



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 05:05 AM UTC

PDB ID : 3G4K / pdb_00003g4k
Title : Crystal structure of human phosphodiesterase 4d with rolipram
Authors : Staker, B.L.
Deposited on : 2009-02-03
Resolution : 1.95 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

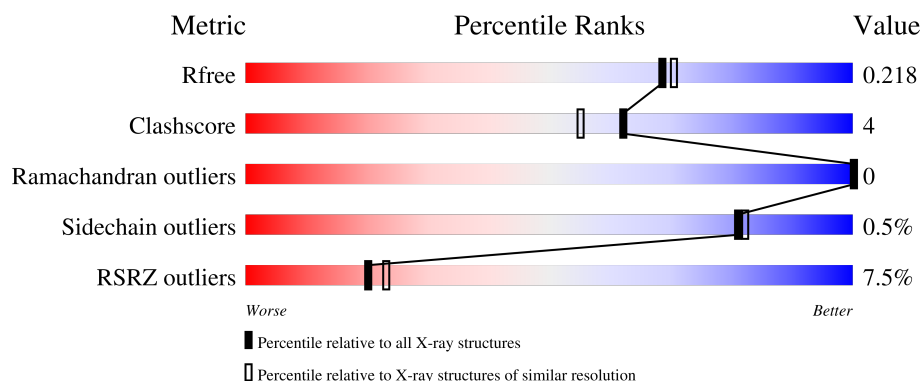
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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}	180053	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	381	 6% 81% 5% 13%
1	B	381	 7% 75% 10% 14%
1	C	381	 7% 77% 8% 14%
1	D	381	 6% 82% 5% 13%

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	C	903[A]	X	-	-	-
5	ROL	D	904[A]	X	-	-	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 11857 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 4D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	330	Total	C	N	O	S	0	0	0
			2667	1690	455	508	14			
1	B	326	Total	C	N	O	S	0	0	0
			2626	1660	446	506	14			
1	C	327	Total	C	N	O	S	0	0	0
			2643	1671	451	507	14			
1	D	333	Total	C	N	O	S	0	0	0
			2688	1700	460	514	14			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	243	MET	-	expression tag	UNP Q08499
A	579	ALA	SER	engineered mutation	UNP Q08499
A	581	ALA	SER	engineered mutation	UNP Q08499
A	618	HIS	-	expression tag	UNP Q08499
A	619	HIS	-	expression tag	UNP Q08499
A	620	HIS	-	expression tag	UNP Q08499
A	621	HIS	-	expression tag	UNP Q08499
A	622	HIS	-	expression tag	UNP Q08499
A	623	HIS	-	expression tag	UNP Q08499
B	243	MET	-	expression tag	UNP Q08499
B	579	ALA	SER	engineered mutation	UNP Q08499
B	581	ALA	SER	engineered mutation	UNP Q08499
B	618	HIS	-	expression tag	UNP Q08499
B	619	HIS	-	expression tag	UNP Q08499
B	620	HIS	-	expression tag	UNP Q08499
B	621	HIS	-	expression tag	UNP Q08499
B	622	HIS	-	expression tag	UNP Q08499
B	623	HIS	-	expression tag	UNP Q08499
C	243	MET	-	expression tag	UNP Q08499
C	579	ALA	SER	engineered mutation	UNP Q08499
C	581	ALA	SER	engineered mutation	UNP Q08499

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Chain	Residue	Modelled	Actual	Comment	Reference
C	618	HIS	-	expression tag	UNP Q08499
C	619	HIS	-	expression tag	UNP Q08499
C	620	HIS	-	expression tag	UNP Q08499
C	621	HIS	-	expression tag	UNP Q08499
C	622	HIS	-	expression tag	UNP Q08499
C	623	HIS	-	expression tag	UNP Q08499
D	243	MET	-	expression tag	UNP Q08499
D	579	ALA	SER	engineered mutation	UNP Q08499
D	581	ALA	SER	engineered mutation	UNP Q08499
D	618	HIS	-	expression tag	UNP Q08499
D	619	HIS	-	expression tag	UNP Q08499
D	620	HIS	-	expression tag	UNP Q08499
D	621	HIS	-	expression tag	UNP Q08499
D	622	HIS	-	expression tag	UNP Q08499
D	623	HIS	-	expression tag	UNP Q08499

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

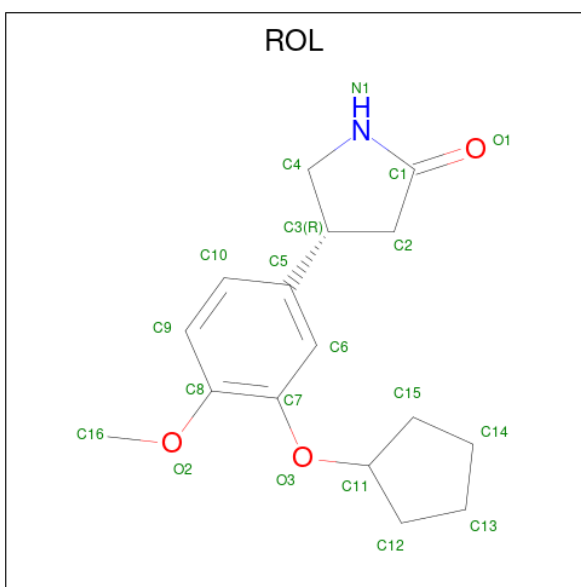
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mg 1 1	0	0
3	B	1	Total Mg 1 1	0	0
3	C	1	Total Mg 1 1	0	0
3	D	1	Total Mg 1 1	0	0

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is ROLIPRAM (CCD ID: ROL) (formula: C₁₆H₂₁NO₃).



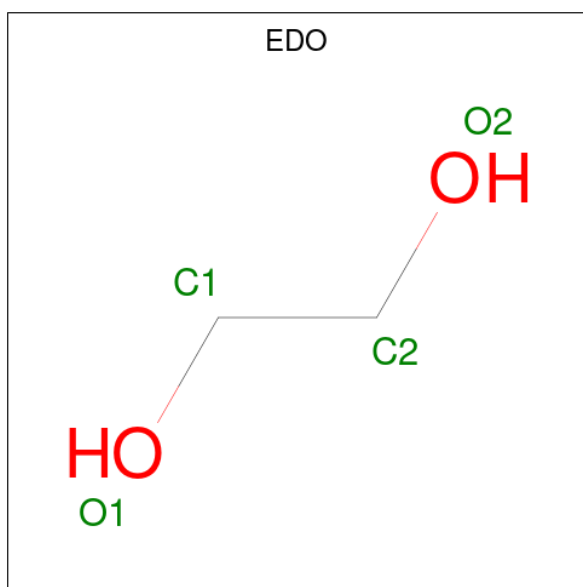
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			20	16	1	3		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	N	O	0	0
			20	16	1	3		
5	C	1	Total	C	N	O	0	1
			40	32	2	6		
5	D	1	Total	C	N	O	0	1
			40	32	2	6		

- Molecule 6 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	272	Total O 272 272	0	0
7	B	249	Total O 249 249	0	0
7	C	240	Total O 240 240	0	0
7	D	273	Total O 273 273	0	0

