



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 26, 2024 – 08:42 AM EDT

PDB ID : 6VYN
Title : N-terminal domain of mouse surfactant protein B with bound lipid, wild type
Authors : Rapoport, T.A.; Bodnar, N.O.
Deposited on : 2020-02-27
Resolution : 2.20 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.37.1
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) : 2.37.1

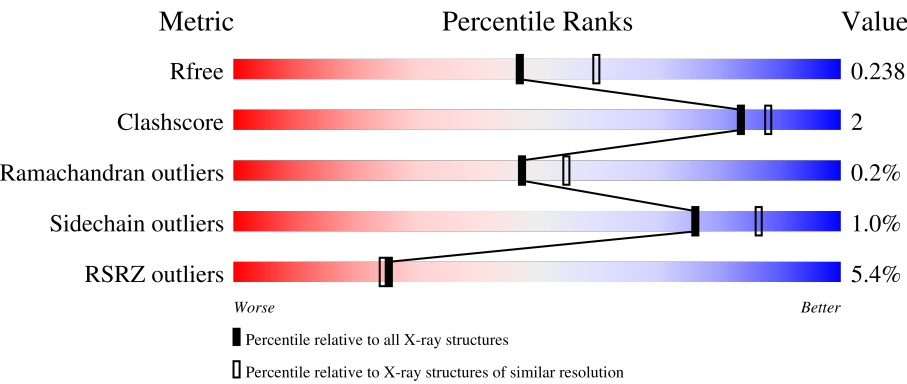
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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 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	87	<div><div></div><div>91%9%</div></div>
1	B	87	<div><div>2%</div><div>86%5%9%</div></div>
1	C	87	<div><div>2%</div><div>86%5%9%</div></div>
1	D	87	<div><div>9%</div><div>82%8%10%</div></div>
1	E	87	<div><div>2%</div><div>84%7%8%</div></div>

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Mol	Chain	Length	Quality of chain
1	F	87	
1	G	87	
1	H	87	

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
2	RXY	D	101	-	-	-	X
2	RXY	F	101[A]	-	-	-	X
2	RXY	F	101[B]	-	-	-	X
2	RXY	F	102	-	-	-	X
2	RXY	G	101[A]	-	-	-	X
2	RXY	G	101[B]	-	-	-	X
2	RXY	G	102	-	-	-	X
2	RXY	H	101	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12402 atoms, of which 6333 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.

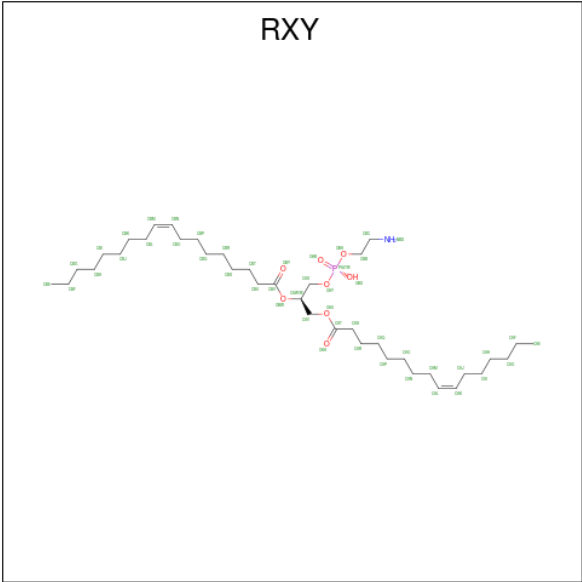
- Molecule 1 is a protein called Pulmonary surfactant-associated protein B.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	79	Total	C	H	N	O	S	0	0	0
			1295	411	653	108	116	7			
1	B	79	Total	C	H	N	O	S	0	1	0
			1308	415	658	110	118	7			
1	C	79	Total	C	H	N	O	S	0	0	0
			1284	409	645	106	117	7			
1	D	78	Total	C	H	N	O	S	0	0	0
			1270	405	639	104	115	7			
1	F	79	Total	C	H	N	O	S	0	0	0
			1284	409	645	106	117	7			
1	H	77	Total	C	H	N	O	S	0	0	0
			1256	400	632	103	114	7			
1	E	80	Total	C	H	N	O	S	0	0	0
			1308	415	658	110	118	7			
1	G	77	Total	C	H	N	O	S	0	0	0
			1258	401	635	103	112	7			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SER	-	expression tag	UNP P50405
B	1	SER	-	expression tag	UNP P50405
C	1	SER	-	expression tag	UNP P50405
D	1	SER	-	expression tag	UNP P50405
F	1	SER	-	expression tag	UNP P50405
H	1	SER	-	expression tag	UNP P50405
E	1	SER	-	expression tag	UNP P50405
G	1	SER	-	expression tag	UNP P50405

- Molecule 2 is (7Z,19R,22R)-25-amino-22-hydroxy-16,22-dioxo-17,21,23-trioxa-22lambda 5 -phosphapentacos-7-en-19-yl (9Z)-octadec-9-enoate (three-letter code: RXY) (formula: C₃₉H₇₄NO₈P).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	P	0	0
			122	39	73	1	8	1		
2	B	1	Total	C	H	N	O	P	0	0
			122	39	73	1	8	1		
2	B	1	Total	C	H	N	O	P	0	0
			122	39	73	1	8	1		
2	C	1	Total	C	H	N	O	P	0	1
			244	78	146	2	16	2		
2	D	1	Total	C	H	N	O	P	0	0
			122	39	73	1	8	1		
2	F	1	Total	C	H	N	O	P	0	1
			244	78	146	2	16	2		
2	F	1	Total	C	H	N	O	P	0	0
			122	39	73	1	8	1		
2	H	1	Total	C	H	N	O	P	0	0
			122	39	73	1	8	1		
2	E	1	Total	C	H	N	O	P	0	1
			244	78	146	2	16	2		
2	E	1	Total	C	H	N	O	P	0	0
			122	39	73	1	8	1		
2	G	1	Total	C	H	N	O	P	0	1
			244	78	146	2	16	2		
2	G	1	Total	C	H	N	O	P	0	0
			122	39	73	1	8	1		

- Molecule 3 is water.

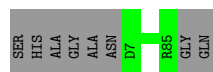
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	45	Total 45	O 45	0	0
3	B	47	Total 47	O 47	0	0
3	C	20	Total 20	O 20	0	0
3	D	7	Total 7	O 7	0	0
3	F	19	Total 19	O 19	0	0
3	H	15	Total 15	O 15	0	0
3	E	23	Total 23	O 23	0	0
3	G	11	Total 11	O 11	0	0

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: Pulmonary surfactant-associated protein B

Chain A: 




- Molecule 1: Pulmonary surfactant-associated protein B

Chain B: 




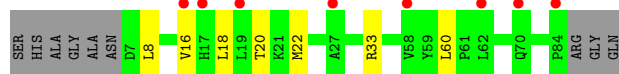
- Molecule 1: Pulmonary surfactant-associated protein B

Chain C: 




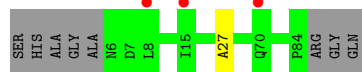
- Molecule 1: Pulmonary surfactant-associated protein B

Chain D: 

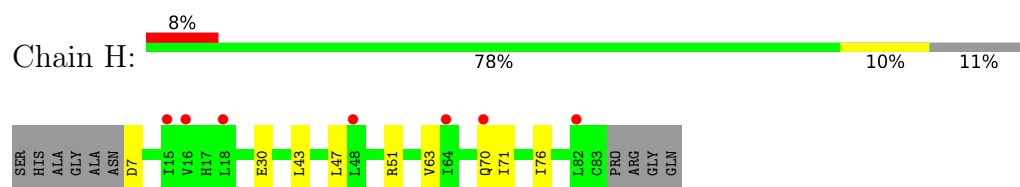


- Molecule 1: Pulmonary surfactant-associated protein B

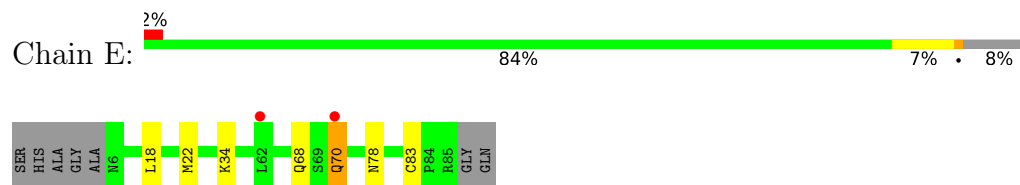
Chain F: 



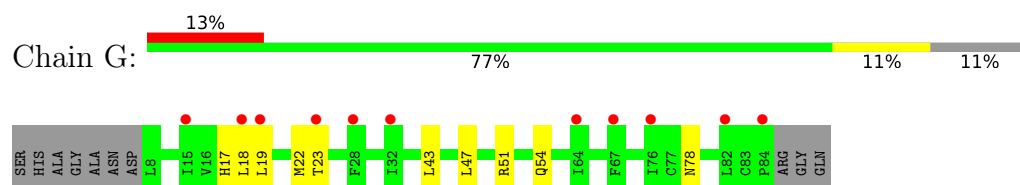
- Molecule 1: Pulmonary surfactant-associated protein B



- Molecule 1: Pulmonary surfactant-associated protein B



- Molecule 1: Pulmonary surfactant-associated protein B



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	93.71Å 108.16Å 114.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	78.70 – 2.20 78.70 – 2.20	Depositor EDS
% Data completeness (in resolution range)	95.2 (78.70-2.20) 95.3 (78.70-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.20 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.17.1 _3660	Depositor
R, R_{free}	0.224 , 0.238 0.224 , 0.238	Depositor DCC
R_{free} test set	1983 reflections (3.47%)	wwPDB-VP
Wilson B-factor (Å ²)	54.9	Xtriage
Anisotropy	0.363	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 61.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12402	wwPDB-VP
Average B, all atoms (Å ²)	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.89% 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: RXY

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	0.25	0/653	0.45	0/884
1	B	0.27	0/661	0.45	0/895
1	C	0.26	0/650	0.45	0/881
1	D	0.25	0/642	0.43	0/870
1	E	0.32	0/661	0.47	0/895
1	F	0.25	0/650	0.42	0/881
1	G	0.25	0/634	0.42	0/859
1	H	0.25	0/634	0.44	0/858
All	All	0.27	0/5185	0.44	0/7023

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	642	653	652	0	0
1	B	650	658	657	3	0
1	C	639	645	645	2	0
1	D	631	639	639	5	0
1	E	650	658	658	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	639	645	645	1	0
1	G	623	635	635	6	0
1	H	624	632	632	6	0
2	A	49	73	0	0	0
2	B	98	146	0	0	0
2	C	98	146	0	0	0
2	D	49	73	0	1	0
2	E	147	219	0	0	0
2	F	147	219	0	0	0
2	G	147	219	0	1	0
2	H	49	73	0	0	0
3	A	45	0	0	0	0
3	B	47	0	0	1	0
3	C	20	0	0	0	0
3	D	7	0	0	0	0
3	E	23	0	0	1	0
3	F	19	0	0	0	0
3	G	11	0	0	0	0
3	H	15	0	0	0	0
All	All	6069	6333	5163	26	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 2.

All (26) 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:D:33:ARG:HD2	1:D:60:LEU:HD23	1.72	0.70
1:G:19:LEU:HD23	1:G:22:MET:CE	2.34	0.57
1:C:18:LEU:O	1:C:22:MET:HG3	2.09	0.53
1:E:78:ASN:OD1	1:E:83:CYS:HB2	2.11	0.50
1:D:8:LEU:HD11	1:F:27:ALA:HB3	1.93	0.49
1:H:43:LEU:HD11	1:H:47:LEU:HD12	1.96	0.47
1:H:7:ASP:N	1:H:7:ASP:OD1	2.48	0.47
1:E:18:LEU:O	1:E:22:MET:HG3	2.16	0.46
1:G:19:LEU:O	1:G:23:THR:HG23	2.16	0.45
1:G:43:LEU:HD11	1:G:47:LEU:HD12	1.99	0.45
1:G:54:GLN:OE1	1:G:54:GLN:N	2.50	0.44
1:H:71:ILE:HD12	1:H:76:ILE:CD1	2.48	0.43
1:H:71:ILE:HD12	1:H:76:ILE:HD12	1.99	0.43
1:B:22:MET:HE2	1:B:28:PHE:CE2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:70:GLN:O	1:E:70:GLN:HG2	2.18	0.43
1:D:33:ARG:HD3	1:H:70:GLN:HG3	2.00	0.43
1:B:74:LYS:NZ	3:B:202:HOH:O	2.52	0.42
1:B:18:LEU:O	1:B:22:MET:HG3	2.20	0.41
1:D:18:LEU:O	1:D:22:MET:HG3	2.20	0.41
1:D:16:VAL:O	1:D:20:THR:HG23	2.20	0.41
1:C:66:TYR:OH	1:C:76:ILE:CD1	2.68	0.41
1:H:63:VAL:HG22	2:G:101[B]:RXY:CBE	2.50	0.41
1:E:68:GLN:NE2	3:E:203:HOH:O	2.52	0.41
1:G:18:LEU:O	1:G:22:MET:HG3	2.20	0.41
1:G:43:LEU:HD11	1:G:47:LEU:CD1	2.51	0.41
2:D:101:RXY:OAY	2:D:101:RXY:CBV	2.69	0.41

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	77/87 (88%)	77 (100%)	0	0	100	100
1	B	78/87 (90%)	76 (97%)	2 (3%)	0	100	100
1	C	77/87 (88%)	76 (99%)	1 (1%)	0	100	100
1	D	76/87 (87%)	75 (99%)	1 (1%)	0	100	100
1	E	78/87 (90%)	77 (99%)	0	1 (1%)	12	9
1	F	77/87 (88%)	76 (99%)	1 (1%)	0	100	100
1	G	75/87 (86%)	75 (100%)	0	0	100	100
1	H	75/87 (86%)	75 (100%)	0	0	100	100
All	All	613/696 (88%)	607 (99%)	5 (1%)	1 (0%)	47	55

