Full wwPDB X-ray Structure Validation Report ⓘ

Oct 5, 2023 – 07:20 AM EDT

PDB ID	:	6VZD
Title	:	N-terminal domain of mouse surfactant protein B (K46E/R51E mutant) with bound lipid
Authors	:	Rapoport, T.A.; Bodnar, N.O.
Deposited on	:	2020-02-28
Resolution	:	1.88 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	:	FAILED
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 1.88 Å.

There are no overall percentile quality scores available for this entry.

MolProbity and EDS failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 6494 atoms, of which 3176 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.

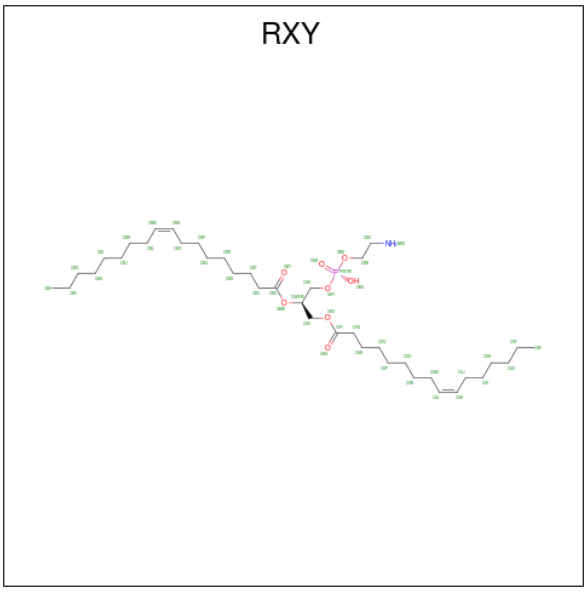
- Molecule 1 is a protein called Pulmonary surfactant-associated protein B.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	79	Total	C	H	N	O	S	0	1	0
			1279	410	638	102	122	7			
1	E	85	Total	C	H	N	O	S	0	2	0
			1369	435	683	113	131	7			
1	B	78	Total	C	H	N	O	S	0	2	0
			1286	412	642	103	122	7			
1	C	78	Total	C	H	N	O	S	0	1	0
			1266	407	629	101	122	7			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SER	-	expression tag	UNP P50405
A	46	GLU	LYS	engineered mutation	UNP P50405
A	51	GLU	ARG	engineered mutation	UNP P50405
E	1	SER	-	expression tag	UNP P50405
E	46	GLU	LYS	engineered mutation	UNP P50405
E	51	GLU	ARG	engineered mutation	UNP P50405
B	1	SER	-	expression tag	UNP P50405
B	46	GLU	LYS	engineered mutation	UNP P50405
B	51	GLU	ARG	engineered mutation	UNP P50405
C	1	SER	-	expression tag	UNP P50405
C	46	GLU	LYS	engineered mutation	UNP P50405
C	51	GLU	ARG	engineered mutation	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: $C_{39}H_{74}NO_8P$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	P	0	1
			244	78	146	2	16	2		
2	A	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	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	1
			244	78	146	2	16	2		
2	B	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	94	Total	O	0	0
			94	94		
3	E	100	Total	O	0	0
			100	100		
3	B	80	Total	O	0	0
			80	80		
3	C	44	Total	O	0	0
			44	44		

MolProbity and EDS failed to run properly - this section is therefore empty.

3 Data and refinement statistics (i)

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	49.79Å 66.12Å 59.62Å 90.00° 97.37° 90.00°	Depositor
Resolution (Å)	59.13 – 1.88	Depositor
% Data completeness (in resolution range)	91.8 (59.13-1.88)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.08 (at 1.88Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.170 , 0.217	Depositor
Wilson B-factor (Å^2)	18.8	Xtriage
Anisotropy	0.001	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6494	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.89% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

4 Model quality

4.1 Standard geometry

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles

4.3.1 Protein backbone

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA

MolProbity failed to run properly - this section is therefore empty.

4.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

4.5 Carbohydrates

There are no monosaccharides in this entry.