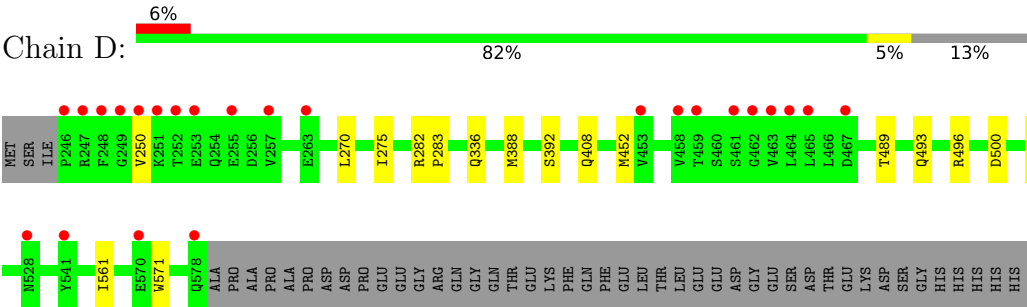
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

- Chain A:
-
- 6% 81% 5% 13%
- NET SER ILE PRO ARG F248 F249 V250 L270 L275 R282 P283 H289 Q293 L341 M388 Q408 E409 M443 K452 V453 E454 T455 K456 K457 V458 T459 S461 S461 T462 V463 L464 L465 L466 D467 Q474 M487 P488 T489 Q493 R508 D511 R512 F513 R514

- Chain B:
-
- Sequence logo for Chain B. The y-axis represents information content in bits (0.00 to 0.25). The x-axis lists amino acids. Red dots indicate positions with high conservation. A green bar at the top shows the overall conservation score: 7% (green), 75% (yellow), 10% (grey), and 14% (white).
- | Position | Amino Acid | Information Content (bits) |
|----------|------------|----------------------------|
| 1 | GLY | 0.25 |
| 2 | GLN | 0.25 |
| 3 | THR | 0.25 |
| 4 | GLU | 0.25 |
| 5 | LYS | 0.25 |
| 6 | PHE | 0.25 |
| 7 | GLN | 0.25 |
| 8 | PHE | 0.25 |
| 9 | LEU | 0.25 |
| 10 | LEU | 0.25 |
| 11 | THR | 0.25 |
| 12 | THR | 0.25 |
| 13 | ASP | 0.25 |
| 14 | GLY | 0.25 |
| 15 | GLY | 0.25 |
| 16 | GLY | 0.25 |
| 17 | GLY | 0.25 |
| 18 | GLY | 0.25 |
| 19 | GLY | 0.25 |
| 20 | GLY | 0.25 |
| 21 | GLY | 0.25 |
| 22 | GLY | 0.25 |
| 23 | GLY | 0.25 |
| 24 | GLY | 0.25 |
| 25 | GLY | 0.25 |

- Chain C:

- 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	98.61Å 112.76Å 160.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 1.95 50.00 – 1.95	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-1.95) 99.6 (50.00-1.95)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.67 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.183 , 0.215 0.188 , 0.218	Depositor DCC
R_{free} test set	6540 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	27.4	Xtriage
Anisotropy	0.026	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 40.2	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	0.96	EDS
Total number of atoms	11857	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.73% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, MG, ZN, ROL, EDO

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	0.61	0/2722	0.75	1/3698 (0.0%)
1	B	0.58	0/2680	0.77	0/3645
1	C	0.58	0/2697	0.76	0/3665
1	D	0.63	0/2744	0.73	0/3729
All	All	0.60	0/10843	0.75	1/14737 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	515	GLU	CB-CA-C	-5.30	101.66	110.68

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	2667	0	2619	19	0
1	B	2626	0	2559	28	0
1	C	2643	0	2593	25	0
1	D	2688	0	2632	18	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	5	0	0	0	0
4	C	5	0	0	0	0
4	D	5	0	0	1	0
5	A	20	0	21	0	0
5	B	20	0	21	0	0
5	C	40	0	42	0	0
5	D	40	0	42	1	0
6	A	32	0	48	3	0
6	B	12	0	18	2	0
6	C	4	0	6	0	0
6	D	8	0	12	0	0
7	A	272	0	0	3	0
7	B	249	0	0	3	0
7	C	240	0	0	4	0
7	D	273	0	0	7	0
All	All	11857	0	10613	88	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 4.