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	70	GLN

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	75/79 (95%)	75 (100%)	0	100	100
1	B	76/79 (96%)	76 (100%)	0	100	100
1	C	75/79 (95%)	75 (100%)	0	100	100
1	D	74/79 (94%)	74 (100%)	0	100	100
1	E	76/79 (96%)	75 (99%)	1 (1%)	69	81
1	F	75/79 (95%)	75 (100%)	0	100	100
1	G	73/79 (92%)	70 (96%)	3 (4%)	30	39
1	H	73/79 (92%)	71 (97%)	2 (3%)	44	57
All	All	597/632 (94%)	591 (99%)	6 (1%)	76	86

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

Mol	Chain	Res	Type
1	H	30	GLU
1	H	51	ARG
1	E	34	LYS
1	G	17	HIS
1	G	51	ARG
1	G	78	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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](#)

16 ligands 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	$\# Z > 2$
2	RXY	G	101[B]	-	48,48,48	1.08	3 (6%)	51,53,53	0.79	2 (3%)
2	RXY	G	101[A]	-	48,48,48	1.07	3 (6%)	51,53,53	0.84	2 (3%)
2	RXY	B	102	-	48,48,48	1.09	3 (6%)	51,53,53	0.85	2 (3%)
2	RXY	A	101	-	48,48,48	1.07	3 (6%)	51,53,53	0.84	2 (3%)
2	RXY	F	101[A]	-	48,48,48	1.07	3 (6%)	51,53,53	0.79	2 (3%)
2	RXY	B	101	-	48,48,48	1.07	3 (6%)	51,53,53	0.86	2 (3%)
2	RXY	C	101[B]	-	48,48,48	1.08	3 (6%)	51,53,53	0.83	2 (3%)
2	RXY	H	101	-	48,48,48	1.08	3 (6%)	51,53,53	0.88	2 (3%)
2	RXY	F	102	-	48,48,48	1.06	3 (6%)	51,53,53	0.87	3 (5%)
2	RXY	C	101[A]	-	48,48,48	1.08	3 (6%)	51,53,53	0.77	2 (3%)
2	RXY	E	102	-	48,48,48	1.08	3 (6%)	51,53,53	0.85	2 (3%)
2	RXY	E	101[B]	-	48,48,48	1.08	3 (6%)	51,53,53	0.82	2 (3%)
2	RXY	E	101[A]	-	48,48,48	1.05	3 (6%)	51,53,53	0.87	2 (3%)
2	RXY	D	101	-	48,48,48	1.07	3 (6%)	51,53,53	0.87	2 (3%)
2	RXY	G	102	-	48,48,48	1.07	2 (4%)	51,53,53	0.97	2 (3%)
2	RXY	F	101[B]	-	48,48,48	1.07	3 (6%)	51,53,53	0.82	2 (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
2	RXY	G	101[B]	-	-	30/52/52/52	-
2	RXY	G	101[A]	-	-	22/52/52/52	-
2	RXY	B	102	-	-	26/52/52/52	-
2	RXY	A	101	-	-	24/52/52/52	-
2	RXY	F	101[A]	-	-	20/52/52/52	-
2	RXY	B	101	-	-	23/52/52/52	-
2	RXY	C	101[B]	-	-	27/52/52/52	-
2	RXY	H	101	-	-	31/52/52/52	-
2	RXY	F	102	-	-	24/52/52/52	-
2	RXY	C	101[A]	-	-	15/52/52/52	-
2	RXY	E	102	-	-	24/52/52/52	-
2	RXY	E	101[B]	-	-	22/52/52/52	-
2	RXY	E	101[A]	-	-	25/52/52/52	-
2	RXY	D	101	-	-	24/52/52/52	-
2	RXY	G	102	-	-	35/52/52/52	-
2	RXY	F	101[B]	-	-	23/52/52/52	-

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	102	RXY	OAU-CAT	3.44	1.43	1.33
2	G	102	RXY	OAU-CAT	3.41	1.43	1.33
2	G	101[B]	RXY	OAU-CAT	3.38	1.43	1.33
2	A	101	RXY	OAU-CAT	3.34	1.43	1.33
2	H	101	RXY	OAU-CAT	3.33	1.43	1.33
2	D	101	RXY	OAU-CAT	3.32	1.43	1.33
2	F	101[B]	RXY	OAU-CAT	3.28	1.42	1.33
2	C	101[B]	RXY	OAU-CAT	3.26	1.42	1.33
2	F	102	RXY	OAU-CAT	3.26	1.42	1.33
2	E	102	RXY	OAU-CAT	3.21	1.42	1.33
2	G	101[A]	RXY	OAU-CAT	3.20	1.42	1.33
2	E	101[B]	RXY	OAU-CAT	3.19	1.42	1.33
2	F	101[A]	RXY	OAU-CAT	3.17	1.42	1.33
2	C	101[A]	RXY	OAU-CAT	3.17	1.42	1.33
2	B	101	RXY	OAU-CAT	3.11	1.42	1.33
2	E	101[A]	RXY	OAU-CAT	3.08	1.42	1.33
2	G	102	RXY	OBW-CBV	2.80	1.42	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	101[B]	RXY	OBW-CBV	2.79	1.42	1.34
2	C	101[A]	RXY	OBW-CBV	2.75	1.42	1.34
2	B	102	RXY	OBW-CBV	2.74	1.42	1.34
2	C	101[B]	RXY	OBW-CBV	2.69	1.41	1.34
2	F	101[A]	RXY	OBW-CBV	2.63	1.41	1.34
2	F	101[B]	RXY	OBW-CBV	2.62	1.41	1.34
2	G	101[A]	RXY	OBW-CBV	2.61	1.41	1.34
2	E	102	RXY	OBW-CBV	2.61	1.41	1.34
2	E	101[A]	RXY	OBW-CBV	2.61	1.41	1.34
2	B	101	RXY	OBW-CBV	2.60	1.41	1.34
2	G	101[B]	RXY	OBW-CBV	2.60	1.41	1.34
2	D	101	RXY	OBW-CBV	2.53	1.41	1.34
2	A	101	RXY	OBW-CBV	2.52	1.41	1.34
2	F	102	RXY	OBW-CBV	2.48	1.41	1.34
2	H	101	RXY	OBW-CAW	-2.48	1.40	1.46
2	F	101[A]	RXY	OBW-CAW	-2.47	1.40	1.46
2	E	101[A]	RXY	OBW-CAW	-2.47	1.40	1.46
2	D	101	RXY	OBW-CAW	-2.47	1.40	1.46
2	F	102	RXY	OBW-CAW	-2.46	1.40	1.46
2	A	101	RXY	OBW-CAW	-2.45	1.40	1.46
2	H	101	RXY	OBW-CBV	2.44	1.41	1.34
2	G	101[A]	RXY	OBW-CAW	-2.44	1.40	1.46
2	C	101[B]	RXY	OBW-CAW	-2.43	1.40	1.46
2	E	101[B]	RXY	OBW-CAW	-2.41	1.40	1.46
2	E	102	RXY	OBW-CAW	-2.40	1.40	1.46
2	B	101	RXY	OBW-CAW	-2.33	1.40	1.46
2	F	101[B]	RXY	OBW-CAW	-2.33	1.40	1.46
2	G	101[B]	RXY	OBW-CAW	-2.29	1.40	1.46
2	B	102	RXY	OBW-CAW	-2.08	1.41	1.46
2	C	101[A]	RXY	OBW-CAW	-2.07	1.41	1.46

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	102	RXY	OBW-CBV-CBU	4.37	120.93	111.50
2	E	102	RXY	OBW-CBV-CBU	4.04	120.20	111.50
2	H	101	RXY	OBW-CBV-CBU	4.01	120.14	111.50
2	B	101	RXY	OBW-CBV-CBU	3.95	120.02	111.50
2	E	101[A]	RXY	OBW-CBV-CBU	3.95	120.01	111.50
2	G	101[A]	RXY	OBW-CBV-CBU	3.77	119.64	111.50
2	D	101	RXY	OBW-CBV-CBU	3.75	119.58	111.50
2	A	101	RXY	OBW-CBV-CBU	3.74	119.56	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	101[B]	RXY	OBW-CBV-CBU	3.67	119.42	111.50
2	C	101[A]	RXY	OBW-CBV-CBU	3.66	119.38	111.50
2	F	101[B]	RXY	OBW-CBV-CBU	3.64	119.34	111.50
2	F	101[A]	RXY	OBW-CBV-CBU	3.62	119.30	111.50
2	F	102	RXY	OBW-CBV-CBU	3.62	119.29	111.50
2	C	101[B]	RXY	OBW-CBV-CBU	3.55	119.16	111.50
2	G	101[B]	RXY	OBW-CBV-CBU	3.54	119.14	111.50
2	B	102	RXY	OBW-CBV-CBU	3.25	118.51	111.50
2	B	102	RXY	OAU-CAT-CAS	3.12	121.70	111.91
2	G	102	RXY	OAU-CAT-CAS	3.02	121.37	111.91
2	D	101	RXY	OAU-CAT-CAS	2.88	120.94	111.91
2	C	101[B]	RXY	OAU-CAT-CAS	2.78	120.64	111.91
2	G	101[B]	RXY	OAU-CAT-CAS	2.76	120.57	111.91
2	G	101[A]	RXY	OAU-CAT-CAS	2.70	120.39	111.91
2	H	101	RXY	OAU-CAT-CAS	2.68	120.32	111.91
2	F	102	RXY	OAU-CAT-CAS	2.60	120.08	111.91
2	F	101[B]	RXY	OAU-CAT-CAS	2.51	119.80	111.91
2	A	101	RXY	OAU-CAT-CAS	2.49	119.71	111.91
2	F	101[A]	RXY	OAU-CAT-CAS	2.42	119.49	111.91
2	E	102	RXY	OAU-CAT-CAS	2.41	119.48	111.91
2	E	101[A]	RXY	OAU-CAT-CAS	2.40	119.44	111.91
2	E	101[B]	RXY	OAU-CAT-CAS	2.39	119.41	111.91
2	C	101[A]	RXY	OAU-CAT-CAS	2.38	119.37	111.91
2	B	101	RXY	OAU-CAT-CAS	2.37	119.36	111.91
2	F	102	RXY	CAW-OBW-CBV	-2.14	112.52	117.79

There are no chirality outliers.

All (395) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	101	RXY	CBU-CBV-OBW-CAW
2	A	101	RXY	OBV-CBV-OBW-CAW
2	A	101	RXY	OBW-CAW-CAX-OAY
2	A	101	RXY	CAX-OAY-PAZ-OBX
2	A	101	RXY	CAX-OAY-PAZ-OAB
2	A	101	RXY	OBA-CBB-CBC-NBD
2	B	101	RXY	CAX-OAY-PAZ-OBX
2	B	101	RXY	CAX-OAY-PAZ-OAB
2	B	101	RXY	CBB-OBA-PAZ-OAY
2	B	101	RXY	CBB-OBA-PAZ-OAB
2	B	101	RXY	OBA-CBB-CBC-NBD
2	B	101	RXY	OAA-CAT-OAU-CAV

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Mol	Chain	Res	Type	Atoms
2	B	102	RXY	CBB-OBA-PAZ-OAB
2	B	102	RXY	OBA-CBB-CBC-NBD
2	C	101[A]	RXY	CAX-OAY-PAZ-OAB
2	C	101[A]	RXY	CBB-OBA-PAZ-OAB
2	C	101[B]	RXY	CBB-OBA-PAZ-OAB
2	C	101[B]	RXY	OBA-CBB-CBC-NBD
2	D	101	RXY	OAU-CAV-CAW-OBW
2	D	101	RXY	CAX-OAY-PAZ-OBX
2	D	101	RXY	CAX-OAY-PAZ-OAB
2	D	101	RXY	CBB-OBA-PAZ-OAB
2	F	101[A]	RXY	CBB-OBA-PAZ-OBX
2	F	101[B]	RXY	CBB-OBA-PAZ-OAB
2	F	102	RXY	CBU-CBV-OBW-CAW
2	H	101	RXY	CAX-OAY-PAZ-OBX
2	H	101	RXY	OBA-CBB-CBC-NBD
2	E	101[A]	RXY	CBB-OBA-PAZ-OBX
2	E	101[A]	RXY	CBB-OBA-PAZ-OAB
2	E	101[A]	RXY	OBA-CBB-CBC-NBD
2	E	102	RXY	CAX-OAY-PAZ-OBX
2	E	102	RXY	CAX-OAY-PAZ-OAB
2	E	102	RXY	OBA-CBB-CBC-NBD
2	G	101[A]	RXY	OBA-CBB-CBC-NBD
2	G	101[B]	RXY	CAX-OAY-PAZ-OBX
2	G	102	RXY	OBY-CBV-OBW-CAW
2	G	102	RXY	CAW-CAX-OAY-PAZ
2	G	102	RXY	CAX-OAY-PAZ-OBX
2	G	102	RXY	CAX-OAY-PAZ-OAB
2	G	102	RXY	CAX-OAY-PAZ-OBA
2	G	102	RXY	CBB-OBA-PAZ-OAY
2	G	102	RXY	CBB-OBA-PAZ-OAB
2	B	101	RXY	CAS-CAT-OAU-CAV
2	F	102	RXY	OBY-CBV-OBW-CAW
2	E	101[A]	RXY	CAS-CAT-OAU-CAV
2	G	102	RXY	CBU-CBV-OBW-CAW
2	C	101[A]	RXY	CAS-CAT-OAU-CAV
2	E	101[B]	RXY	CAS-CAT-OAU-CAV
2	C	101[A]	RXY	OAA-CAT-OAU-CAV
2	E	101[A]	RXY	OAA-CAT-OAU-CAV
2	D	101	RXY	CBU-CBV-OBW-CAW
2	B	101	RXY	CBH-CBI-CBJ-CBK
2	H	101	RXY	CAG-CAH-CAI-CAJ
2	E	101[B]	RXY	OAA-CAT-OAU-CAV