4.6 Ligand geometry

8 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	A	102	-	48,48,48	1.07	3 (6%)	51,53,53	0.90	2 (3%)
2	RXY	E	201	-	48,48,48	1.05	3 (6%)	51,53,53	0.90	2 (3%)
2	RXY	B	403	-	48,48,48	1.09	3 (6%)	51,53,53	0.91	2 (3%)
2	RXY	B	401	-	48,48,48	1.05	3 (6%)	51,53,53	0.82	2 (3%)
2	RXY	B	402[B]	-	48,48,48	1.07	3 (6%)	51,53,53	0.84	2 (3%)
2	RXY	A	101[A]	-	48,48,48	1.08	3 (6%)	51,53,53	0.84	2 (3%)
2	RXY	A	101[B]	-	48,48,48	1.06	3 (6%)	51,53,53	0.79	2 (3%)
2	RXY	B	402[A]	-	48,48,48	1.09	3 (6%)	51,53,53	0.93	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	A	102	-	-	32/52/52/52	-
2	RXY	E	201	-	-	21/52/52/52	-
2	RXY	B	403	-	-	16/52/52/52	-
2	RXY	B	401	-	-	26/52/52/52	-
2	RXY	B	402[B]	-	-	26/52/52/52	-
2	RXY	A	101[A]	-	-	21/52/52/52	-
2	RXY	A	101[B]	-	-	24/52/52/52	-
2	RXY	B	402[A]	-	-	21/52/52/52	-

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	403	RXY	OAU-CAT	3.36	1.43	1.33
2	B	402[A]	RXY	OAU-CAT	3.28	1.42	1.33
2	B	401	RXY	OAU-CAT	3.28	1.42	1.33
2	A	102	RXY	OAU-CAT	3.26	1.42	1.33
2	A	101[A]	RXY	OAU-CAT	3.26	1.42	1.33
2	E	201	RXY	OAU-CAT	3.16	1.42	1.33
2	A	101[B]	RXY	OAU-CAT	3.15	1.42	1.33
2	B	402[B]	RXY	OAU-CAT	3.03	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	403	RXY	OBW-CBV	2.78	1.42	1.34
2	B	403	RXY	OBW-CAW	-2.73	1.39	1.46
2	A	101[B]	RXY	OBW-CBV	2.70	1.41	1.34
2	B	402[A]	RXY	OBW-CBV	2.70	1.41	1.34
2	E	201	RXY	OBW-CBV	2.60	1.41	1.34
2	A	102	RXY	OBW-CBV	2.60	1.41	1.34
2	A	101[A]	RXY	OBW-CBV	2.59	1.41	1.34
2	B	402[B]	RXY	OBW-CBV	2.58	1.41	1.34
2	B	402[A]	RXY	OBW-CAW	-2.53	1.40	1.46
2	A	102	RXY	OBW-CAW	-2.52	1.40	1.46
2	B	401	RXY	OBW-CBV	2.49	1.41	1.34
2	B	402[B]	RXY	OBW-CAW	-2.48	1.40	1.46
2	E	201	RXY	OBW-CAW	-2.44	1.40	1.46
2	A	101[A]	RXY	OBW-CAW	-2.39	1.40	1.46
2	A	101[B]	RXY	OBW-CAW	-2.25	1.41	1.46
2	B	401	RXY	OBW-CAW	-2.11	1.41	1.46

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	402[A]	RXY	OBW-CBV-CBU	4.10	120.34	111.50
2	A	102	RXY	OBW-CBV-CBU	4.08	120.30	111.50
2	E	201	RXY	OBW-CBV-CBU	4.03	120.19	111.50
2	A	101[A]	RXY	OBW-CBV-CBU	4.02	120.16	111.50
2	B	403	RXY	OBW-CBV-CBU	4.01	120.13	111.50
2	B	401	RXY	OBW-CBV-CBU	3.89	119.88	111.50
2	A	101[B]	RXY	OBW-CBV-CBU	3.49	119.02	111.50
2	B	402[B]	RXY	OBW-CBV-CBU	3.36	118.74	111.50
2	A	102	RXY	OAU-CAT-CAS	2.86	120.87	111.91
2	B	402[B]	RXY	OAU-CAT-CAS	2.83	120.78	111.91
2	E	201	RXY	OAU-CAT-CAS	2.80	120.69	111.91
2	B	402[A]	RXY	OAU-CAT-CAS	2.64	120.18	111.91
2	B	403	RXY	OAU-CAT-CAS	2.63	120.17	111.91
2	A	101[B]	RXY	OAU-CAT-CAS	2.63	120.16	111.91
2	A	101[A]	RXY	OAU-CAT-CAS	2.44	119.56	111.91
2	B	401	RXY	OAU-CAT-CAS	2.38	119.38	111.91

There are no chirality outliers.