All (88) 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:575:THR:HG21	7:A:104:HOH:O	1.77	0.85
1:B:387:LEU:HG	7:B:717:HOH:O	1.84	0.77
1:A:408:GLN:OE1	1:D:408:GLN:OE1	2.07	0.73
1:A:575:THR:HG22	1:A:575:THR:O	1.92	0.68
1:B:496:ARG:HD3	1:B:571:TRP:CH2	2.29	0.68
1:C:459:THR:HG22	1:C:463:VAL:O	1.93	0.68
1:C:320:HIS:HE1	1:C:369:ASP:OD1	1.78	0.66
1:B:350:VAL:CG2	1:B:463:VAL:CG1	2.75	0.64
1:B:346:ALA:O	1:B:463:VAL:HG13	1.99	0.62
1:C:464:LEU:HD21	1:C:553:LEU:HD11	1.82	0.62
1:C:496:ARG:HD3	1:C:571:TRP:CH2	2.34	0.62
1:B:350:VAL:HG23	1:B:463:VAL:HG11	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:496:ARG:HD3	1:D:571:TRP:CH2	2.35	0.61
1:C:408:GLN:NE2	7:C:125:HOH:O	2.34	0.60
1:B:420:LYS:HG2	1:B:424:GLN:HE21	1.65	0.60
1:D:500:ASP:OD1	7:D:956:HOH:O	2.16	0.59
1:B:489:THR:HB	1:B:561:ILE:HG23	1.86	0.58
1:B:270:LEU:HD22	1:B:336:GLN:HG3	1.84	0.58
1:A:270:LEU:HD11	1:A:275:ILE:HD11	1.85	0.57
1:B:262:LEU:HD11	1:B:286:VAL:CG1	2.35	0.56
1:C:573:GLN:NE2	1:C:576:ILE:HD12	2.21	0.56
1:B:512:ARG:HD2	7:D:69:HOH:O	2.05	0.55
1:A:512:ARG:HD2	7:C:116:HOH:O	2.07	0.55
1:A:489:THR:HB	1:A:561:ILE:HG23	1.89	0.55
1:D:388:MET:HA	1:D:388:MET:HE2	1.89	0.54
1:B:350:VAL:HG23	1:B:463:VAL:CG1	2.36	0.54
1:B:262:LEU:O	1:B:265:VAL:HG23	2.08	0.54
1:D:452:MET:CE	7:D:162:HOH:O	2.56	0.53
1:A:511:ASP:O	1:A:515:GLU:HG3	2.09	0.52
1:B:511:ASP:OD1	1:B:514:ARG:NH2	2.43	0.52
1:C:573:GLN:HE21	1:C:576:ILE:HD12	1.74	0.52
1:A:575:THR:O	1:A:575:THR:CG2	2.58	0.52
1:A:409:GLU:HG3	6:A:624:EDO:H12	1.93	0.51
1:C:320:HIS:HD2	7:C:52:HOH:O	1.93	0.51
1:C:573:GLN:HE21	1:C:573:GLN:HA	1.76	0.50
7:A:88:HOH:O	1:C:512:ARG:HD2	2.11	0.50
1:B:411:ASN:ND2	7:B:693:HOH:O	2.39	0.50
1:A:289:HIS:CE1	1:A:293:GLN:HE21	2.30	0.50
1:C:448:ASP:C	1:C:474:GLN:NE2	2.70	0.50
1:D:392:SER:HB2	7:D:738:HOH:O	2.10	0.50
1:D:270:LEU:HD22	1:D:336:GLN:HG3	1.92	0.49
1:C:571:TRP:O	1:C:575:THR:HG23	2.12	0.49
1:C:489:THR:HB	1:C:561:ILE:HG23	1.93	0.49
1:C:455:THR:O	1:C:455:THR:HG22	2.14	0.48
7:B:121:HOH:O	1:D:512:ARG:HD2	2.14	0.48
1:D:270:LEU:HD11	1:D:275:ILE:CD1	2.45	0.47
1:A:388:MET:HA	1:A:388:MET:HE2	1.97	0.47
1:C:348:GLU:O	1:C:463:VAL:HG11	2.14	0.47
1:B:496:ARG:HD3	1:B:571:TRP:CZ3	2.50	0.47
1:B:494:LEU:HD21	6:B:11:EDO:O1	2.16	0.46
1:C:270:LEU:HD22	1:C:336:GLN:HG3	1.96	0.46
1:D:452:MET:HE3	7:D:162:HOH:O	2.15	0.46
1:C:448:ASP:O	1:C:474:GLN:NE2	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:309:ILE:CG2	1:B:313:MET:HE3	2.46	0.46
1:D:493:GLN:NE2	4:D:2:SO4:O3	2.49	0.46
1:D:496:ARG:HD3	1:D:571:TRP:CZ3	2.51	0.46
6:A:624:EDO:H22	1:C:384:GLU:HB2	1.99	0.45
1:C:492:LEU:HD21	1:C:571:TRP:CE2	2.52	0.45
1:C:492:LEU:HD21	1:C:571:TRP:CD2	2.52	0.45
1:D:282:ARG:N	1:D:283:PRO:CD	2.81	0.44
1:B:344:THR:HG22	1:B:347:LEU:HD12	2.00	0.44
1:A:511:ASP:OD1	1:A:514:ARG:NH2	2.47	0.44
1:A:512:ARG:CD	7:C:116:HOH:O	2.65	0.44
1:B:262:LEU:HD11	1:B:286:VAL:HG13	2.00	0.44
1:C:253:GLU:O	1:C:257:VAL:HG23	2.18	0.43
1:B:282:ARG:N	1:B:283:PRO:CD	2.81	0.43
1:A:270:LEU:HD11	1:A:275:ILE:CD1	2.47	0.43
1:A:341:LEU:HD23	6:A:14:EDO:H12	2.00	0.43
1:D:270:LEU:HD11	1:D:275:ILE:HD11	2.01	0.43
1:C:405:LYS:NZ	1:D:388:MET:HE1	2.34	0.43
1:A:388:MET:HE1	1:B:405:LYS:NZ	2.34	0.43
1:B:362:ALA:O	1:B:366:HIS:HB3	2.19	0.43
1:D:489:THR:HB	1:D:561:ILE:HG23	2.01	0.42
1:B:494:LEU:CD2	6:B:11:EDO:O1	2.67	0.42
1:A:487:ASN:HB2	1:A:488:PRO:HD3	2.00	0.42
1:B:464:LEU:HD21	1:B:553:LEU:HG	2.02	0.42
1:A:493:GLN:NE2	7:A:637:HOH:O	2.52	0.42
1:A:282:ARG:N	1:A:283:PRO:CD	2.82	0.42
1:B:490:LYS:HB3	1:B:491:PRO:HD2	2.02	0.42
1:B:395:LEU:HD23	1:B:395:LEU:HA	1.91	0.41
1:B:326:HIS:ND1	1:B:505:GLU:OE2	2.40	0.41
1:D:452:MET:SD	7:D:162:HOH:O	2.62	0.41
1:C:282:ARG:N	1:C:283:PRO:CD	2.84	0.41
1:C:504:GLU:OE2	1:C:508:ARG:NH2	2.54	0.41
1:D:510:GLY:HA3	1:D:524:CYS:O	2.20	0.41
1:B:264:ASP:HB2	1:B:270:LEU:HD12	2.03	0.40
5:D:904[A]:ROL:H142	7:D:59:HOH:O	2.20	0.40
1:C:350:VAL:HG11	1:C:466:LEU:HD12	2.02	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	328/381 (86%)	321 (98%)	7 (2%)	0	100	100
1	B	324/381 (85%)	317 (98%)	7 (2%)	0	100	100
1	C	325/381 (85%)	319 (98%)	6 (2%)	0	100	100
1	D	331/381 (87%)	327 (99%)	4 (1%)	0	100	100
All	All	1308/1524 (86%)	1284 (98%)	24 (2%)	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	299/345 (87%)	299 (100%)	0	100	100
1	B	295/345 (86%)	293 (99%)	2 (1%)	76	76
1	C	298/345 (86%)	295 (99%)	3 (1%)	68	67
1	D	302/345 (88%)	301 (100%)	1 (0%)	86	87
All	All	1194/1380 (86%)	1188 (100%)	6 (0%)	81	82

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

Mol	Chain	Res	Type
1	B	258	LEU
1	B	508	ARG

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Mol	Chain	Res	Type
1	C	408	GLN
1	C	523	MET
1	C	573	GLN
1	D	250	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	254	GLN
1	A	289	HIS
1	A	411	ASN
1	A	416	GLN
1	A	474	GLN
1	A	528	ASN
1	B	254	GLN
1	B	289	HIS
1	B	376	GLN
1	B	411	ASN
1	B	424	GLN
1	B	555	HIS
1	B	573	GLN
1	C	320	HIS
1	C	376	GLN
1	C	408	GLN
1	C	411	ASN
1	C	535	GLN
1	C	559	GLN
1	C	573	GLN
1	D	289	HIS
1	D	293	GLN
1	D	411	ASN
1	D	474	GLN
1	D	555	HIS
1	D	573	GLN

5.3.3 RNA ⓘ

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 31 ligands modelled in this entry, 8 are monoatomic - leaving 23 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	$\# Z > 2$
6	EDO	A	9	-	3,3,3	0.41	0	2,2,2	0.41	0
5	ROL	C	903[A]	-	22,22,22	1.01	1 (4%)	30,30,30	1.23	2 (6%)
6	EDO	D	10	-	3,3,3	0.42	0	2,2,2	0.31	0
4	SO4	A	1	-	4,4,4	0.22	0	6,6,6	0.36	0
4	SO4	D	2	-	4,4,4	0.35	0	6,6,6	0.49	0
6	EDO	B	8	-	3,3,3	0.42	0	2,2,2	0.25	0
6	EDO	A	14	-	3,3,3	0.38	0	2,2,2	0.27	0
6	EDO	A	7	-	3,3,3	0.41	0	2,2,2	0.46	0
6	EDO	C	5	-	3,3,3	0.41	0	2,2,2	0.35	0
4	SO4	C	3	-	4,4,4	0.19	0	6,6,6	0.30	0
6	EDO	A	4	-	3,3,3	0.51	0	2,2,2	0.13	0
6	EDO	A	13	-	3,3,3	0.40	0	2,2,2	0.43	0
5	ROL	B	902	-	22,22,22	0.93	1 (4%)	30,30,30	1.19	2 (6%)
6	EDO	A	624	-	3,3,3	0.46	0	2,2,2	0.51	0
5	ROL	A	901	-	22,22,22	0.96	1 (4%)	30,30,30	1.09	2 (6%)
5	ROL	D	904[B]	-	22,22,22	0.97	1 (4%)	30,30,30	1.28	4 (13%)
6	EDO	A	12	-	3,3,3	0.39	0	2,2,2	0.44	0
5	ROL	D	904[A]	-	22,22,22	0.95	1 (4%)	30,30,30	1.27	3 (10%)
6	EDO	B	3	-	3,3,3	0.38	0	2,2,2	0.46	0
6	EDO	A	6	-	3,3,3	0.36	0	2,2,2	0.52	0
6	EDO	D	624	-	3,3,3	0.46	0	2,2,2	0.05	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	ROL	C	903[B]	-	22,22,22	0.98	1 (4%)	30,30,30	1.14	2 (6%)
6	EDO	B	11	-	3,3,3	0.23	0	2,2,2	0.75	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
6	EDO	A	9	-	-	1/1/1/1	-
5	ROL	C	903[A]	-	1/1/3/4	2/10/26/26	0/3/3/3
6	EDO	D	10	-	-	0/1/1/1	-
6	EDO	B	8	-	-	0/1/1/1	-
6	EDO	A	14	-	-	1/1/1/1	-
6	EDO	A	7	-	-	1/1/1/1	-
6	EDO	C	5	-	-	0/1/1/1	-
6	EDO	A	4	-	-	0/1/1/1	-
6	EDO	A	13	-	-	0/1/1/1	-
5	ROL	B	902	-	-	2/10/26/26	0/3/3/3
6	EDO	A	624	-	-	1/1/1/1	-
5	ROL	A	901	-	-	0/10/26/26	0/3/3/3
5	ROL	D	904[B]	-	-	1/10/26/26	0/3/3/3
6	EDO	A	12	-	-	0/1/1/1	-
5	ROL	D	904[A]	-	1/1/3/4	5/10/26/26	0/3/3/3
6	EDO	B	3	-	-	0/1/1/1	-
6	EDO	A	6	-	-	0/1/1/1	-
6	EDO	D	624	-	-	0/1/1/1	-
5	ROL	C	903[B]	-	-	2/10/26/26	0/3/3/3
6	EDO	B	11	-	-	0/1/1/1	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	903[A]	ROL	C8-C7	4.03	1.49	1.40
5	D	904[A]	ROL	C8-C7	3.95	1.49	1.40
5	C	903[B]	ROL	C8-C7	3.85	1.48	1.40
5	D	904[B]	ROL	C8-C7	3.55	1.48	1.40
5	A	901	ROL	C8-C7	3.36	1.47	1.40
5	B	902	ROL	C8-C7	3.17	1.47	1.40