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Mol	Chain	Res	Type	Atoms
2	B	102	RXY	CAG-CAH-CAI-CAJ
2	H	101	RXY	CBI-CBJ-CBK-CBL
2	A	101	RXY	CAS-CAT-OAU-CAV
2	F	101[A]	RXY	CAS-CAT-OAU-CAV
2	E	102	RXY	CAS-CAT-OAU-CAV
2	A	101	RXY	CAQ-CAR-CAS-CAT
2	F	101[A]	RXY	OAA-CAT-OAU-CAV
2	B	102	RXY	CAQ-CAR-CAS-CAT
2	D	101	RXY	OBY-CBV-OBW-CAW
2	G	102	RXY	CAQ-CAR-CAS-CAT
2	B	101	RXY	CBU-CBV-OBW-CAW
2	A	101	RXY	OAA-CAT-OAU-CAV
2	E	102	RXY	OAA-CAT-OAU-CAV
2	C	101[A]	RXY	CBJ-CBK-CBL-CBM
2	A	101	RXY	CAX-OAY-PAZ-OBA
2	A	101	RXY	CBB-OBA-PAZ-OAY
2	B	101	RXY	CAX-OAY-PAZ-OBA
2	B	102	RXY	CBB-OBA-PAZ-OAY
2	C	101[A]	RXY	CAX-OAY-PAZ-OBA
2	D	101	RXY	CAX-OAY-PAZ-OBA
2	F	101[A]	RXY	CBB-OBA-PAZ-OAY
2	F	102	RXY	CBB-OBA-PAZ-OAY
2	H	101	RXY	CAX-OAY-PAZ-OBA
2	E	101[A]	RXY	CBB-OBA-PAZ-OAY
2	E	101[B]	RXY	CAX-OAY-PAZ-OBA
2	E	102	RXY	CAX-OAY-PAZ-OBA
2	G	101[A]	RXY	CAX-OAY-PAZ-OBA
2	G	101[B]	RXY	CAX-OAY-PAZ-OBA
2	C	101[B]	RXY	CAQ-CAR-CAS-CAT
2	B	101	RXY	OBY-CBV-OBW-CAW
2	F	101[B]	RXY	CBN-CBO-CBP-CBQ
2	A	101	RXY	CBI-CBJ-CBK-CBL
2	C	101[B]	RXY	CBH-CBI-CBJ-CBK
2	E	101[B]	RXY	CAP-CAQ-CAR-CAS
2	F	101[B]	RXY	CBU-CBV-OBW-CAW
2	B	101	RXY	CAF-CAG-CAH-CAI
2	G	102	RXY	CAF-CAG-CAH-CAI
2	E	101[A]	RXY	CAG-CAH-CAI-CAJ
2	G	101[B]	RXY	CBO-CBP-CBQ-CBR
2	B	101	RXY	CAV-CAW-OBW-CBV
2	F	101[B]	RXY	OBY-CBV-OBW-CAW
2	E	102	RXY	CBF-CBG-CBH-CBI

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Mol	Chain	Res	Type	Atoms
2	B	101	RXY	CAO-CAP-CAQ-CAR
2	E	101[A]	RXY	CAM-CAN-CAO-CAP
2	A	101	RXY	CAF-CAG-CAH-CAI
2	E	101[B]	RXY	CAM-CAN-CAO-CAP
2	B	101	RXY	CAG-CAH-CAI-CAJ
2	B	102	RXY	CAM-CAN-CAO-CAP
2	G	102	RXY	CBQ-CBR-CBS-CBT
2	C	101[B]	RXY	CBQ-CBR-CBS-CBT
2	C	101[B]	RXY	CBN-CBO-CBP-CBQ
2	D	101	RXY	CAL-CAM-CAN-CAO
2	E	101[A]	RXY	CAL-CAM-CAN-CAO
2	G	101[B]	RXY	CAH-CAI-CAJ-CAK
2	F	102	RXY	CBI-CBJ-CBK-CBL
2	E	102	RXY	CAF-CAG-CAH-CAI
2	C	101[B]	RXY	CBS-CBT-CBU-CBV
2	C	101[B]	RXY	CBR-CBS-CBT-CBU
2	C	101[B]	RXY	CAO-CAP-CAQ-CAR
2	F	101[A]	RXY	CAG-CAH-CAI-CAJ
2	G	102	RXY	CBG-CBH-CBI-CBJ
2	B	102	RXY	CBR-CBS-CBT-CBU
2	B	102	RXY	CBF-CBG-CBH-CBI
2	F	102	RXY	CAF-CAG-CAH-CAI
2	G	102	RXY	CBH-CBI-CBJ-CBK
2	H	101	RXY	CAF-CAG-CAH-CAI
2	A	101	RXY	CAH-CAI-CAJ-CAK
2	B	102	RXY	CBJ-CBK-CBL-CBM
2	B	102	RXY	CAH-CAI-CAJ-CAK
2	C	101[A]	RXY	CBN-CBO-CBP-CBQ
2	F	101[B]	RXY	CAL-CAM-CAN-CAO
2	E	101[A]	RXY	CAQ-CAR-CAS-CAT
2	B	101	RXY	CBG-CBH-CBI-CBJ
2	E	102	RXY	CAM-CAN-CAO-CAP
2	A	101	RXY	CBQ-CBR-CBS-CBT
2	H	101	RXY	CBG-CBH-CBI-CBJ
2	F	101[B]	RXY	CBQ-CBR-CBS-CBT
2	E	102	RXY	CBP-CBQ-CBR-CBS
2	F	101[B]	RXY	CBH-CBI-CBJ-CBK
2	G	101[A]	RXY	CAM-CAN-CAO-CAP
2	G	102	RXY	CAS-CAT-OAU-CAV
2	E	101[A]	RXY	CAO-CAP-CAQ-CAR
2	E	102	RXY	CBG-CBH-CBI-CBJ
2	E	101[A]	RXY	CAH-CAI-CAJ-CAK

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Mol	Chain	Res	Type	Atoms
2	G	101[B]	RXY	CBJ-CBK-CBL-CBM
2	G	101[B]	RXY	CBN-CBO-CBP-CBQ
2	E	101[B]	RXY	CAQ-CAR-CAS-CAT
2	H	101	RXY	CAS-CAT-OAU-CAV
2	G	101[A]	RXY	CBP-CBQ-CBR-CBS
2	G	102	RXY	CBR-CBS-CBT-CBU
2	B	102	RXY	CBH-CBI-CBJ-CBK
2	G	101[B]	RXY	CAF-CAG-CAH-CAI
2	G	101[B]	RXY	CBS-CBT-CBU-CBV
2	E	102	RXY	CBR-CBS-CBT-CBU
2	G	102	RXY	OAA-CAT-OAU-CAV
2	H	101	RXY	CBU-CBV-OBW-CAW
2	G	101[A]	RXY	CBU-CBV-OBW-CAW
2	H	101	RXY	OBW-CAW-CAX-OAY
2	E	102	RXY	OBW-CAW-CAX-OAY
2	H	101	RXY	OBY-CBV-OBW-CAW
2	G	101[A]	RXY	OBY-CBV-OBW-CAW
2	G	101[B]	RXY	CBF-CBG-CBH-CBI
2	E	102	RXY	CBN-CBO-CBP-CBQ
2	C	101[B]	RXY	CAP-CAQ-CAR-CAS
2	G	101[A]	RXY	CBG-CBH-CBI-CBJ
2	G	101[A]	RXY	CAP-CAQ-CAR-CAS
2	C	101[B]	RXY	CBO-CBP-CBQ-CBR
2	E	101[A]	RXY	CBR-CBS-CBT-CBU
2	A	101	RXY	CAV-CAW-CAX-OAY
2	G	101[B]	RXY	CAV-CAW-CAX-OAY
2	G	102	RXY	CAV-CAW-CAX-OAY
2	H	101	RXY	CBR-CBS-CBT-CBU
2	G	101[B]	RXY	CAN-CAO-CAP-CAQ
2	H	101	RXY	CBN-CBO-CBP-CBQ
2	G	101[A]	RXY	CBN-CBO-CBP-CBQ
2	G	101[A]	RXY	CAH-CAI-CAJ-CAK
2	D	101	RXY	OAU-CAV-CAW-CAX
2	F	102	RXY	OAU-CAV-CAW-CAX
2	E	101[A]	RXY	OAU-CAV-CAW-CAX
2	G	101[B]	RXY	OAU-CAV-CAW-CAX
2	B	101	RXY	CAN-CAO-CAP-CAQ
2	B	102	RXY	CBO-CBP-CBQ-CBR
2	G	101[B]	RXY	CAM-CAN-CAO-CAP
2	H	101	RXY	OAA-CAT-OAU-CAV
2	A	101	RXY	CBN-CBO-CBP-CBQ
2	A	101	RXY	CAL-CAM-CAN-CAO

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Mol	Chain	Res	Type	Atoms
2	D	101	RXY	CAH-CAI-CAJ-CAK
2	E	102	RXY	CAH-CAI-CAJ-CAK
2	G	101[A]	RXY	CBJ-CBK-CBL-CBM
2	G	101[B]	RXY	CBU-CBV-OBW-CAW
2	F	102	RXY	CBE-CBF-CBG-CBH
2	F	102	RXY	CBP-CBQ-CBR-CBS
2	H	101	RXY	CBH-CBI-CBJ-CBK
2	B	102	RXY	CAS-CAT-OAU-CAV
2	G	101[B]	RXY	CAS-CAT-OAU-CAV
2	B	101	RXY	CBE-CBF-CBG-CBH
2	G	102	RXY	CAM-CAN-CAO-CAP
2	G	101[B]	RXY	CBI-CBJ-CBK-CBL
2	G	101[A]	RXY	CBO-CBP-CBQ-CBR
2	B	102	RXY	CAO-CAP-CAQ-CAR
2	B	102	RXY	CBM-CBN-CBO-CBP
2	C	101[B]	RXY	CAV-CAW-CAX-OAY
2	H	101	RXY	CAV-CAW-CAX-OAY
2	E	102	RXY	CAV-CAW-CAX-OAY
2	F	101[A]	RXY	OBA-CBB-CBC-NBD
2	C	101[B]	RXY	CAS-CAT-OAU-CAV
2	A	101	RXY	CBE-CBF-CBG-CBH
2	D	101	RXY	CAW-CAX-OAY-PAZ
2	B	102	RXY	OAA-CAT-OAU-CAV
2	G	101[B]	RXY	CBG-CBH-CBI-CBJ
2	H	101	RXY	CBS-CBT-CBU-CBV
2	F	101[A]	RXY	OAU-CAV-CAW-CAX
2	E	101[B]	RXY	OAU-CAV-CAW-CAX
2	E	102	RXY	CAN-CAO-CAP-CAQ
2	D	101	RXY	CBF-CBG-CBH-CBI
2	F	102	RXY	CAM-CAN-CAO-CAP
2	C	101[B]	RXY	CBB-OBA-PAZ-OAY
2	G	101[B]	RXY	OAA-CAT-OAU-CAV
2	C	101[B]	RXY	OBW-CAW-CAX-OAY
2	E	101[B]	RXY	OBW-CAW-CAX-OAY
2	G	101[B]	RXY	OBW-CAW-CAX-OAY
2	G	102	RXY	OBW-CAW-CAX-OAY
2	G	101[B]	RXY	OBY-CBV-OBW-CAW
2	F	102	RXY	OAU-CAV-CAW-OBW
2	E	101[B]	RXY	OAU-CAV-CAW-OBW
2	G	102	RXY	OAU-CAV-CAW-OBW
2	G	102	RXY	CBP-CBQ-CBR-CBS
2	B	102	RXY	CAW-CAX-OAY-PAZ

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Mol	Chain	Res	Type	Atoms
2	C	101[B]	RXY	CAW-CAX-OAY-PAZ
2	C	101[B]	RXY	CAL-CAM-CAN-CAO
2	F	101[B]	RXY	CBJ-CBK-CBL-CBM
2	A	101	RXY	CBK-CBL-CBM-CBN
2	D	101	RXY	CBQ-CBR-CBS-CBT
2	G	101[A]	RXY	CBI-CBJ-CBK-CBL
2	C	101[B]	RXY	CBU-CBV-OBW-CAW
2	E	101[A]	RXY	CAE-CAF-CAG-CAH
2	F	101[B]	RXY	CBS-CBT-CBU-CBV
2	F	101[B]	RXY	CAF-CAG-CAH-CAI
2	F	101[B]	RXY	CBR-CBS-CBT-CBU
2	F	102	RXY	CBG-CBH-CBI-CBJ
2	G	102	RXY	CBO-CBP-CBQ-CBR
2	C	101[B]	RXY	OBY-CBV-OBW-CAW
2	G	101[B]	RXY	CAP-CAQ-CAR-CAS
2	G	102	RXY	CAX-CAW-OBW-CBV
2	B	101	RXY	CBP-CBQ-CBR-CBS
2	F	101[B]	RXY	CAS-CAT-OAU-CAV
2	E	101[B]	RXY	CBJ-CBK-CBL-CBM
2	E	101[B]	RXY	CAH-CAI-CAJ-CAK
2	H	101	RXY	OAU-CAV-CAW-CAX
2	F	101[A]	RXY	CAP-CAQ-CAR-CAS
2	E	101[B]	RXY	CBO-CBP-CBQ-CBR
2	C	101[B]	RXY	OAA-CAT-OAU-CAV
2	H	101	RXY	OAU-CAV-CAW-OBW
2	G	101[B]	RXY	OAU-CAV-CAW-OBW
2	E	102	RXY	CBO-CBP-CBQ-CBR
2	E	101[A]	RXY	CAF-CAG-CAH-CAI
2	F	102	RXY	CBS-CBT-CBU-CBV
2	D	101	RXY	CAG-CAH-CAI-CAJ
2	H	101	RXY	CBO-CBP-CBQ-CBR
2	C	101[B]	RXY	CAX-OAY-PAZ-OBA
2	D	101	RXY	CBB-OBA-PAZ-OAY
2	A	101	RXY	CBB-OBA-PAZ-OBX
2	A	101	RXY	CBB-OBA-PAZ-OAB
2	B	102	RXY	CBB-OBA-PAZ-OBX
2	C	101[A]	RXY	CAX-OAY-PAZ-OBX
2	F	101[A]	RXY	CBB-OBA-PAZ-OAB
2	F	102	RXY	CBB-OBA-PAZ-OBX
2	F	102	RXY	CBB-OBA-PAZ-OAB
2	H	101	RXY	CAX-OAY-PAZ-OAB
2	E	101[B]	RXY	CAX-OAY-PAZ-OBX