All (187) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	101[A]	RXY	CBB-OBA-PAZ-OAY

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Mol	Chain	Res	Type	Atoms
2	A	101[A]	RXY	CBB-OBA-PAZ-OBX
2	A	101[A]	RXY	CBB-OBA-PAZ-OAB
2	A	101[A]	RXY	OBA-CBB-CBC-NBD
2	A	101[B]	RXY	CBB-OBA-PAZ-OAB
2	A	102	RXY	CBU-CBV-OBW-CAW
2	A	102	RXY	OBY-CBV-OBW-CAW
2	A	102	RXY	CBC-CBB-OBA-PAZ
2	E	201	RXY	OBY-CBV-OBW-CAW
2	E	201	RXY	OBA-CBB-CBC-NBD
2	B	401	RXY	CAX-OAY-PAZ-OBX
2	B	401	RXY	CAX-OAY-PAZ-OAB
2	B	401	RXY	OBA-CBB-CBC-NBD
2	B	402[A]	RXY	CBU-CBV-OBW-CAW
2	B	402[A]	RXY	CBB-OBA-PAZ-OBX
2	B	402[B]	RXY	CBB-OBA-PAZ-OBX
2	B	402[B]	RXY	CBB-OBA-PAZ-OAB
2	B	402[B]	RXY	OBA-CBB-CBC-NBD
2	B	403	RXY	CBB-OBA-PAZ-OBX
2	B	403	RXY	OBA-CBB-CBC-NBD
2	B	402[B]	RXY	OAA-CAT-OAU-CAV
2	B	402[A]	RXY	OBY-CBV-OBW-CAW
2	B	401	RXY	CAS-CAT-OAU-CAV
2	E	201	RXY	CBU-CBV-OBW-CAW
2	A	102	RXY	CAS-CAT-OAU-CAV
2	B	402[B]	RXY	CAS-CAT-OAU-CAV
2	A	102	RXY	OAA-CAT-OAU-CAV
2	B	401	RXY	OAA-CAT-OAU-CAV
2	A	101[B]	RXY	CAS-CAT-OAU-CAV
2	A	101[B]	RXY	OAA-CAT-OAU-CAV
2	B	402[A]	RXY	CAS-CAT-OAU-CAV
2	B	401	RXY	CBO-CBP-CBQ-CBR
2	B	403	RXY	CBS-CBT-CBU-CBV
2	A	101[B]	RXY	CAQ-CAR-CAS-CAT
2	A	102	RXY	CAQ-CAR-CAS-CAT
2	E	201	RXY	CAQ-CAR-CAS-CAT
2	B	402[B]	RXY	CAW-CAX-OAY-PAZ
2	B	402[A]	RXY	OAA-CAT-OAU-CAV
2	B	402[B]	RXY	CBI-CBJ-CBK-CBL
2	A	102	RXY	CAX-OAY-PAZ-OBA
2	B	401	RXY	CAX-OAY-PAZ-OBA
2	B	402[A]	RXY	CBB-OBA-PAZ-OAY
2	B	402[B]	RXY	CBB-OBA-PAZ-OAY

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Mol	Chain	Res	Type	Atoms
2	B	403	RXY	CBB-OBA-PAZ-OAY
2	B	402[B]	RXY	CBS-CBT-CBU-CBV
2	E	201	RXY	CAO-CAP-CAQ-CAR
2	A	101[A]	RXY	CBU-CBV-OBW-CAW
2	A	101[A]	RXY	CBH-CBI-CBJ-CBK
2	A	102	RXY	CAP-CAQ-CAR-CAS
2	B	401	RXY	CAF-CAG-CAH-CAI
2	B	402[B]	RXY	CAM-CAN-CAO-CAP
2	E	201	RXY	CAN-CAO-CAP-CAQ
2	A	101[A]	RXY	OBY-CBV-OBW-CAW
2	A	101[A]	RXY	CAN-CAO-CAP-CAQ
2	B	402[B]	RXY	CBG-CBH-CBI-CBJ
2	A	102	RXY	CAN-CAO-CAP-CAQ
2	B	402[A]	RXY	CAP-CAQ-CAR-CAS
2	E	201	RXY	CAS-CAT-OAU-CAV
2	B	403	RXY	CAG-CAH-CAI-CAJ
2	A	102	RXY	CBO-CBP-CBQ-CBR
2	B	402[B]	RXY	CAO-CAP-CAQ-CAR
2	B	401	RXY	CBP-CBQ-CBR-CBS
2	B	402[A]	RXY	CAM-CAN-CAO-CAP
2	B	402[B]	RXY	CBO-CBP-CBQ-CBR
2	A	102	RXY	CBI-CBJ-CBK-CBL
2	E	201	RXY	CAP-CAQ-CAR-CAS
2	A	101[A]	RXY	CBR-CBS-CBT-CBU
2	A	101[B]	RXY	CAM-CAN-CAO-CAP
2	B	402[B]	RXY	CAN-CAO-CAP-CAQ
2	A	102	RXY	CBH-CBI-CBJ-CBK
2	E	201	RXY	CBH-CBI-CBJ-CBK
2	B	402[A]	RXY	CBR-CBS-CBT-CBU
2	A	101[A]	RXY	CBO-CBP-CBQ-CBR
2	A	101[B]	RXY	CBS-CBT-CBU-CBV
2	B	402[B]	RXY	CAG-CAH-CAI-CAJ
2	A	102	RXY	CAM-CAN-CAO-CAP
2	E	201	RXY	OAA-CAT-OAU-CAV
2	A	101[A]	RXY	CAG-CAH-CAI-CAJ
2	A	102	RXY	CBN-CBO-CBP-CBQ
2	A	101[A]	RXY	CBS-CBT-CBU-CBV
2	B	402[A]	RXY	CBO-CBP-CBQ-CBR
2	B	401	RXY	CBQ-CBR-CBS-CBT
2	B	402[B]	RXY	CBR-CBS-CBT-CBU
2	A	102	RXY	OAU-CAV-CAW-OBW
2	A	101[B]	RXY	CAL-CAM-CAN-CAO

