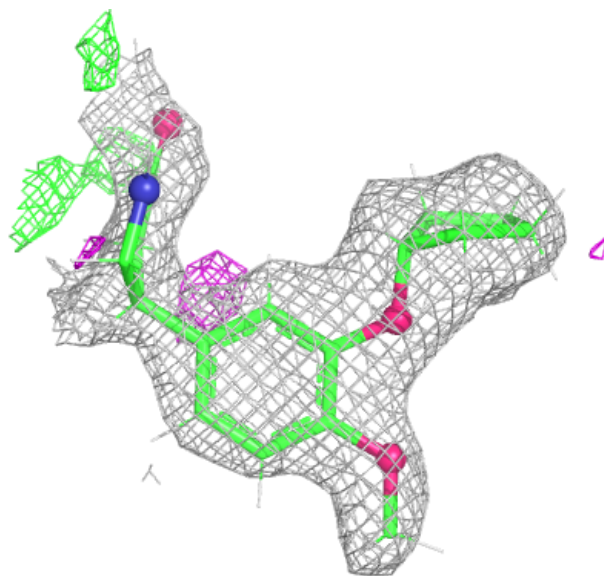
Electron density around ROL B 602 (A):

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



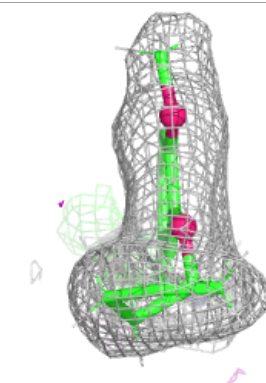
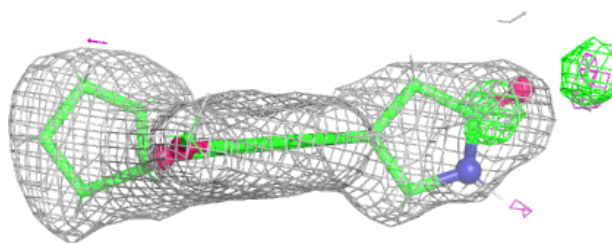
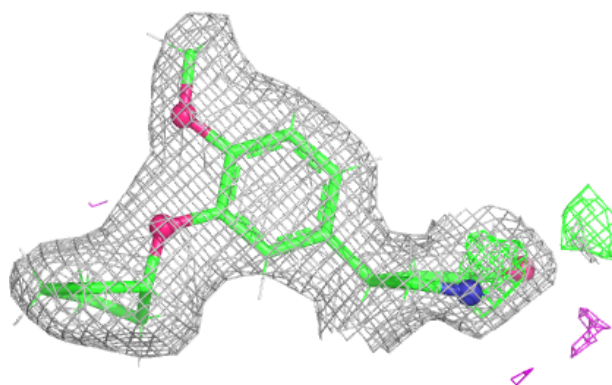
Electron density around ROL B 602 (B):

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and green (positive)



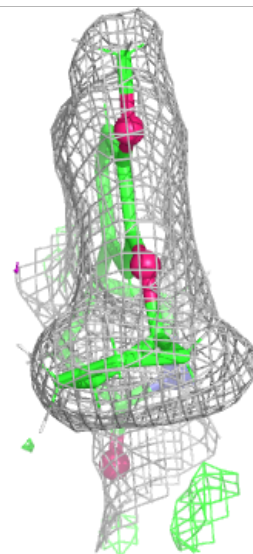
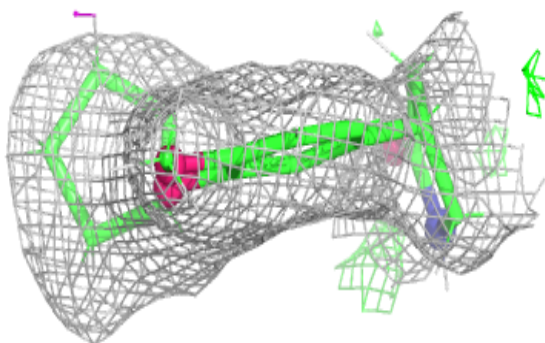
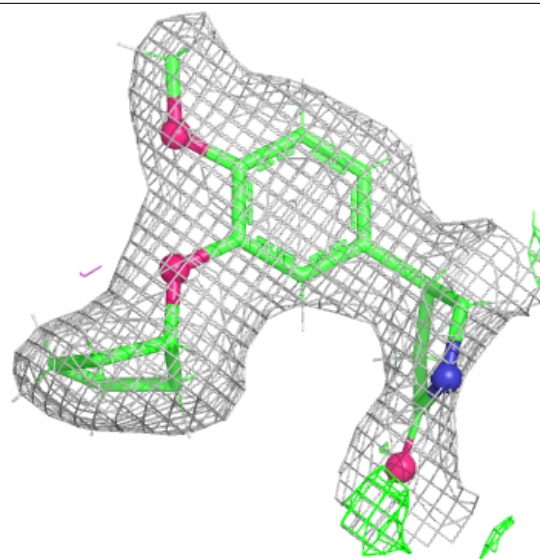
Electron density around ROL A 601 (A):

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



Electron density around ROL 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.