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Mol	Chain	Res	Type	Atoms
2	E	101[B]	RXY	CAX-OAY-PAZ-OAB
2	G	101[A]	RXY	CAX-OAY-PAZ-OBX
2	B	101	RXY	CBO-CBP-CBQ-CBR
2	E	101[A]	RXY	CBQ-CBR-CBS-CBT
2	F	101[B]	RXY	OAA-CAT-OAU-CAV
2	B	102	RXY	CBE-CBF-CBG-CBH
2	G	101[B]	RXY	CAO-CAP-CAQ-CAR
2	H	101	RXY	CBC-CBB-OBA-PAZ
2	F	102	RXY	CAH-CAI-CAJ-CAK
2	B	101	RXY	CBI-CBJ-CBK-CBL
2	F	102	RXY	CAS-CAT-OAU-CAV
2	F	102	RXY	CBR-CBS-CBT-CBU
2	D	101	RXY	CBE-CBF-CBG-CBH
2	F	101[B]	RXY	CBO-CBP-CBQ-CBR
2	G	102	RXY	CAP-CAQ-CAR-CAS
2	F	101[A]	RXY	CAQ-CAR-CAS-CAT
2	H	101	RXY	CAP-CAQ-CAR-CAS
2	G	102	RXY	OAU-CAV-CAW-CAX
2	F	101[A]	RXY	OAU-CAV-CAW-OBW
2	E	101[A]	RXY	OAU-CAV-CAW-OBW
2	A	101	RXY	CBR-CBS-CBT-CBU
2	F	101[A]	RXY	CAF-CAG-CAH-CAI
2	F	102	RXY	CBH-CBI-CBJ-CBK
2	G	102	RXY	CAG-CAH-CAI-CAJ
2	G	102	RXY	CAE-CAF-CAG-CAH
2	F	101[A]	RXY	CBN-CBO-CBP-CBQ
2	E	102	RXY	CAL-CAM-CAN-CAO
2	F	101[B]	RXY	CAN-CAO-CAP-CAQ
2	F	102	RXY	CAE-CAF-CAG-CAH
2	F	102	RXY	OAA-CAT-OAU-CAV
2	E	101[B]	RXY	CBF-CBG-CBH-CBI
2	C	101[A]	RXY	CAV-CAW-OBW-CBV
2	D	101	RXY	CBT-CBU-CBV-OBW
2	F	101[B]	RXY	CAW-CAX-OAY-PAZ
2	C	101[A]	RXY	CBK-CBL-CBM-CBN
2	B	102	RXY	CAN-CAO-CAP-CAQ
2	B	102	RXY	CAF-CAG-CAH-CAI
2	C	101[A]	RXY	CBB-OBA-PAZ-OAY
2	F	101[A]	RXY	CAX-OAY-PAZ-OBA
2	F	101[B]	RXY	CAX-OAY-PAZ-OBA
2	H	101	RXY	CBB-OBA-PAZ-OAY
2	E	101[A]	RXY	CAX-OAY-PAZ-OBA

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Mol	Chain	Res	Type	Atoms
2	E	102	RXY	CBB-OBA-PAZ-OAY
2	G	101[A]	RXY	CBB-OBA-PAZ-OAY
2	G	101[B]	RXY	CBB-OBA-PAZ-OAY
2	G	101[B]	RXY	CBQ-CBR-CBS-CBT
2	C	101[B]	RXY	CAI-CAJ-CAK-CAL
2	C	101[A]	RXY	CBQ-CBR-CBS-CBT
2	E	102	RXY	CAP-CAQ-CAR-CAS
2	C	101[A]	RXY	CAK-CAL-CAM-CAN
2	F	101[A]	RXY	CAI-CAJ-CAK-CAL
2	H	101	RXY	CAK-CAL-CAM-CAN
2	G	101[B]	RXY	CAL-CAM-CAN-CAO
2	G	102	RXY	CBN-CBO-CBP-CBQ
2	G	102	RXY	CAH-CAI-CAJ-CAK
2	D	101	RXY	CAF-CAG-CAH-CAI
2	E	101[B]	RXY	CAV-CAW-CAX-OAY
2	E	102	RXY	CAG-CAH-CAI-CAJ
2	F	101[B]	RXY	CAE-CAF-CAG-CAH
2	C	101[B]	RXY	CAN-CAO-CAP-CAQ
2	G	101[A]	RXY	CAN-CAO-CAP-CAQ
2	D	101	RXY	CAN-CAO-CAP-CAQ
2	D	101	RXY	CBO-CBP-CBQ-CBR
2	H	101	RXY	CBP-CBQ-CBR-CBS
2	G	101[B]	RXY	CBR-CBS-CBT-CBU
2	E	101[B]	RXY	CBH-CBI-CBJ-CBK
2	B	102	RXY	CBG-CBH-CBI-CBJ
2	B	102	RXY	CAV-CAW-OBW-CBV
2	D	101	RXY	CAX-CAW-OBW-CBV
2	F	101[A]	RXY	CBK-CBL-CBM-CBN
2	F	102	RXY	CAK-CAL-CAM-CAN
2	E	101[A]	RXY	CAP-CAQ-CAR-CAS
2	F	101[B]	RXY	OBW-CAW-CAX-OAY
2	E	101[A]	RXY	CBO-CBP-CBQ-CBR
2	B	102	RXY	CAK-CAL-CAM-CAN
2	E	101[B]	RXY	CBS-CBT-CBU-CBV
2	F	101[A]	RXY	CAK-CAL-CAM-CAN
2	G	102	RXY	CAK-CAL-CAM-CAN
2	F	102	RXY	CAG-CAH-CAI-CAJ
2	H	101	RXY	CBF-CBG-CBH-CBI
2	B	101	RXY	CBM-CBN-CBO-CBP
2	F	101[A]	RXY	CBS-CBT-CBU-CBV
2	G	101[B]	RXY	CAE-CAF-CAG-CAH
2	B	101	RXY	CBR-CBS-CBT-CBU

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Mol	Chain	Res	Type	Atoms
2	G	101[A]	RXY	CAI-CAJ-CAK-CAL
2	H	101	RXY	CAH-CAI-CAJ-CAK
2	D	101	RXY	CAK-CAL-CAM-CAN
2	E	101[A]	RXY	CBK-CBL-CBM-CBN
2	C	101[B]	RXY	CBK-CBL-CBM-CBN
2	F	101[A]	RXY	CAH-CAI-CAJ-CAK
2	C	101[A]	RXY	CBM-CBN-CBO-CBP
2	D	101	RXY	CBK-CBL-CBM-CBN
2	F	101[B]	RXY	CAI-CAJ-CAK-CAL
2	H	101	RXY	CAI-CAJ-CAK-CAL
2	E	101[A]	RXY	CBM-CBN-CBO-CBP
2	E	101[A]	RXY	CAK-CAL-CAM-CAN
2	E	101[A]	RXY	CAI-CAJ-CAK-CAL
2	F	102	RXY	CBT-CBU-CBV-OBW
2	F	101[B]	RXY	CAV-CAW-CAX-OAY
2	D	101	RXY	CBM-CBN-CBO-CBP
2	C	101[B]	RXY	CBT-CBU-CBV-OBW
2	E	101[B]	RXY	CBK-CBL-CBM-CBN
2	G	101[B]	RXY	CAI-CAJ-CAK-CAL
2	G	102	RXY	CBE-CBF-CBG-CBH
2	B	102	RXY	CBQ-CBR-CBS-CBT
2	G	101[A]	RXY	CBM-CBN-CBO-CBP
2	G	102	RXY	CBK-CBL-CBM-CBN
2	G	102	RXY	CBM-CBN-CBO-CBP
2	H	101	RXY	CAR-CAS-CAT-OAU
2	C	101[B]	RXY	CAX-OAY-PAZ-OAB
2	F	102	RXY	CAX-OAY-PAZ-OBX
2	G	101[B]	RXY	CBB-OBA-PAZ-OAB
2	G	101[A]	RXY	CAQ-CAR-CAS-CAT
2	F	101[B]	RXY	OBA-CBB-CBC-NBD
2	E	101[B]	RXY	OBA-CBB-CBC-NBD
2	G	102	RXY	CAR-CAS-CAT-OAU
2	G	101[A]	RXY	CAO-CAP-CAQ-CAR
2	F	101[B]	RXY	CBM-CBN-CBO-CBP
2	A	101	RXY	CBC-CBB-OBA-PAZ
2	C	101[A]	RXY	CBC-CBB-OBA-PAZ
2	G	101[A]	RXY	CBC-CBB-OBA-PAZ
2	E	101[B]	RXY	CBM-CBN-CBO-CBP
2	E	101[B]	RXY	CAK-CAL-CAM-CAN
2	E	102	RXY	CAI-CAJ-CAK-CAL
2	G	101[A]	RXY	CBT-CBU-CBV-OBW
2	C	101[B]	RXY	CBT-CBU-CBV-OBY

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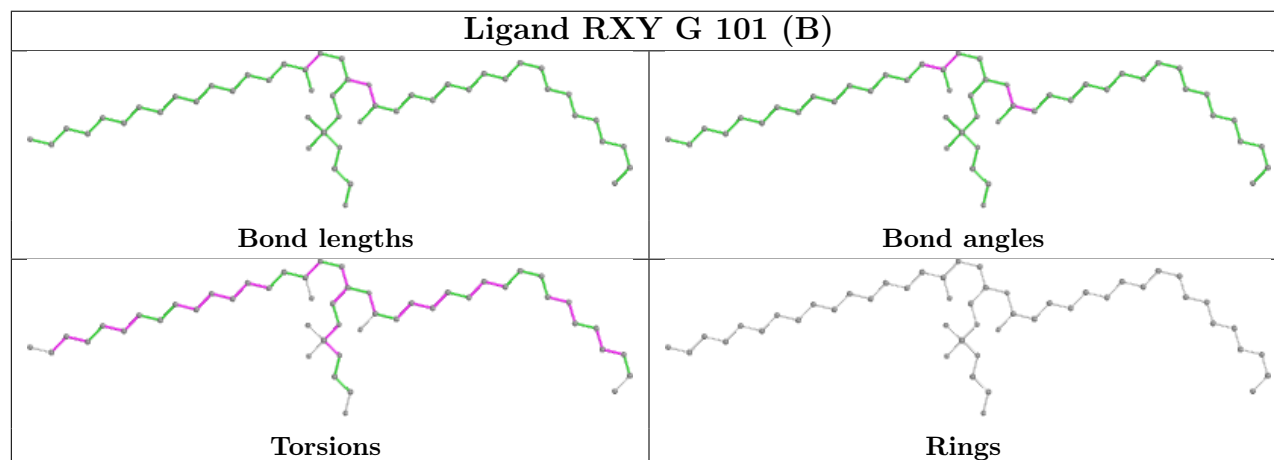
Mol	Chain	Res	Type	Atoms
2	H	101	RXY	CAR-CAS-CAT-OAA
2	G	102	RXY	CAI-CAJ-CAK-CAL
2	B	102	RXY	CBT-CBU-CBV-OBW
2	F	101[A]	RXY	CAN-CAO-CAP-CAQ
2	E	102	RXY	CBK-CBL-CBM-CBN