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Mol	Chain	Res	Type	Atoms
2	B	402[A]	RXY	CBN-CBO-CBP-CBQ
2	B	401	RXY	CBH-CBI-CBJ-CBK
2	B	401	RXY	CAG-CAH-CAI-CAJ
2	A	101[B]	RXY	CAX-OAY-PAZ-OBA
2	A	101[B]	RXY	CBB-OBA-PAZ-OAY
2	E	201	RXY	CBP-CBQ-CBR-CBS
2	B	403	RXY	CBF-CBG-CBH-CBI
2	A	101[A]	RXY	CBN-CBO-CBP-CBQ
2	A	102	RXY	CAH-CAI-CAJ-CAK
2	B	401	RXY	CAH-CAI-CAJ-CAK
2	B	402[A]	RXY	CBJ-CBK-CBL-CBM
2	B	403	RXY	CBR-CBS-CBT-CBU
2	A	102	RXY	OAU-CAV-CAW-CAX
2	A	101[A]	RXY	CAI-CAJ-CAK-CAL
2	B	402[B]	RXY	CAL-CAM-CAN-CAO
2	B	401	RXY	CBU-CBV-OBW-CAW
2	B	402[A]	RXY	CAG-CAH-CAI-CAJ
2	A	102	RXY	CBG-CBH-CBI-CBJ
2	B	403	RXY	CAM-CAN-CAO-CAP
2	A	102	RXY	CBF-CBG-CBH-CBI
2	B	401	RXY	CBF-CBG-CBH-CBI
2	B	403	RXY	CAF-CAG-CAH-CAI
2	E	201	RXY	CBN-CBO-CBP-CBQ
2	A	102	RXY	CAW-CAV-OAU-CAT
2	A	101[B]	RXY	CAW-CAX-OAY-PAZ
2	A	101[A]	RXY	CAL-CAM-CAN-CAO
2	E	201	RXY	OAU-CAV-CAW-CAX
2	B	402[B]	RXY	OAU-CAV-CAW-CAX
2	B	402[B]	RXY	OBW-CAW-CAX-OAY
2	B	401	RXY	OBY-CBV-OBW-CAW
2	A	101[A]	RXY	CAM-CAN-CAO-CAP
2	B	403	RXY	CAE-CAF-CAG-CAH
2	A	101[B]	RXY	CAO-CAP-CAQ-CAR
2	A	101[B]	RXY	CBG-CBH-CBI-CBJ
2	E	201	RXY	CAH-CAI-CAJ-CAK
2	B	403	RXY	CAL-CAM-CAN-CAO
2	A	101[B]	RXY	CBR-CBS-CBT-CBU
2	B	402[A]	RXY	CAN-CAO-CAP-CAQ
2	A	101[B]	RXY	CAE-CAF-CAG-CAH
2	A	102	RXY	CBQ-CBR-CBS-CBT
2	B	401	RXY	CAN-CAO-CAP-CAQ
2	B	401	RXY	OBW-CAW-CAX-OAY