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	901	ROL	C16-O2-C8	3.93	123.28	117.51
5	D	904[A]	ROL	O2-C8-C7	3.79	120.54	115.40
5	C	903[B]	ROL	C16-O2-C8	3.69	122.93	117.51
5	C	903[A]	ROL	O2-C8-C7	3.47	120.10	115.40
5	B	902	ROL	C16-O2-C8	3.24	122.26	117.51
5	C	903[A]	ROL	C16-O2-C8	3.14	122.12	117.51
5	D	904[B]	ROL	O2-C8-C7	3.03	119.51	115.40
5	C	903[B]	ROL	O2-C8-C7	2.66	119.00	115.40
5	D	904[A]	ROL	C2-C3-C5	-2.53	110.09	115.29
5	B	902	ROL	C6-C5-C3	-2.39	114.98	120.88
5	D	904[B]	ROL	O1-C1-C2	-2.33	123.51	126.48
5	D	904[B]	ROL	C3-C2-C1	-2.33	101.92	104.96
5	D	904[B]	ROL	C6-C5-C3	-2.24	115.32	120.88
5	D	904[A]	ROL	C16-O2-C8	2.17	120.70	117.51
5	A	901	ROL	O2-C8-C7	2.04	118.17	115.40

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	C	903[A]	ROL	C3
5	D	904[A]	ROL	C3

All (16) torsion outliers are listed below:

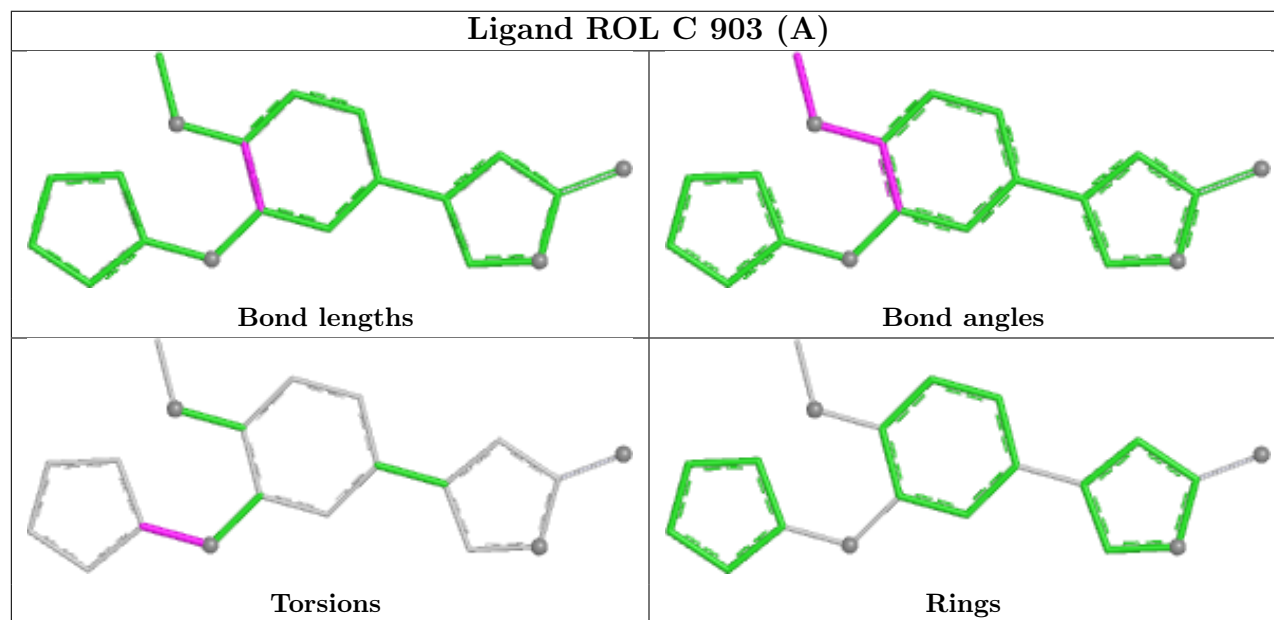
Mol	Chain	Res	Type	Atoms
5	B	902	ROL	C15-C11-O3-C7
5	C	903[A]	ROL	C15-C11-O3-C7
5	C	903[A]	ROL	C12-C11-O3-C7
5	C	903[B]	ROL	C15-C11-O3-C7
5	C	903[B]	ROL	C12-C11-O3-C7
5	D	904[A]	ROL	C15-C11-O3-C7
5	D	904[A]	ROL	C12-C11-O3-C7
5	D	904[A]	ROL	C7-C8-O2-C16
5	B	902	ROL	C12-C11-O3-C7
6	A	624	EDO	O1-C1-C2-O2
6	A	14	EDO	O1-C1-C2-O2
5	D	904[A]	ROL	C9-C8-O2-C16
6	A	9	EDO	O1-C1-C2-O2
5	D	904[A]	ROL	C8-C7-O3-C11
6	A	7	EDO	O1-C1-C2-O2
5	D	904[B]	ROL	C7-C8-O2-C16

There are no ring outliers.