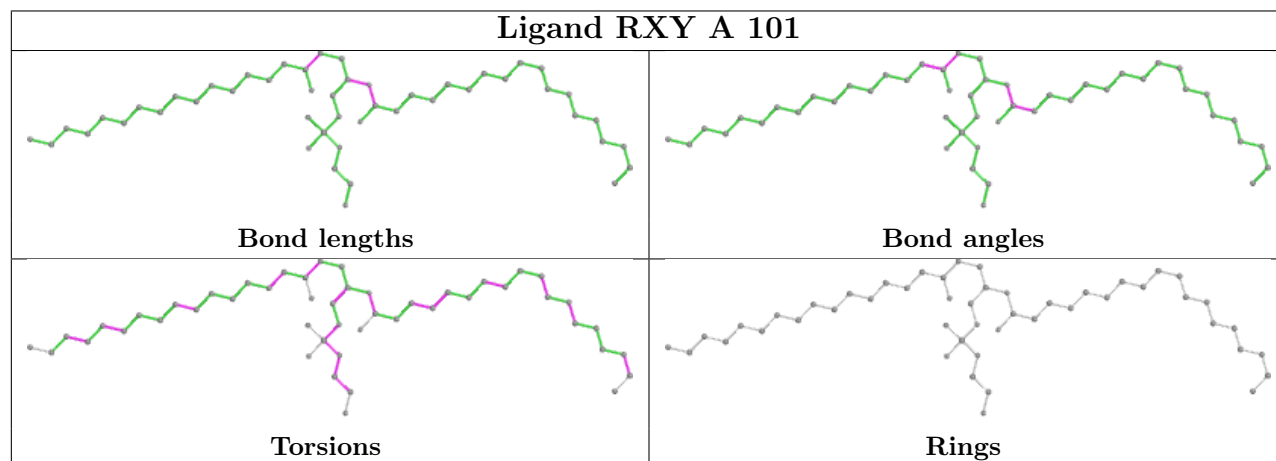
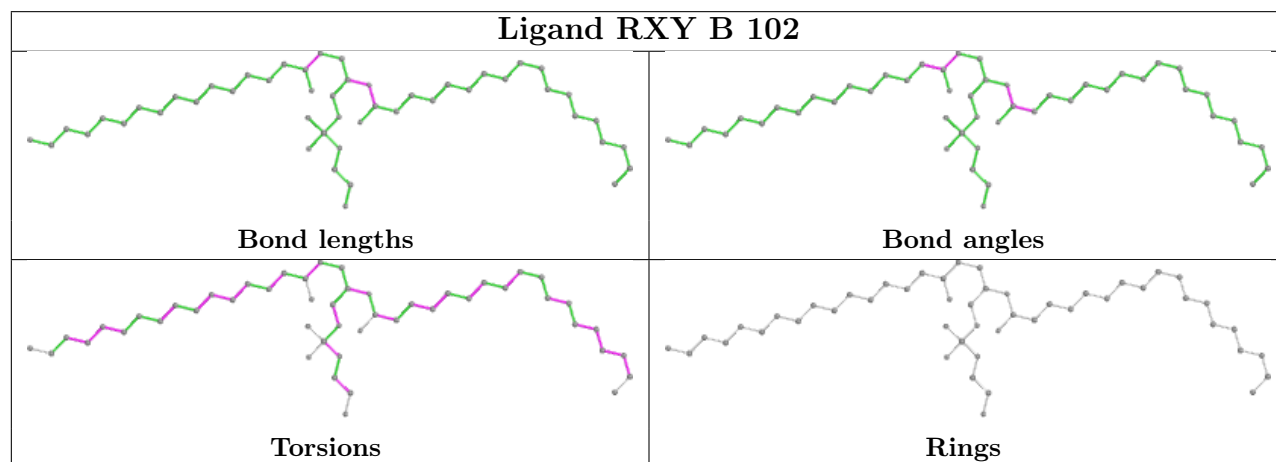
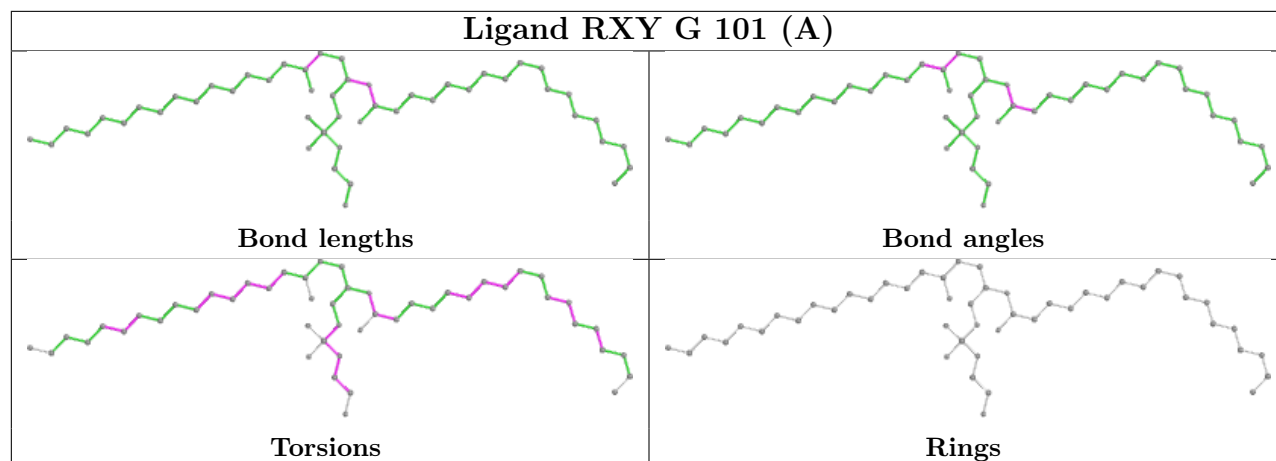
There are no ring outliers.

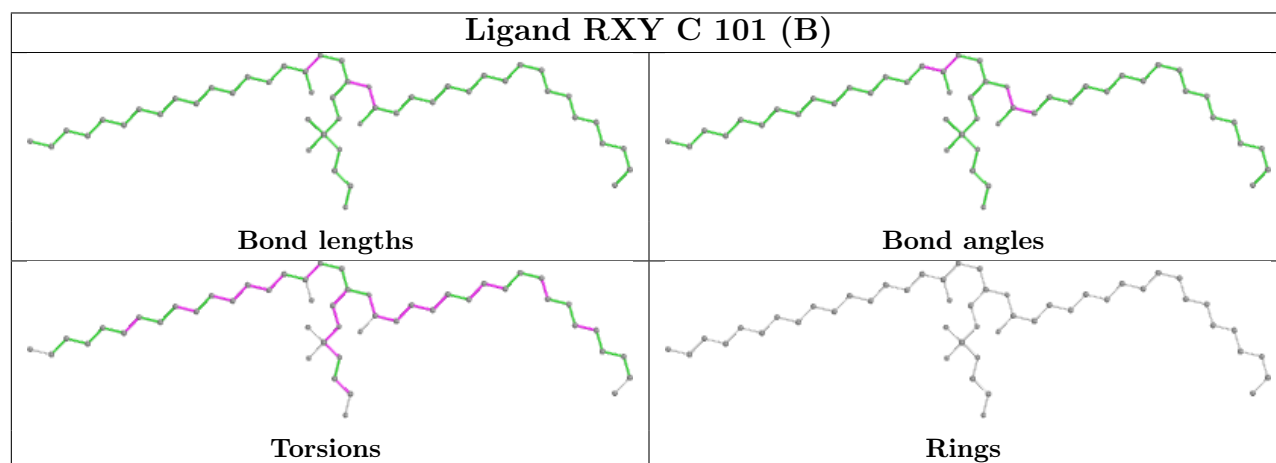
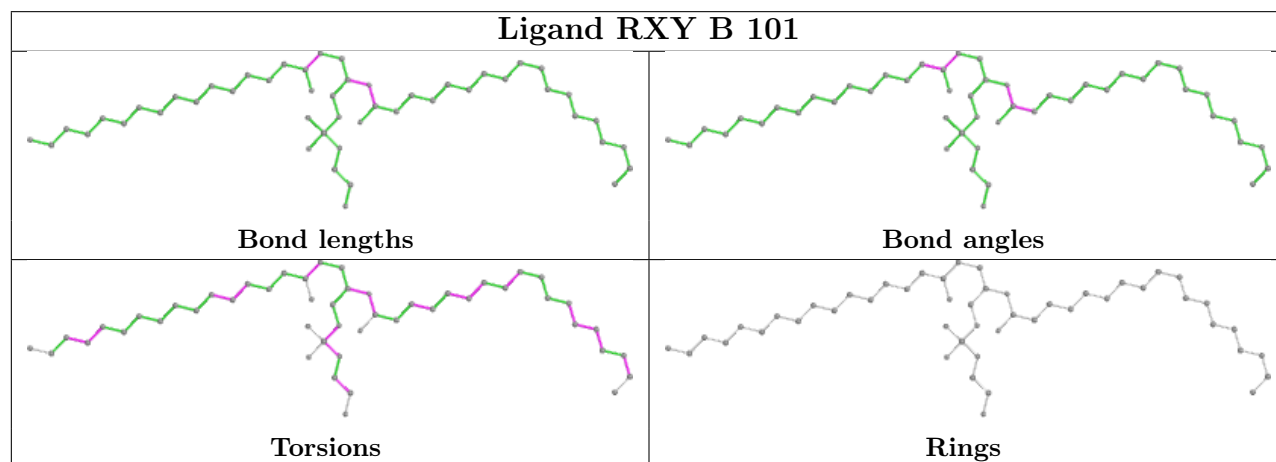
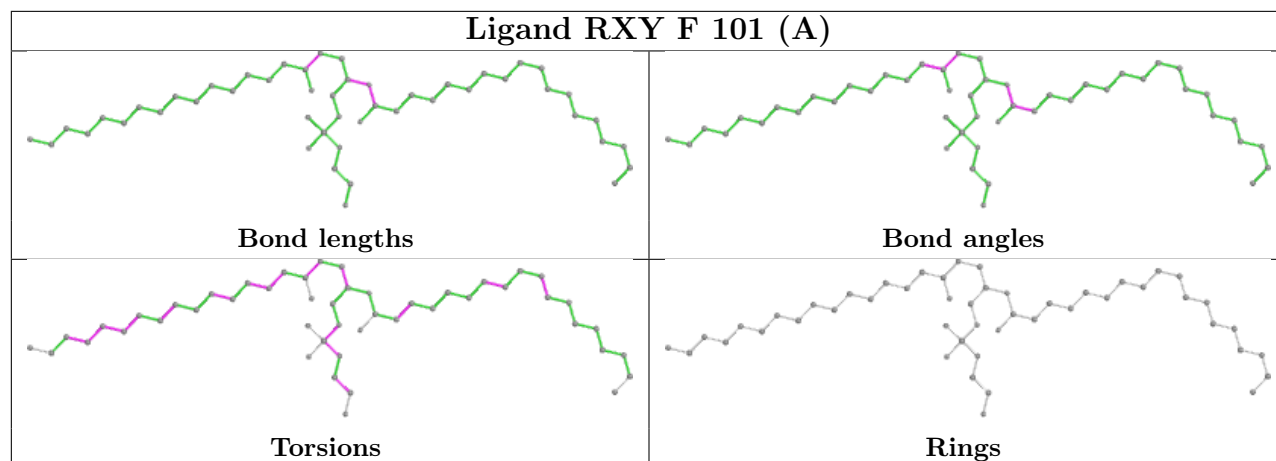
2 monomers are involved in 2 short contacts:

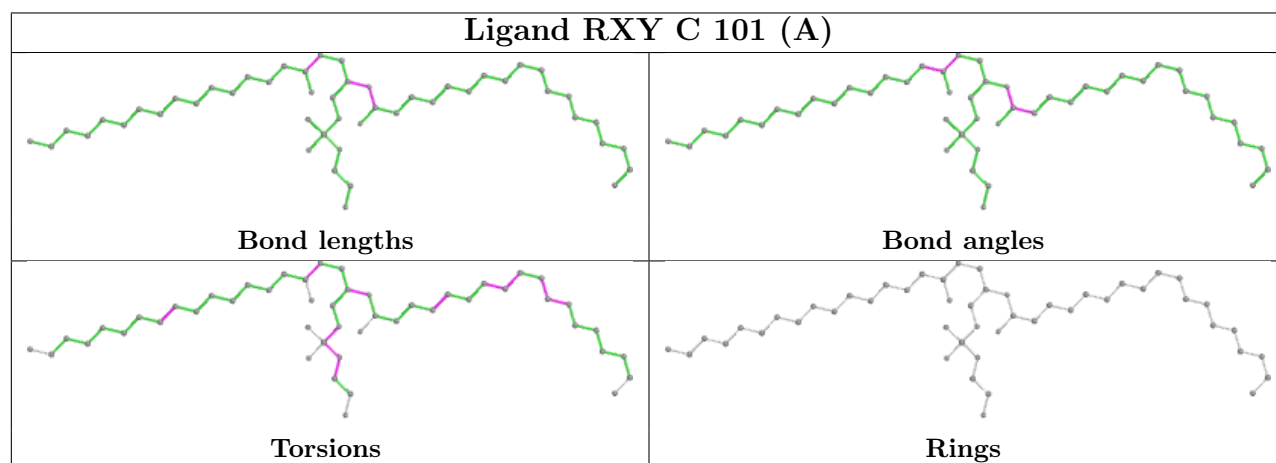
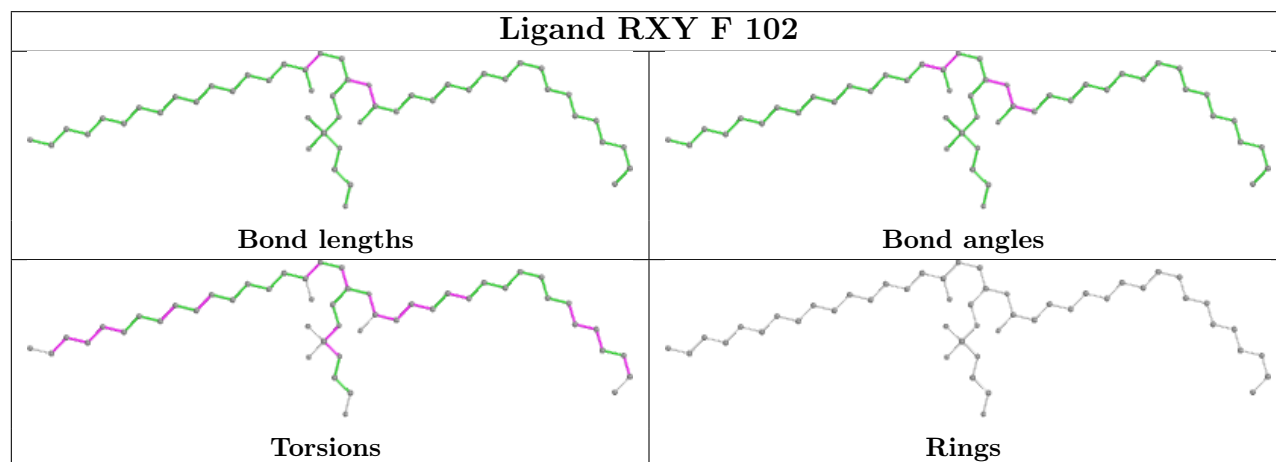
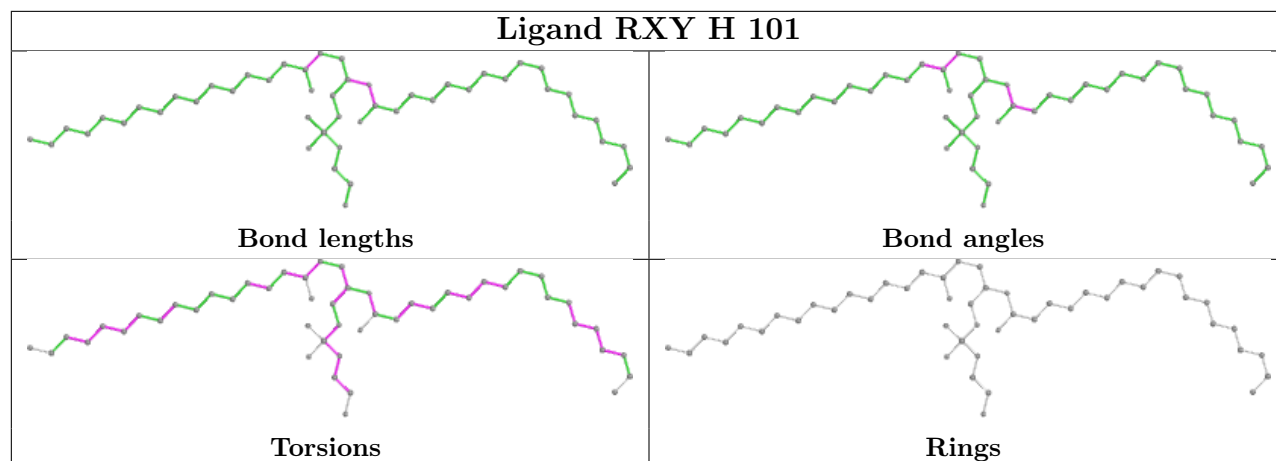
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	101[B]	RXY	1	0
2	D	101	RXY	1	0