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Mol	Chain	Res	Type	Atoms
2	E	201	RXY	OAU-CAV-CAW-OBW
2	B	402[A]	RXY	CAO-CAP-CAQ-CAR
2	B	401	RXY	CBE-CBF-CBG-CBH
2	A	102	RXY	CBB-OBA-PAZ-OAY
2	A	101[B]	RXY	CAX-OAY-PAZ-OAB
2	A	102	RXY	CAX-OAY-PAZ-OBX
2	A	102	RXY	CBB-OBA-PAZ-OBX
2	A	102	RXY	CBB-OBA-PAZ-OAB
2	B	402[A]	RXY	CBB-OBA-PAZ-OAB
2	B	401	RXY	CAV-CAW-CAX-OAY
2	B	403	RXY	CBC-CBB-OBA-PAZ
2	B	402[B]	RXY	CAH-CAI-CAJ-CAK
2	B	402[B]	RXY	OAU-CAV-CAW-OBW
2	B	402[A]	RXY	CBG-CBH-CBI-CBJ
2	E	201	RXY	CBK-CBL-CBM-CBN
2	E	201	RXY	CAE-CAF-CAG-CAH
2	B	402[B]	RXY	CAX-OAY-PAZ-OBA
2	B	402[B]	RXY	CBM-CBN-CBO-CBP
2	B	402[A]	RXY	CAF-CAG-CAH-CAI
2	B	402[B]	RXY	CBK-CBL-CBM-CBN
2	B	401	RXY	CAP-CAQ-CAR-CAS
2	A	101[B]	RXY	OBA-CBB-CBC-NBD
2	B	401	RXY	CAM-CAN-CAO-CAP
2	A	102	RXY	CAE-CAF-CAG-CAH
2	B	401	RXY	CBI-CBJ-CBK-CBL
2	E	201	RXY	CAK-CAL-CAM-CAN
2	B	401	RXY	CBK-CBL-CBM-CBN
2	B	403	RXY	CAH-CAI-CAJ-CAK
2	B	402[B]	RXY	CAV-CAW-CAX-OAY
2	B	403	RXY	CAN-CAO-CAP-CAQ
2	B	402[B]	RXY	CAI-CAJ-CAK-CAL
2	A	102	RXY	CAR-CAS-CAT-OAU
2	A	101[A]	RXY	CAK-CAL-CAM-CAN
2	A	101[B]	RXY	CAI-CAJ-CAK-CAL
2	A	102	RXY	CBK-CBL-CBM-CBN
2	B	402[A]	RXY	CAI-CAJ-CAK-CAL
2	B	403	RXY	CAI-CAJ-CAK-CAL
2	A	101[B]	RXY	CAR-CAS-CAT-OAU
2	A	101[B]	RXY	CBK-CBL-CBM-CBN
2	B	402[A]	RXY	CBK-CBL-CBM-CBN
2	B	403	RXY	CBK-CBL-CBM-CBN
2	A	101[B]	RXY	CBF-CBG-CBH-CBI

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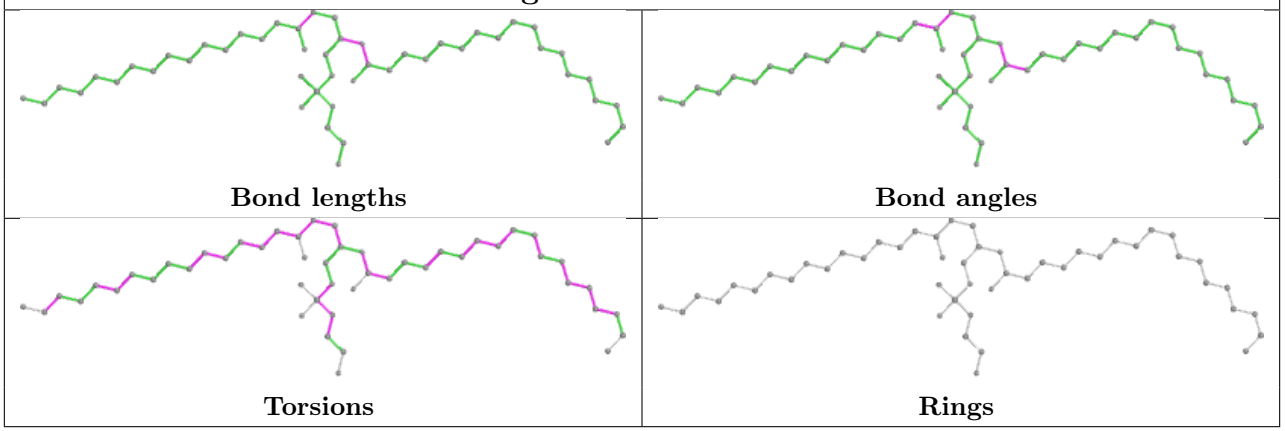
Mol	Chain	Res	Type	Atoms
2	A	102	RXY	CAI-CAJ-CAK-CAL
2	A	101[A]	RXY	CBK-CBL-CBM-CBN
2	A	101[A]	RXY	CBT-CBU-CBV-OBW
2	B	402[A]	RXY	CAK-CAL-CAM-CAN
2	A	101[B]	RXY	CAR-CAS-CAT-OAA
2	A	101[B]	RXY	CBH-CBI-CBJ-CBK
2	E	201	RXY	CBF-CBG-CBH-CBI
2	A	102	RXY	CAR-CAS-CAT-OAA
2	A	101[B]	RXY	CAK-CAL-CAM-CAN
2	E	201	RXY	CBB-OBA-PAZ-OAB
2	E	201	RXY	CBC-CBB-OBA-PAZ
2	B	401	RXY	CBS-CBT-CBU-CBV
2	B	401	RXY	CBM-CBN-CBO-CBP
2	A	101[B]	RXY	CBQ-CBR-CBS-CBT
2	A	101[A]	RXY	CBT-CBU-CBV-OBY
2	A	102	RXY	CBT-CBU-CBV-OBW
2	A	101[A]	RXY	CAH-CAI-CAJ-CAK
2	A	102	RXY	CBM-CBN-CBO-CBP

There are no ring outliers.