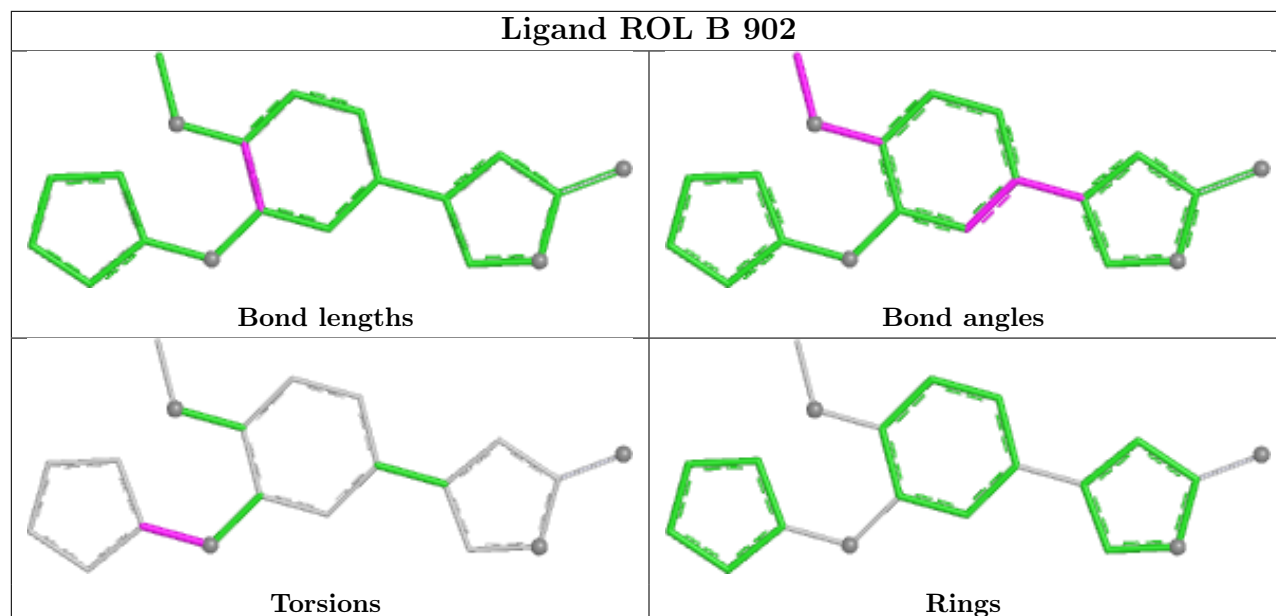
5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	2	SO4	1	0
6	A	14	EDO	1	0
6	A	624	EDO	2	0
5	D	904[A]	ROL	1	0
6	B	11	EDO	2	0

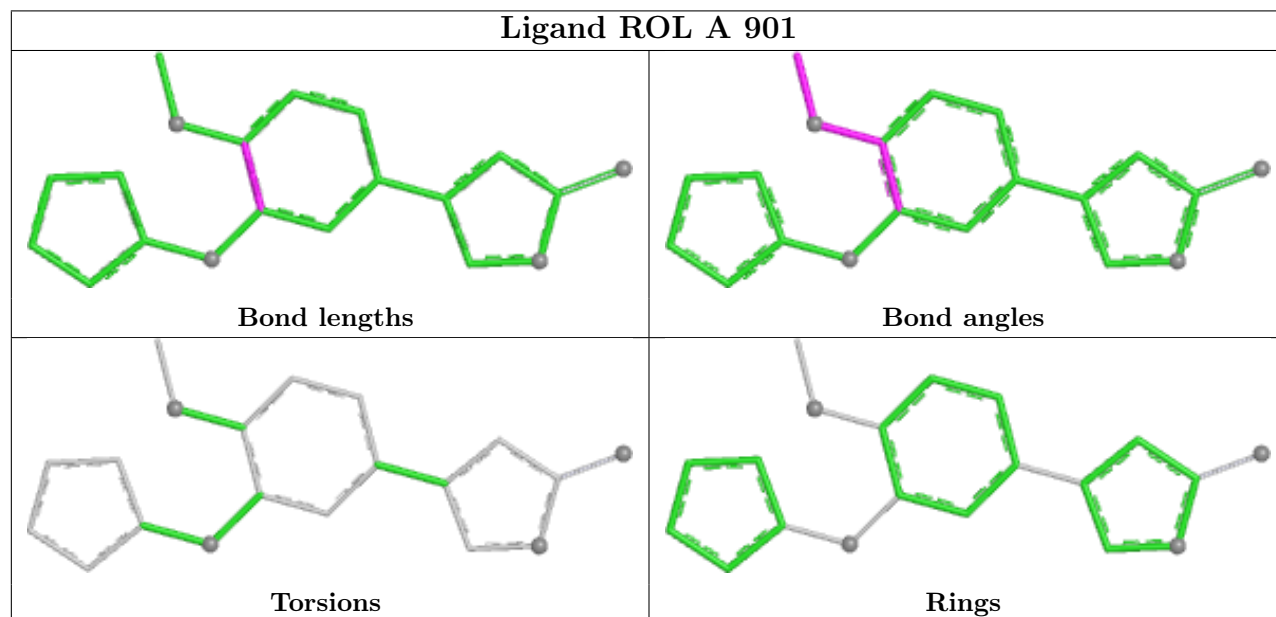
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