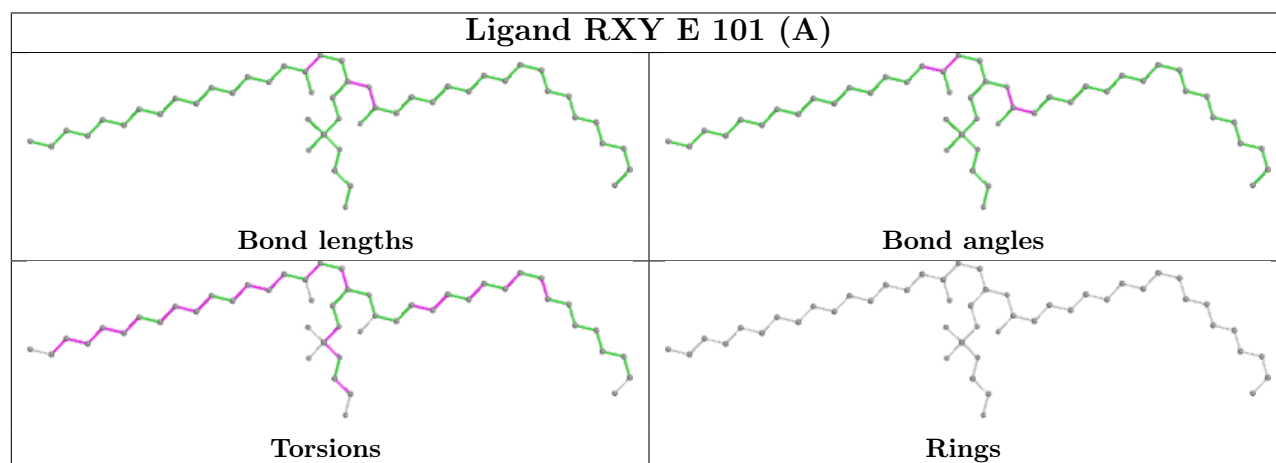
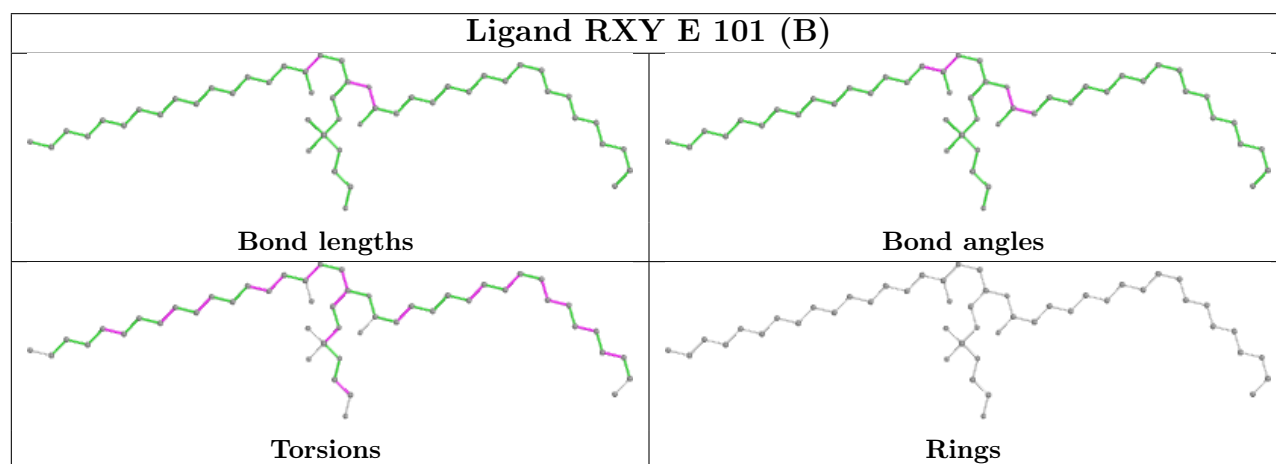
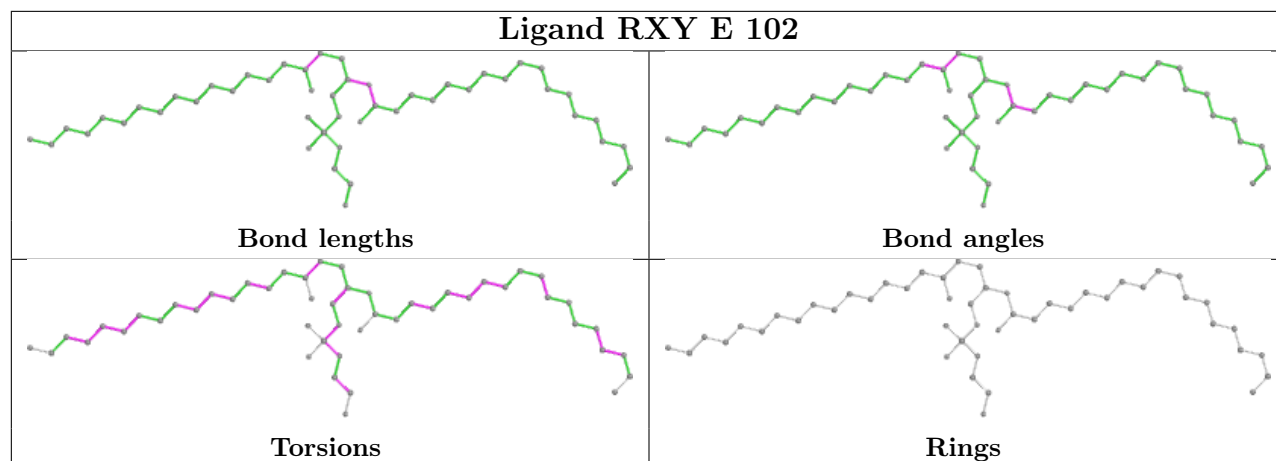
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

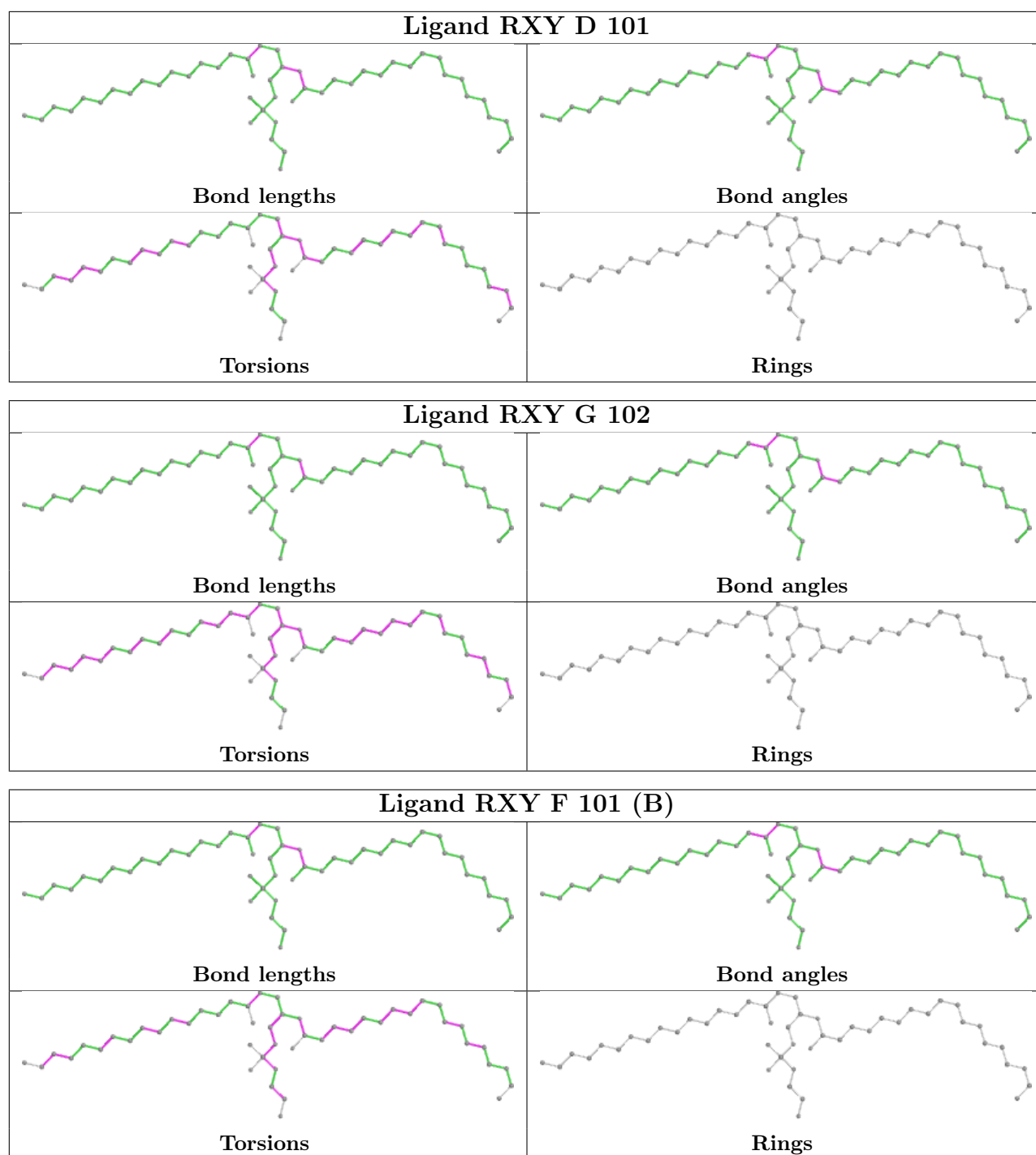












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [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	79/87 (90%)	0.58	0 100 100	48, 59, 85, 113	0
1	B	79/87 (90%)	0.61	1 (1%) 77 75	50, 58, 83, 120	0
1	C	79/87 (90%)	0.64	2 (2%) 57 55	52, 72, 101, 156	0
1	D	78/87 (89%)	0.66	8 (10%) 6 5	56, 96, 134, 157	0
1	E	80/87 (91%)	0.70	2 (2%) 57 55	49, 71, 113, 141	0
1	F	79/87 (90%)	0.54	3 (3%) 40 38	53, 89, 122, 155	0
1	G	77/87 (88%)	0.86	11 (14%) 2 2	54, 104, 139, 189	0
1	H	77/87 (88%)	0.82	7 (9%) 9 8	52, 105, 138, 169	0
All	All	628/696 (90%)	0.68	34 (5%) 25 24	48, 76, 133, 189	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	70	GLN	5.0
1	E	70	GLN	4.8
1	G	82	LEU	4.4
1	D	84	PRO	4.1
1	G	18	LEU	3.6
1	H	82	LEU	3.5
1	G	67	PHE	3.2
1	H	15	ILE	3.2
1	F	70	GLN	2.9
1	D	70	GLN	2.7
1	H	18	LEU	2.7
1	F	15	ILE	2.7
1	D	62	LEU	2.7
1	G	19	LEU	2.6
1	G	64	ILE	2.6
1	C	47	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	G	15	ILE	2.5
1	H	70	GLN	2.4
1	H	48	LEU	2.4
1	G	28	PHE	2.4
1	G	76	ILE	2.4
1	H	64	ILE	2.3
1	G	32	ILE	2.3
1	H	16	VAL	2.3
1	G	23	THR	2.2
1	D	58	VAL	2.1
1	D	17	HIS	2.1
1	D	16	VAL	2.1
1	G	84	PRO	2.1
1	F	8	LEU	2.0
1	B	34	LYS	2.0
1	D	19	LEU	2.0
1	E	62	LEU	2.0
1	D	27	ALA	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, 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.