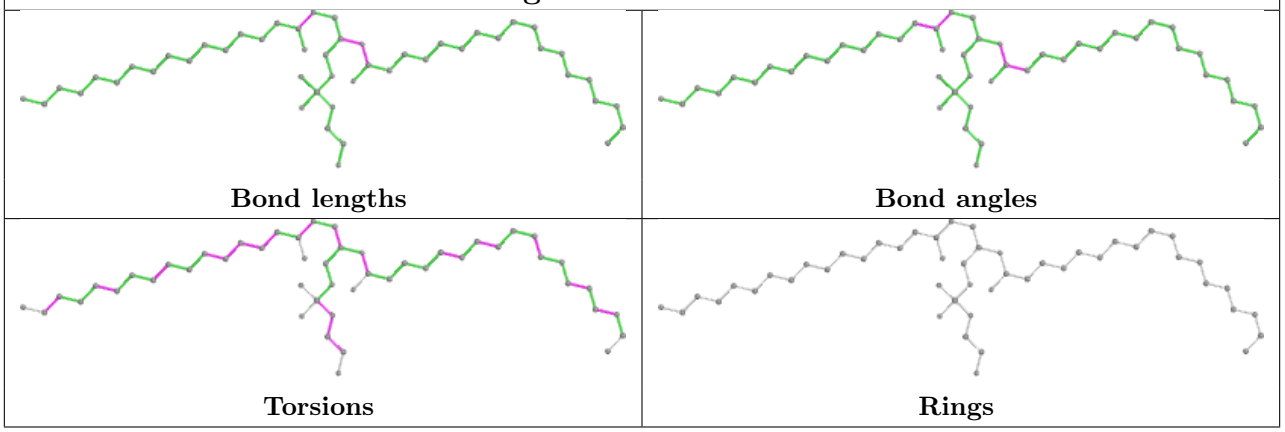
No monomer is involved in short contacts.

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 then 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.