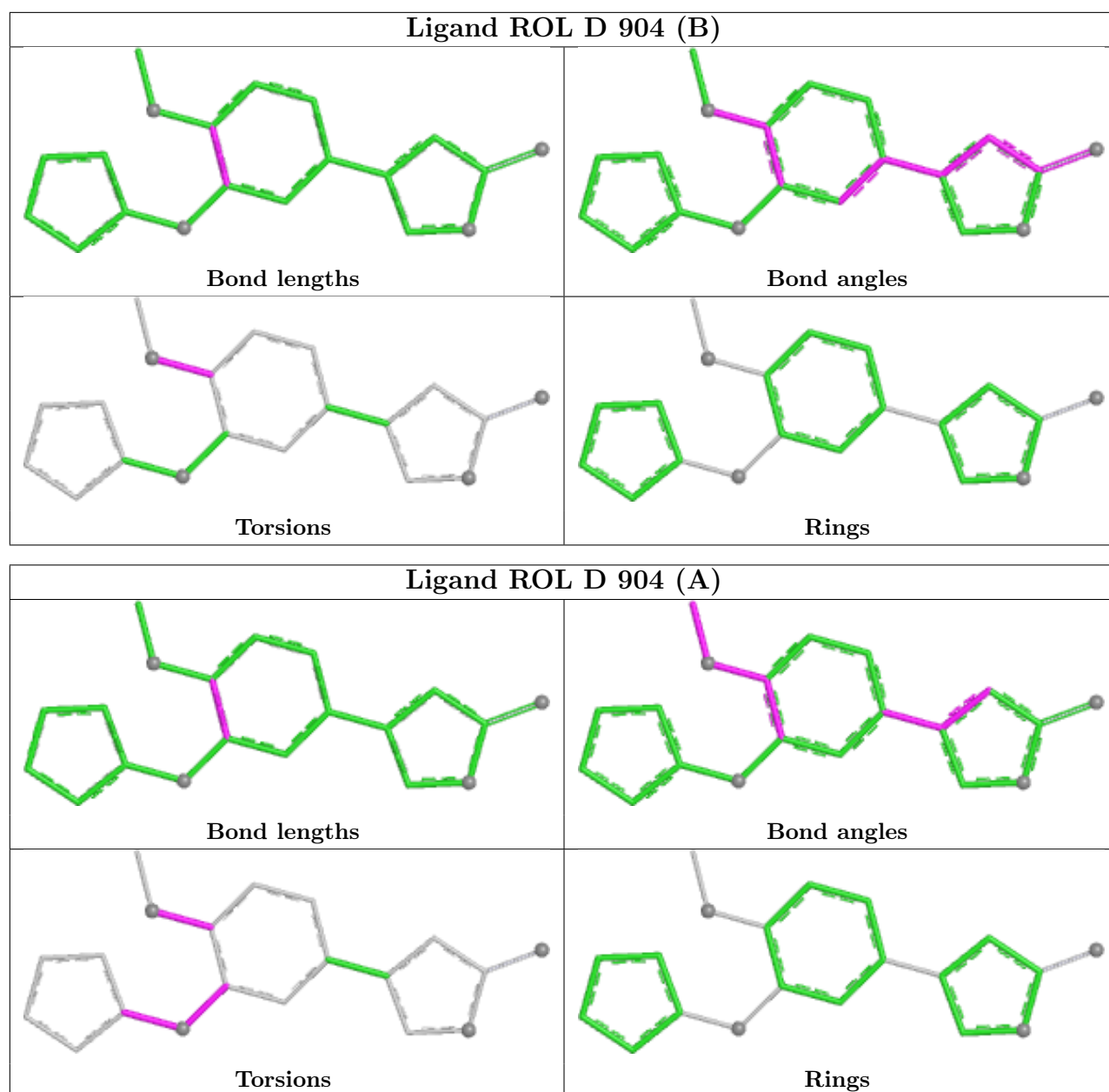


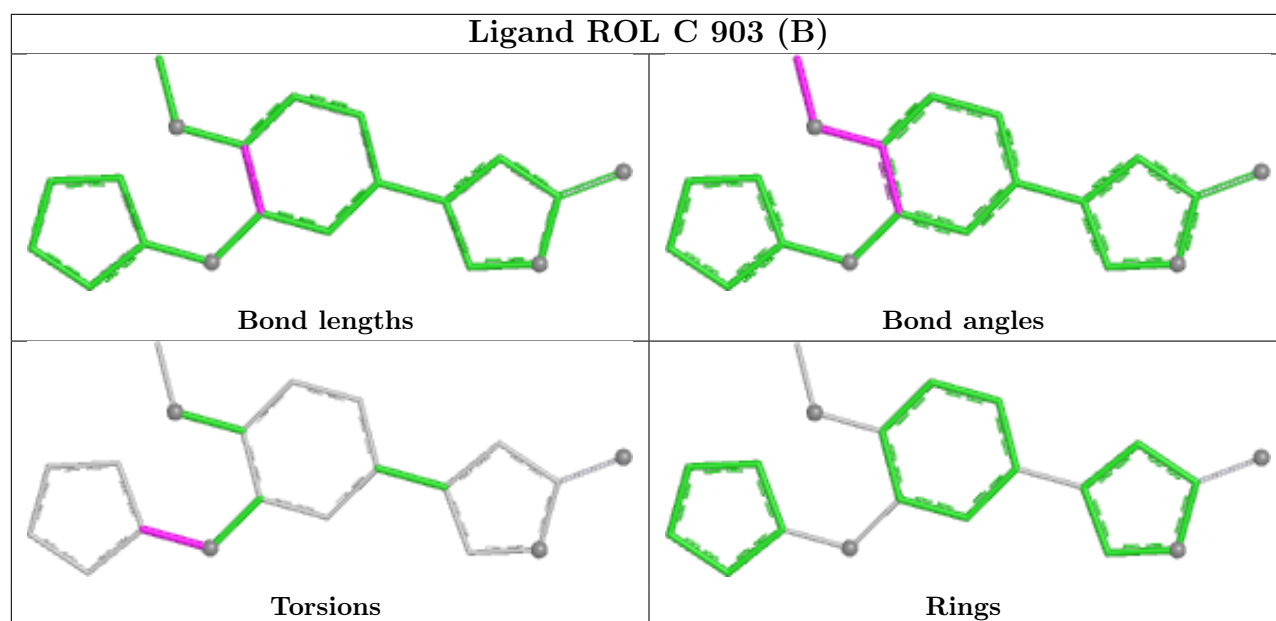
Ligand ROL B 902



Ligand ROL A 901







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	330/381 (86%)	0.28	24 (7%) 21 24	16, 27, 48, 56	0
1	B	326/381 (85%)	0.51	26 (7%) 18 21	17, 29, 49, 69	0
1	C	327/381 (85%)	0.42	25 (7%) 20 22	16, 29, 50, 65	0
1	D	333/381 (87%)	0.30	24 (7%) 21 25	15, 27, 52, 68	0
All	All	1316/1524 (86%)	0.37	99 (7%) 20 23	15, 28, 50, 69	0

All (99) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	248	PHE	6.1
1	D	250	VAL	5.8
1	C	460	SER	4.9
1	A	461	SER	4.9
1	A	248	PHE	4.7
1	C	461	SER	4.7
1	C	252	THR	4.6
1	A	460	SER	4.5
1	D	578	GLN	4.5
1	C	459	THR	4.4
1	C	462	GLY	4.3
1	A	459	THR	4.2
1	D	249	GLY	4.0
1	A	577	PRO	3.9
1	C	254	GLN	3.8
1	C	467	ASP	3.7
1	A	465	LEU	3.7
1	D	461	SER	3.6
1	B	467	ASP	3.6
1	A	575	THR	3.6
1	C	465	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	257	VAL	3.5
1	A	467	ASP	3.5
1	D	247	ARG	3.5
1	B	458	VAL	3.4
1	D	246	PRO	3.1
1	A	529	ALA	3.1
1	B	253	GLU	3.1
1	D	462	GLY	3.1
1	B	461	SER	3.0
1	D	251	LYS	3.0
1	C	458	VAL	3.0
1	B	463	VAL	2.9
1	C	463	VAL	2.9
1	D	570	GLU	2.9
1	D	541	TYR	2.9
1	C	256	ASP	2.9
1	C	577	PRO	2.8
1	C	541	TYR	2.8
1	D	467	ASP	2.8
1	D	252	THR	2.7
1	C	464	LEU	2.7
1	A	250	VAL	2.6
1	B	254	GLN	2.6
1	A	519	GLU	2.6
1	C	453	VAL	2.6
1	A	452	MET	2.5
1	B	258	LEU	2.5
1	B	265	VAL	2.5
1	B	462	GLY	2.5
1	A	462	GLY	2.4
1	A	474	GLN	2.4
1	B	459	THR	2.4
1	D	458	VAL	2.4
1	A	508	ARG	2.4
1	D	253	GLU	2.4
1	D	463	VAL	2.4
1	A	528	ASN	2.4
1	B	465	LEU	2.4
1	B	466	LEU	2.4
1	B	575	THR	2.4
1	C	570	GLU	2.4
1	B	457	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	464	LEU	2.3
1	D	459	THR	2.3
1	B	560	ASP	2.3
1	B	349	ALA	2.3
1	A	457	LYS	2.3
1	A	453	VAL	2.3
1	B	570	GLU	2.3
1	A	493	GLN	2.3
1	B	493	GLN	2.3
1	B	578	GLN	2.3
1	B	571	TRP	2.3
1	C	575	THR	2.3
1	B	460	SER	2.2
1	A	458	VAL	2.2
1	C	578	GLN	2.2
1	C	529	ALA	2.2
1	C	561	ILE	2.2
1	A	464	LEU	2.2
1	B	558	ALA	2.2
1	C	408	GLN	2.1
1	D	453	VAL	2.1
1	B	574	SER	2.1
1	D	465	LEU	2.1
1	D	528	ASN	2.1
1	B	455	THR	2.1
1	A	455	THR	2.1
1	D	263	GLU	2.1
1	D	257	VAL	2.1
1	C	447	ALA	2.1
1	C	306	ASP	2.1
1	A	443	MET	2.0
1	A	573	GLN	2.0
1	D	255	GLU	2.0
1	C	470	SER	2.0
1	B	561	ILE	2.0
1	C	257	VAL	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 ⓘ