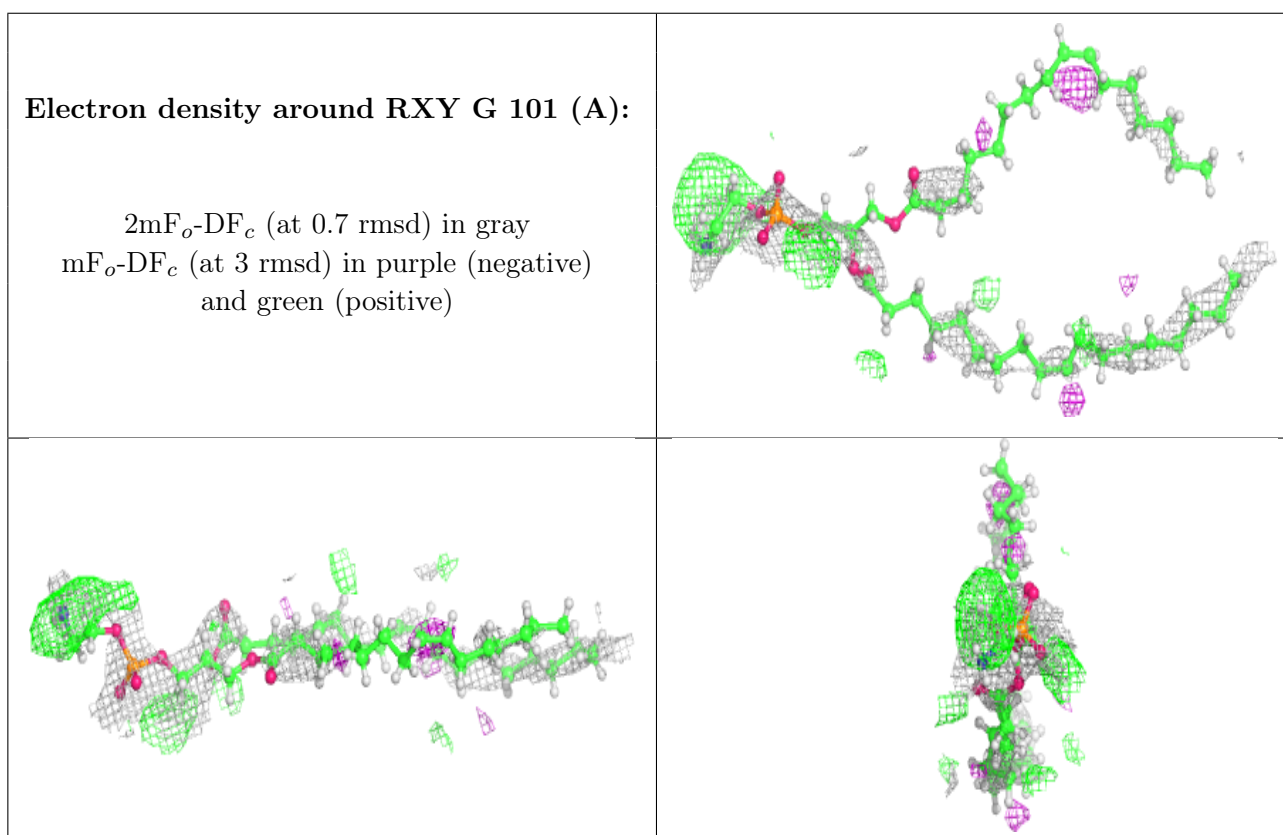
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	RXY	G	101[A]	49/49	0.35	0.74	79,106,126,128	122
2	RXY	G	101[B]	49/49	0.35	0.74	82,106,125,128	122
2	RXY	F	101[A]	49/49	0.47	0.48	63,100,116,118	122
2	RXY	F	101[B]	49/49	0.47	0.48	79,101,116,118	122
2	RXY	E	101[A]	49/49	0.56	0.37	54,83,99,102	122

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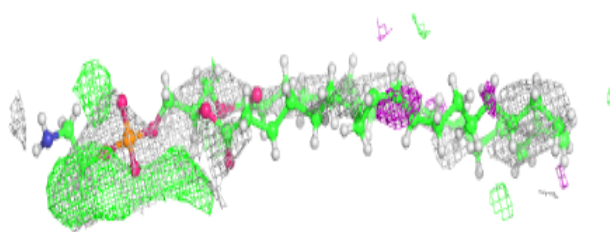
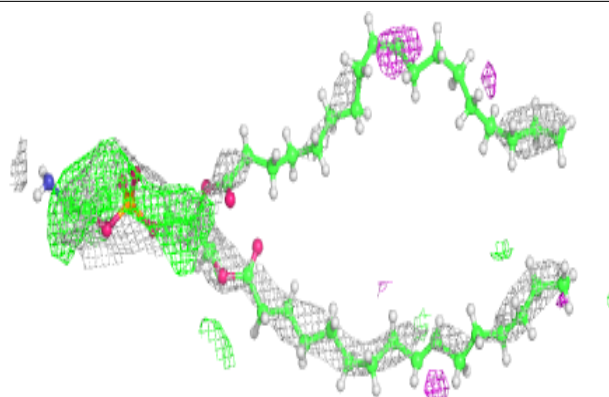
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	RXY	E	101[B]	49/49	0.56	0.37	65,85,99,103	122
2	RXY	G	102	49/49	0.56	0.44	81,127,156,172	0
2	RXY	F	102	49/49	0.61	0.47	81,114,147,159	0
2	RXY	C	101[A]	49/49	0.61	0.39	58,90,101,108	122
2	RXY	C	101[B]	49/49	0.61	0.39	69,91,104,110	122
2	RXY	H	101	49/49	0.62	0.53	90,127,154,176	0
2	RXY	B	102	49/49	0.69	0.34	65,101,145,159	0
2	RXY	D	101	49/49	0.77	0.40	72,113,149,163	0
2	RXY	B	101	49/49	0.78	0.25	62,93,128,140	0
2	RXY	E	102	49/49	0.81	0.23	67,94,128,143	0
2	RXY	A	101	49/49	0.85	0.24	64,92,117,130	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.

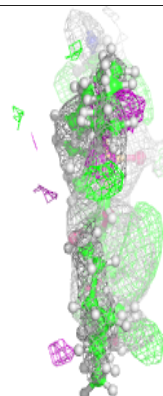
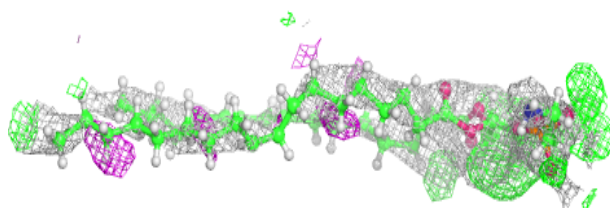
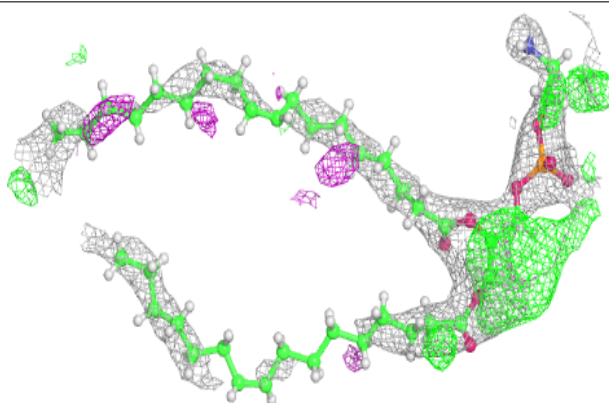


Electron density around RXY G 101 (B):

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

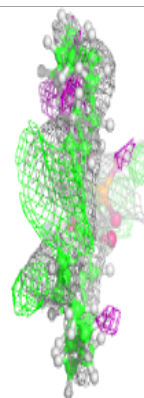
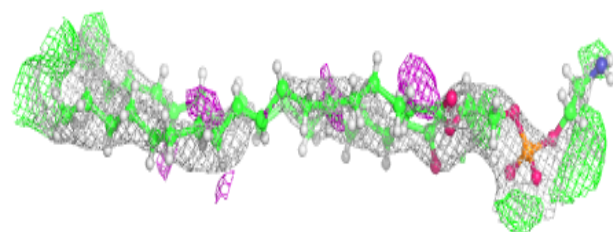
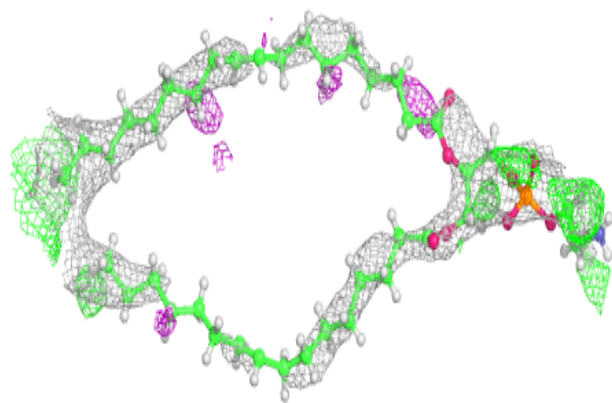
**Electron density around RXY F 101 (A):**

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

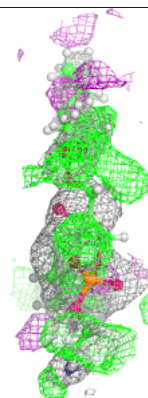
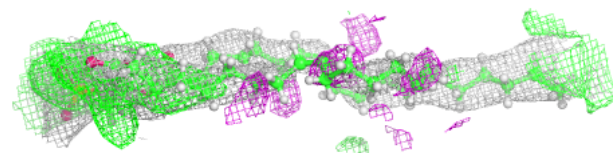
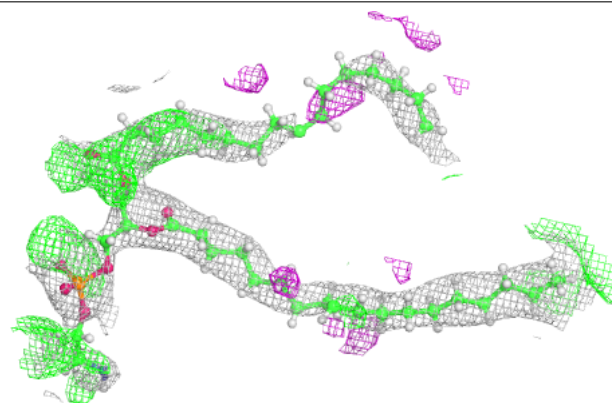


Electron density around RXY F 101 (B):

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

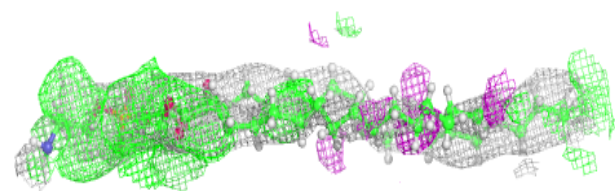
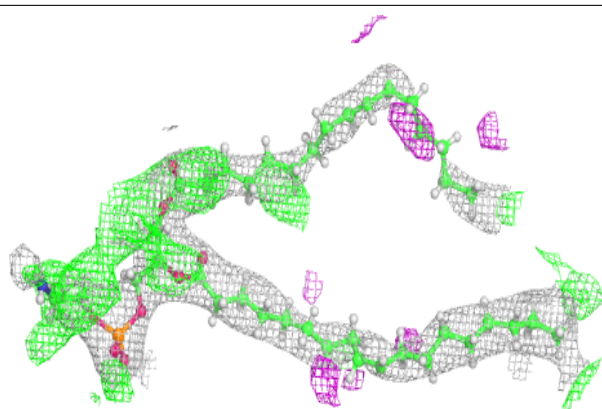
**Electron density around RXY E 101 (A):**

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

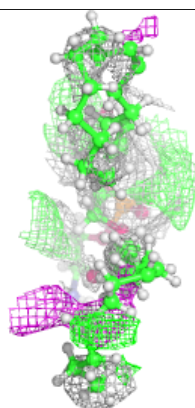
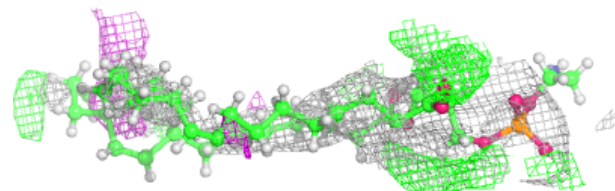
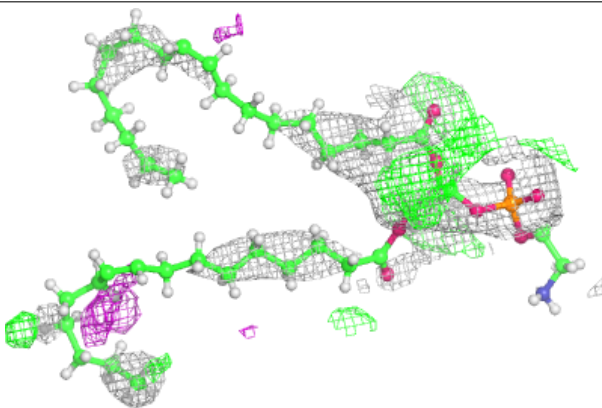


Electron density around RXY E 101 (B):