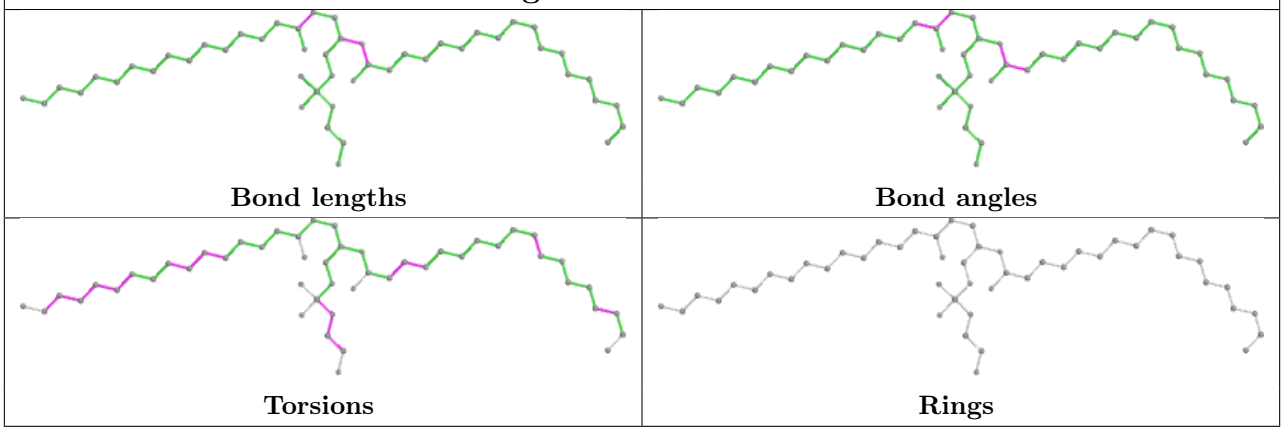
Ligand RXY A 102



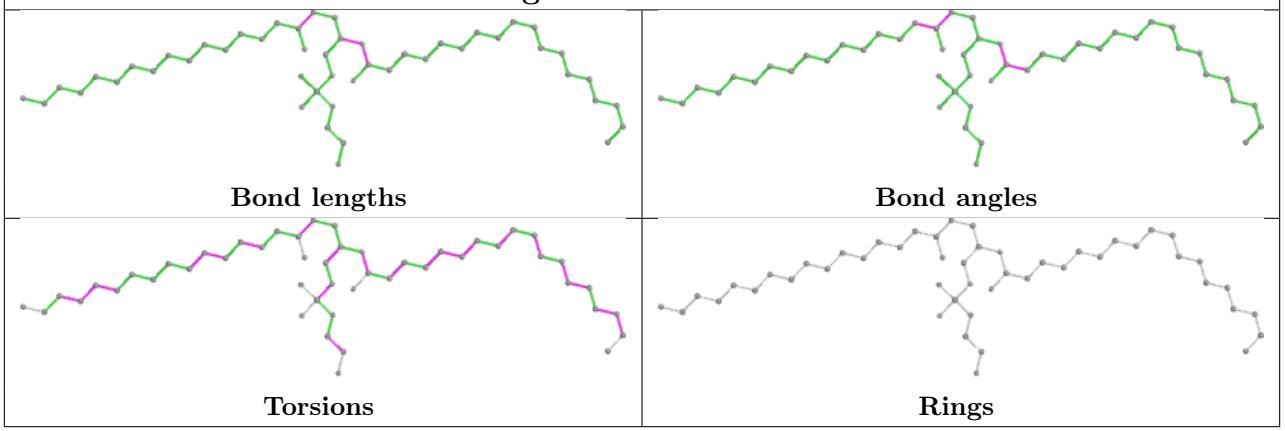
Ligand RXY E 201



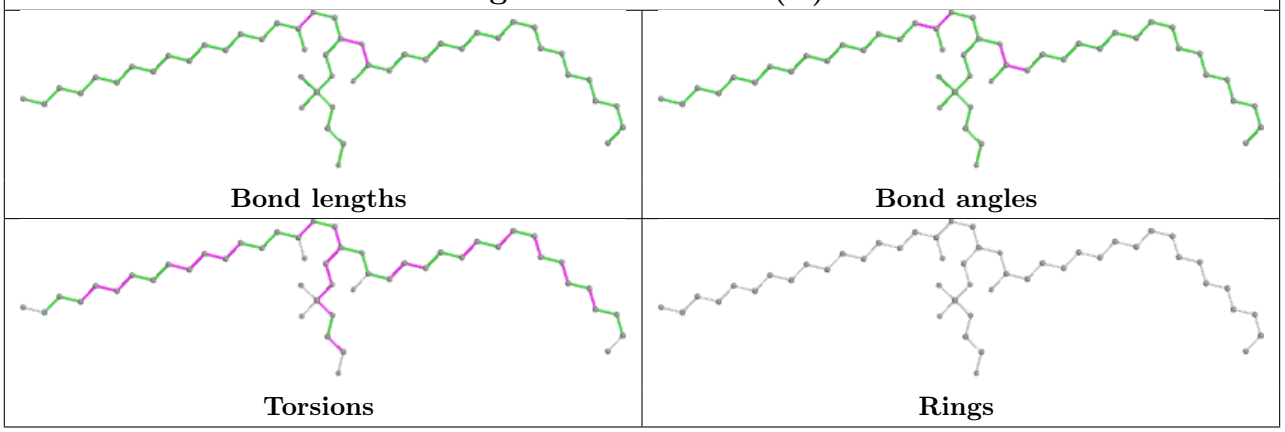
Ligand RXY B 403



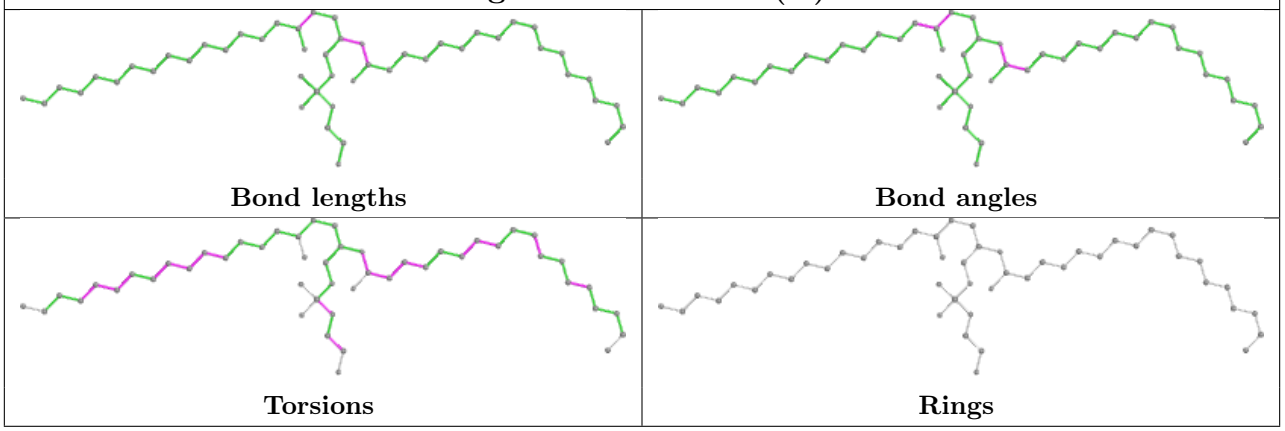
Ligand RXY B 401

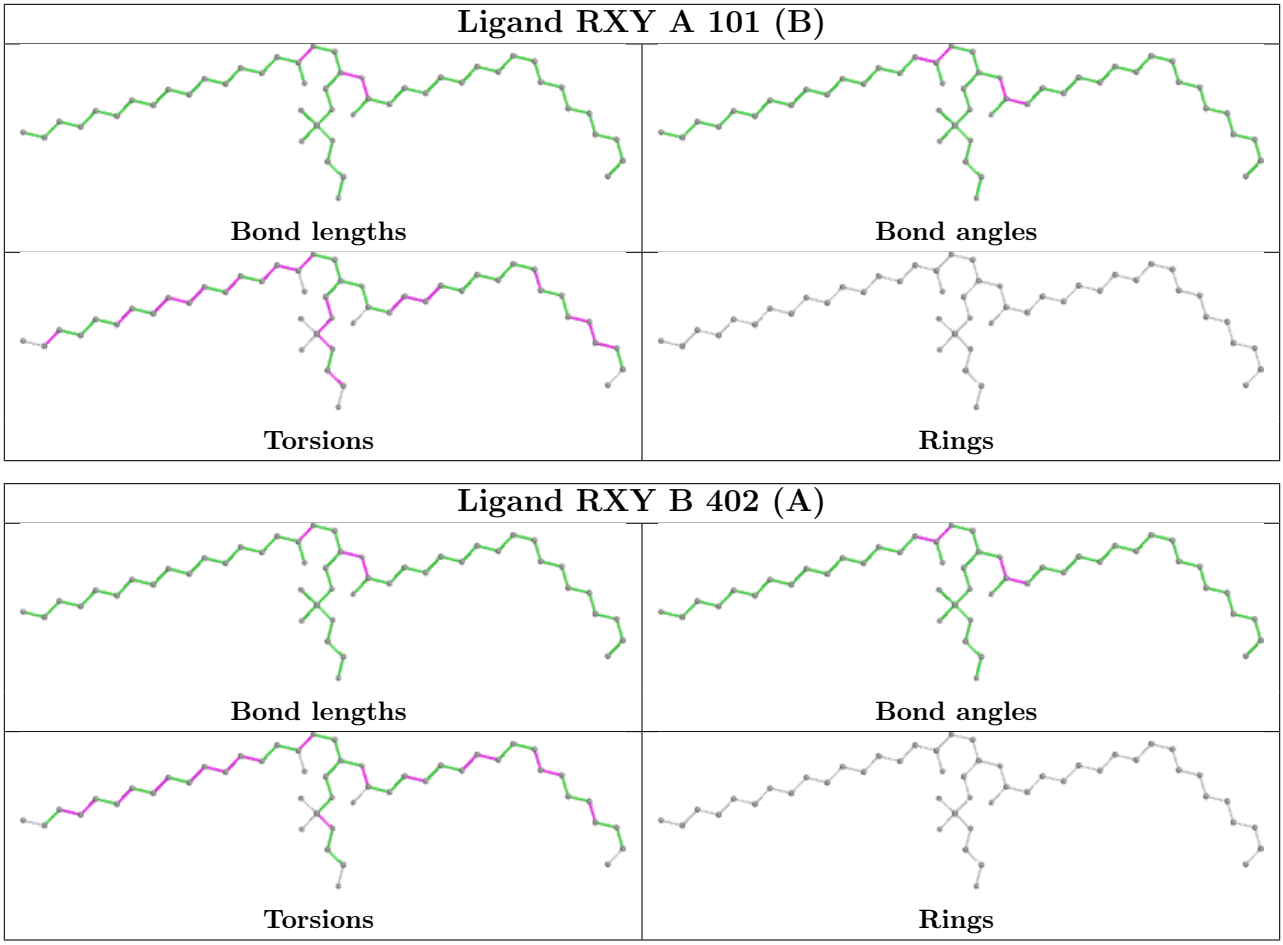


Ligand RXY B 402 (B)



Ligand RXY A 101 (A)





4.7 Other polymers (i)

There are no such residues in this entry.

4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

5 Fit of model and data

5.1 Protein, DNA and RNA chains

EDS failed to run properly - this section is therefore empty.

5.2 Non-standard residues in protein, DNA, RNA chains

EDS failed to run properly - this section is therefore empty.

5.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

5.4 Ligands

EDS failed to run properly - this section is therefore empty.

5.5 Other polymers

EDS failed to run properly - this section is therefore empty.