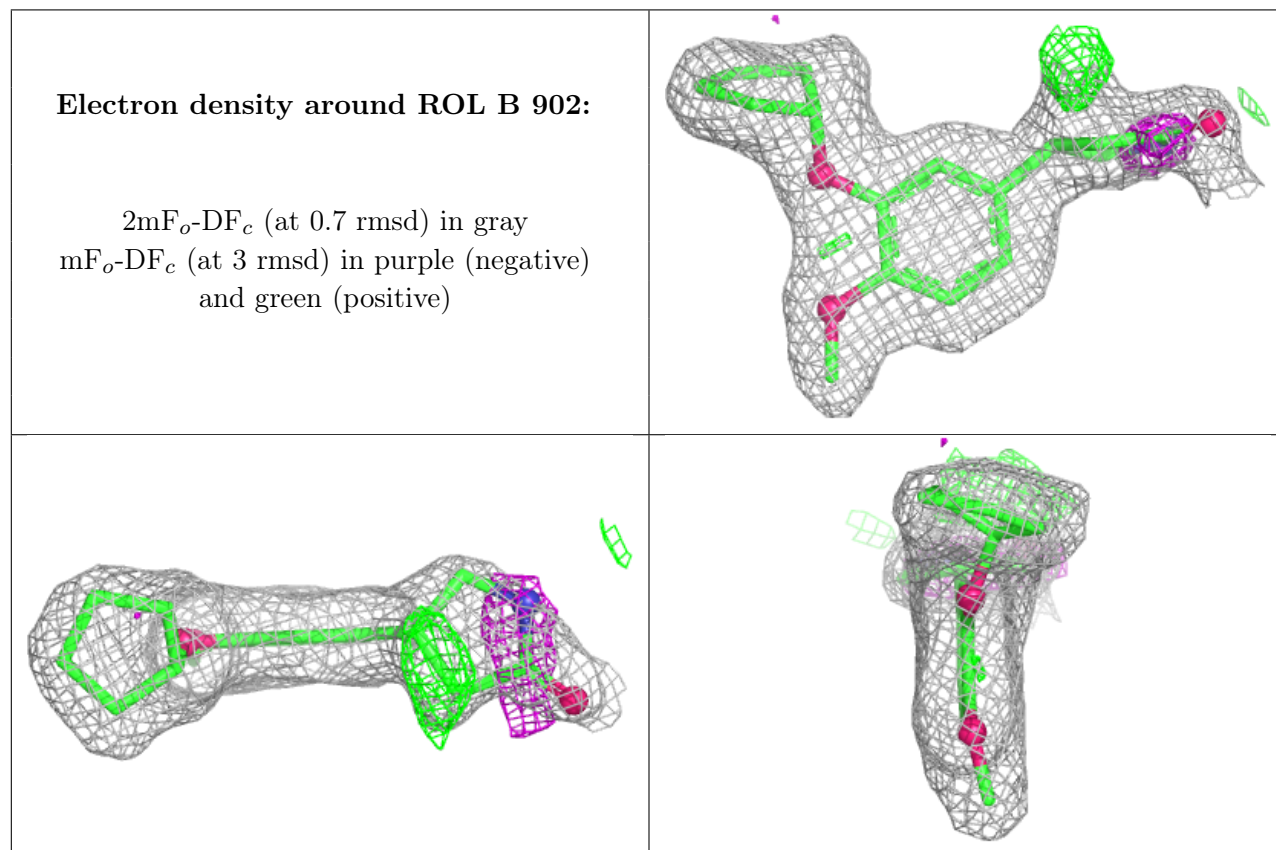
There are no oligosaccharides in this entry.

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.

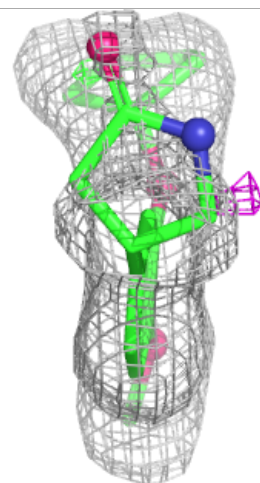
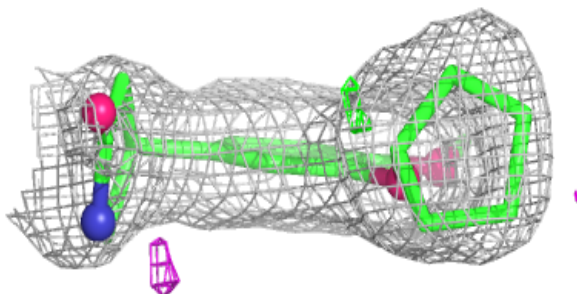
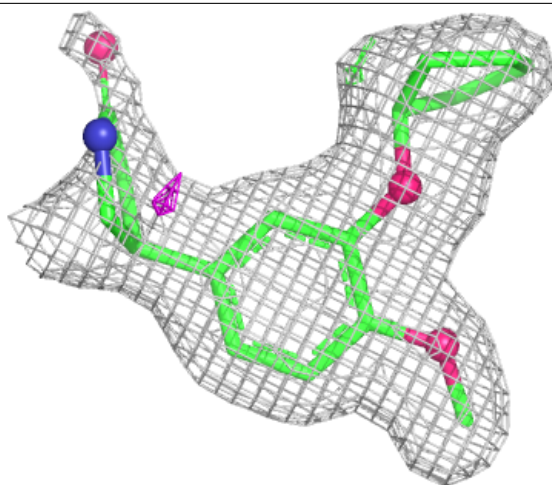
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	EDO	A	6	4/4	0.76	0.28	43,43,44,47	0
3	MG	A	802	1/1	0.78	0.12	47,47,47,47	0
6	EDO	A	9	4/4	0.81	0.14	49,50,51,51	0
6	EDO	B	11	4/4	0.83	0.26	44,45,47,49	0
6	EDO	A	12	4/4	0.85	0.17	42,43,44,46	0
6	EDO	B	3	4/4	0.86	0.14	39,39,40,40	0
6	EDO	A	7	4/4	0.86	0.15	41,43,43,44	0
4	SO4	C	3	5/5	0.88	0.14	58,61,62,63	0
6	EDO	A	624	4/4	0.88	0.28	21,27,28,30	0
5	ROL	B	902	20/20	0.89	0.13	29,37,42,42	0
6	EDO	D	10	4/4	0.90	0.11	32,34,34,35	0
5	ROL	C	903[A]	20/20	0.91	0.14	37,39,41,41	20
6	EDO	A	14	4/4	0.91	0.14	46,46,46,47	0
5	ROL	C	903[B]	20/20	0.91	0.14	21,25,28,28	20
5	ROL	D	904[A]	20/20	0.91	0.14	37,38,41,41	20
5	ROL	D	904[B]	20/20	0.91	0.14	17,21,25,26	20
4	SO4	D	2	5/5	0.92	0.16	41,46,48,48	0
3	MG	D	808	1/1	0.93	0.18	43,43,43,43	0
5	ROL	A	901	20/20	0.93	0.09	29,33,38,39	0
4	SO4	A	1	5/5	0.93	0.13	39,44,46,47	0
3	MG	C	806	1/1	0.93	0.14	41,41,41,41	0
6	EDO	A	13	4/4	0.94	0.10	34,34,35,35	0
6	EDO	B	8	4/4	0.94	0.08	31,32,32,32	0
3	MG	B	804	1/1	0.95	0.14	47,47,47,47	0
6	EDO	C	5	4/4	0.95	0.07	31,31,32,32	0
6	EDO	D	624	4/4	0.95	0.09	26,27,27,27	0
6	EDO	A	4	4/4	0.95	0.08	28,30,30,32	0
2	ZN	A	801	1/1	0.99	0.02	21,21,21,21	0
2	ZN	B	803	1/1	1.00	0.01	25,25,25,25	0
2	ZN	C	805	1/1	1.00	0.02	23,23,23,23	0
2	ZN	D	807	1/1	1.00	0.02	21,21,21,21	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.