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

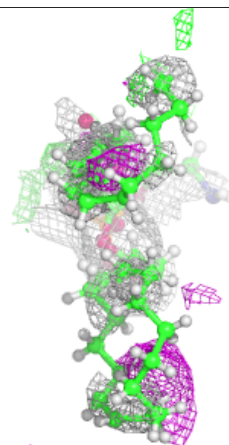
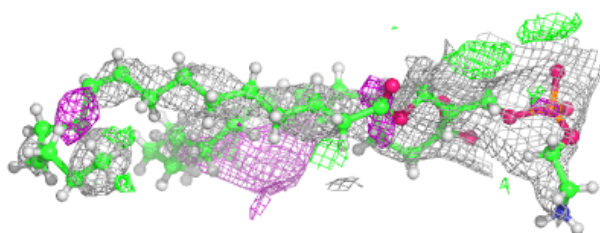
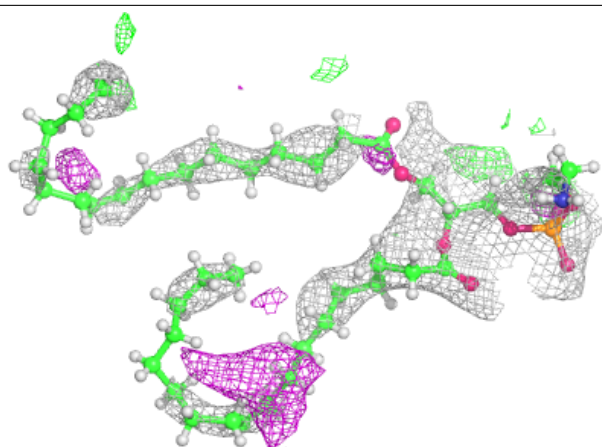
**Electron density around RXY G 102:**

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

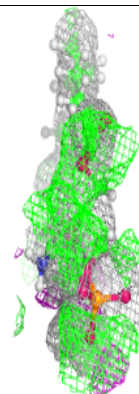
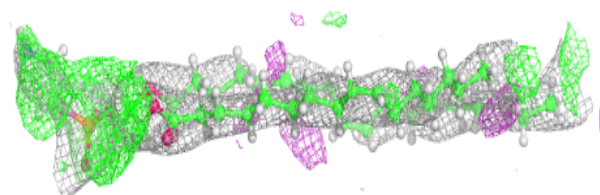
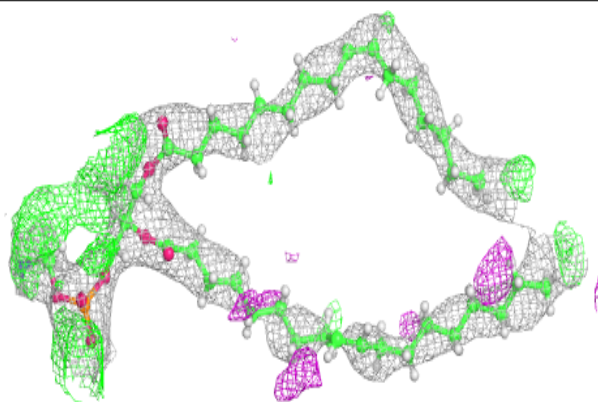


Electron density around RXY F 102:

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

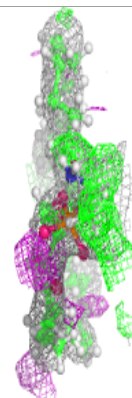
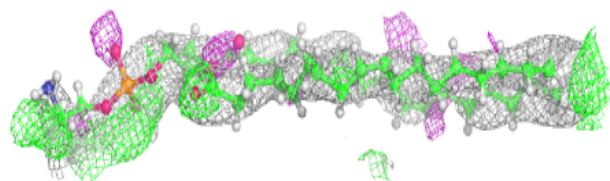
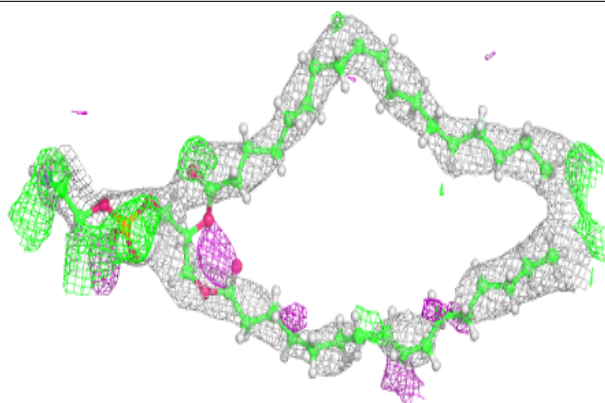
**Electron density around RXY C 101 (A):**

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

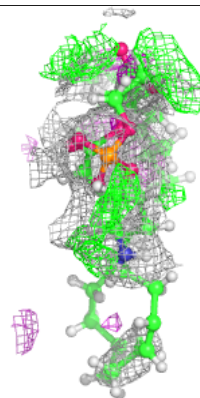
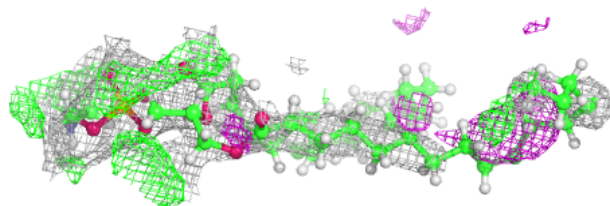
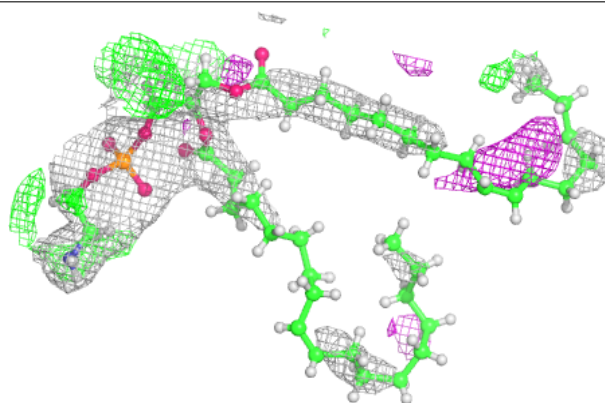


Electron density around RXY C 101 (B):

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

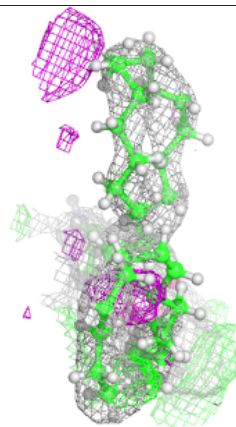
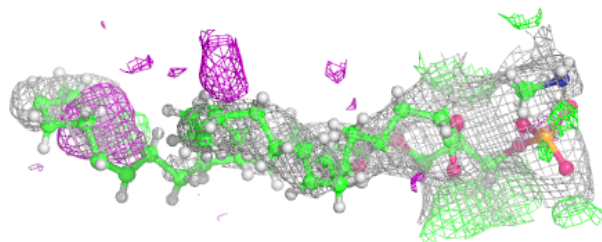
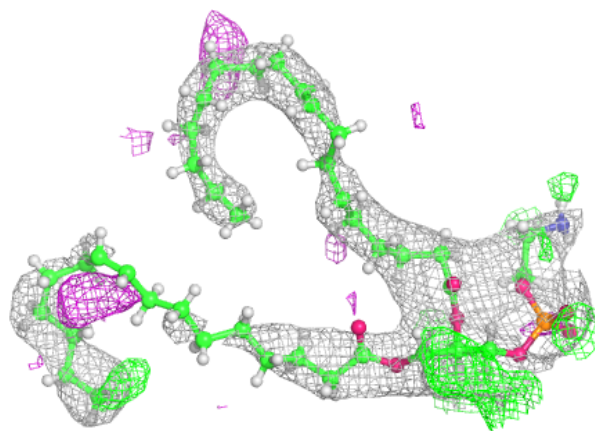
**Electron density around RXY H 101:**

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



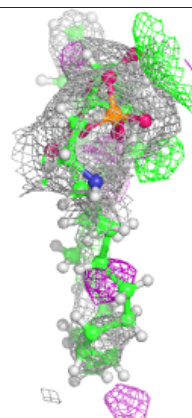
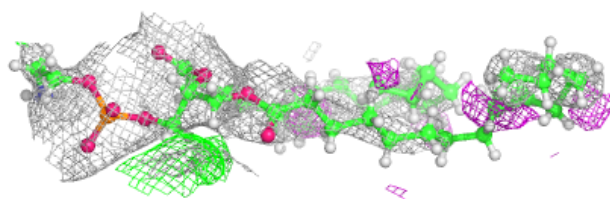
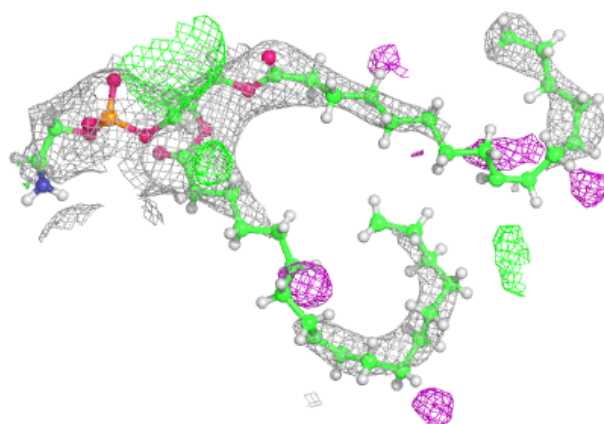
Electron density around RXY B 102:

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

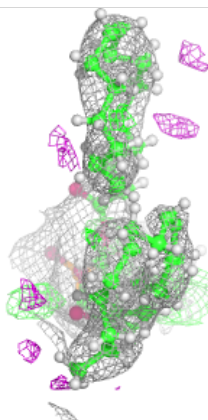
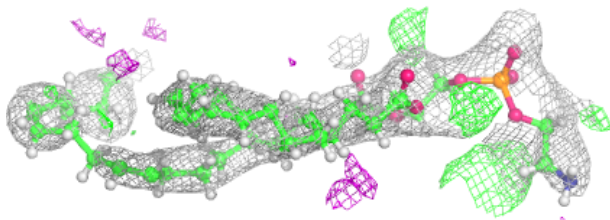
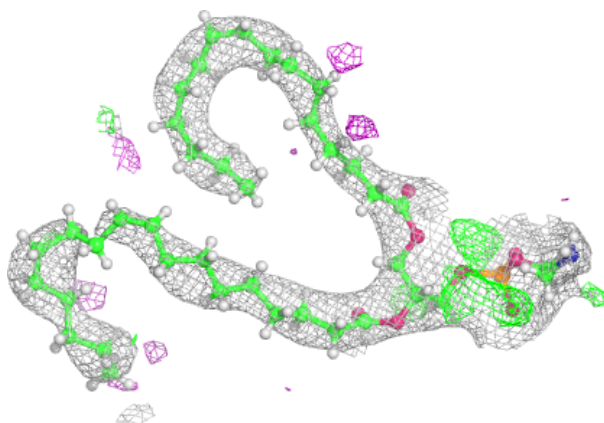


Electron density around RXY D 101:

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

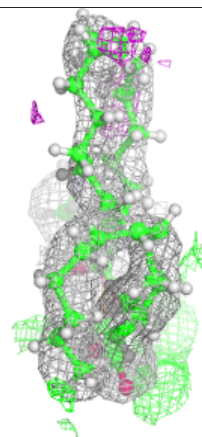
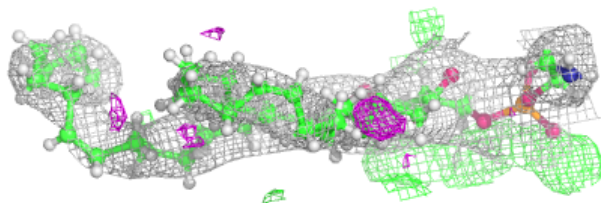
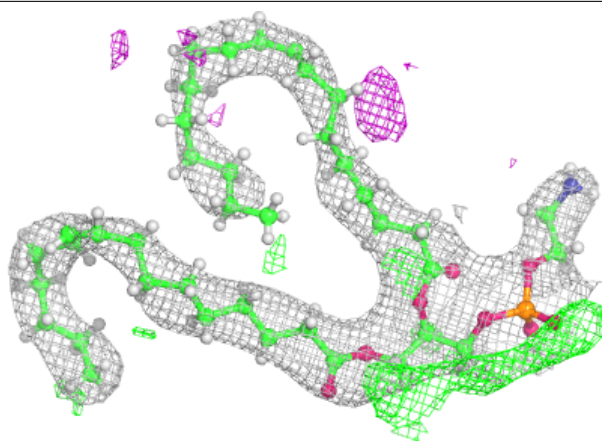
**Electron density around RXY B 101:**

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

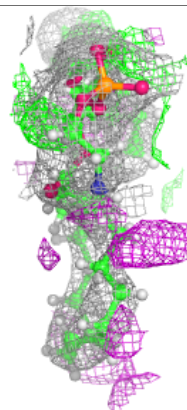
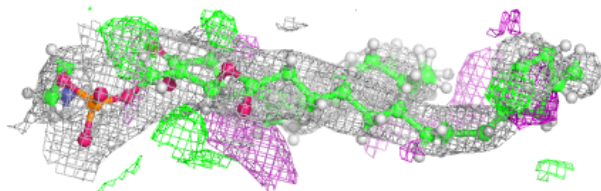
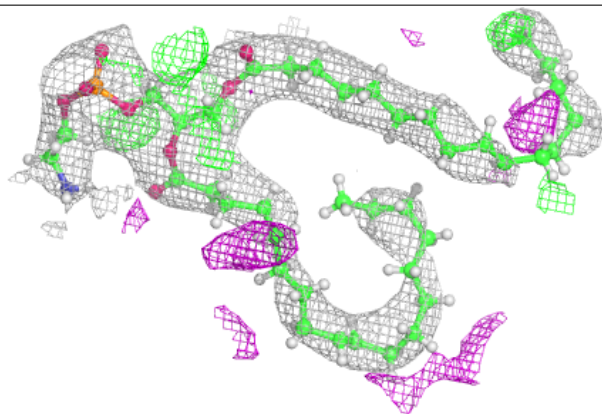


Electron density around RXY E 102:

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

**Electron density around RXY A 101:**

$2mF_o-DF_c$ (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.