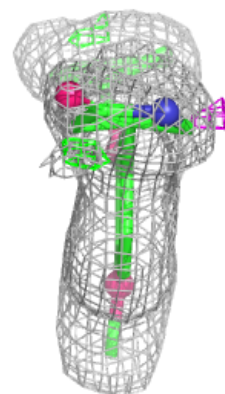
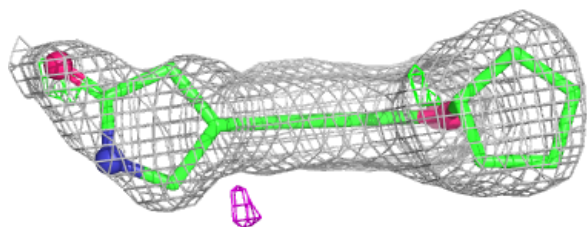
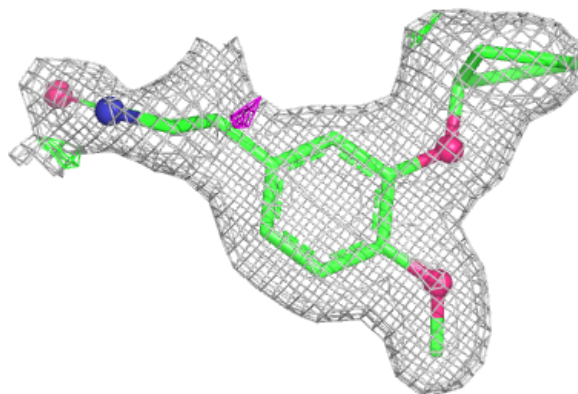
Electron density around ROL C 903 (A):

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



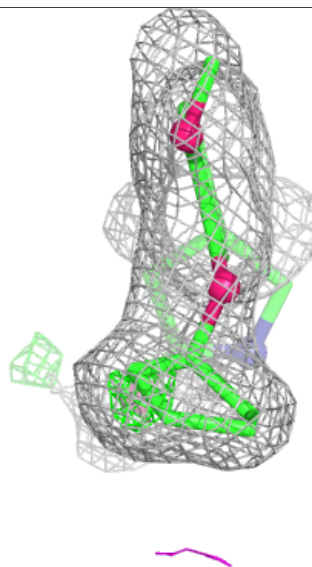
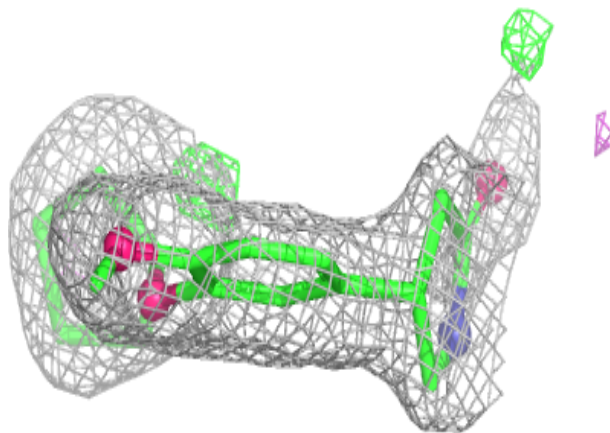
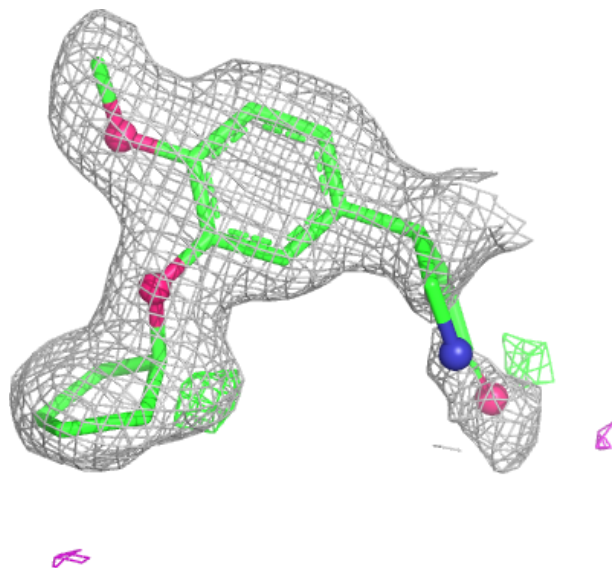
Electron density around ROL C 903 (B):

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



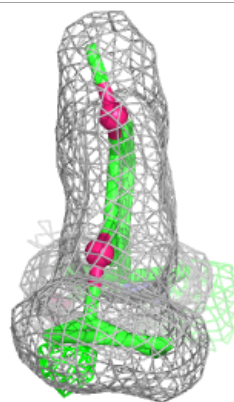
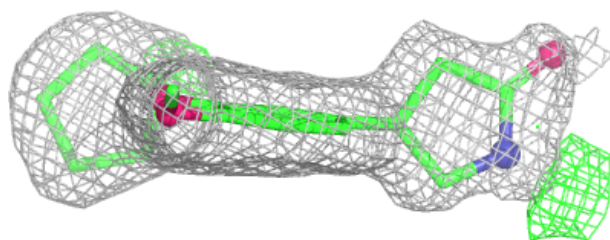
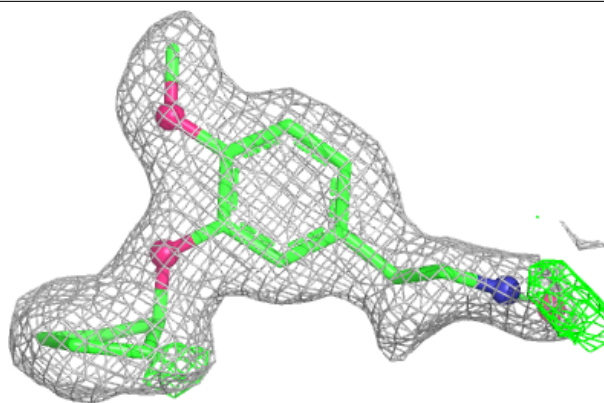
Electron density around ROL D 904 (A):

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

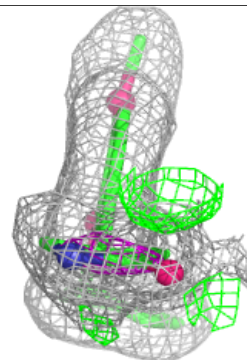
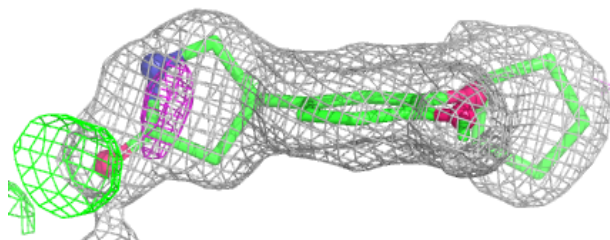
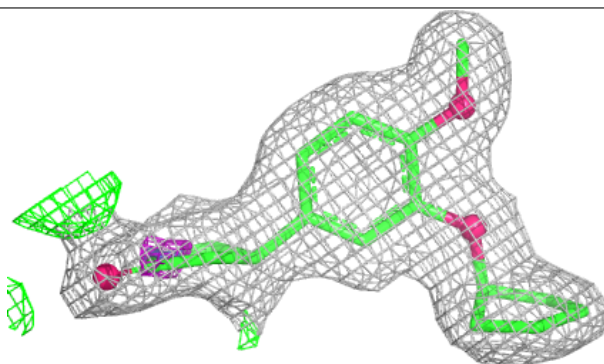


Electron density around ROL D 904 (B):

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

**Electron density around ROL A 901:**

$2mF_o-DF_c$ (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.