Full wwPDB X-ray Structure Validation Report (i)

Nov 14, 2023 – 11:41 PM JST

PDB ID	:	6IIU
Title	:	Crystal structure of the human thromboxane A2 receptor bound to ramatroban
Authors	:	Fan, H.; Zhao, Q.; Wu, B.
Deposited on	:	2018-10-07
Resolution	:	2.50 Å(reported)

The following versions of software and data (see references (i)) 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	:	2.36
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)	:	2.36

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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.
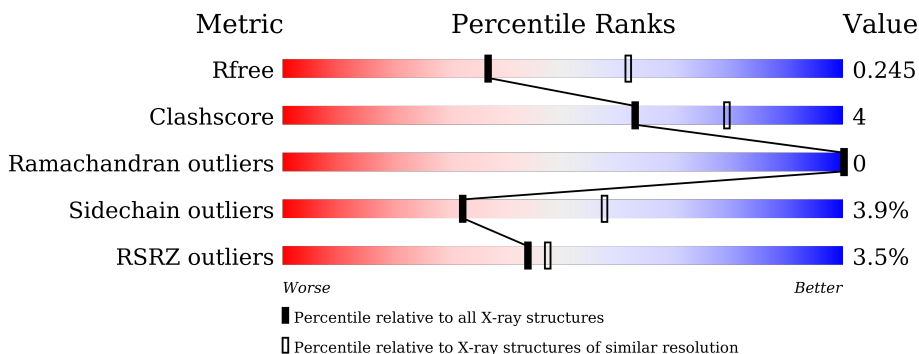
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 <=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	484	3% / 84% / 10% / · 5%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 3565 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 Soluble cytochrome b562,Thromboxane A2 receptor,Rubredo xin,Thromboxane A2 receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	460	3458	2229	577	629	23	0	0	0

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	991	ASP	-	expression tag	UNP P0ABE7
A	992	TYR	-	expression tag	UNP P0ABE7
A	993	LYS	-	expression tag	UNP P0ABE7
A	994	ASP	-	expression tag	UNP P0ABE7
A	995	ASP	-	expression tag	UNP P0ABE7
A	996	ASP	-	expression tag	UNP P0ABE7
A	997	ASP	-	expression tag	UNP P0ABE7
A	998	GLY	-	expression tag	UNP P0ABE7
A	999	ALA	-	expression tag	UNP P0ABE7
A	1000	PRO	-	expression tag	UNP P0ABE7
A	1007	TRP	MET	engineered mutation	UNP P0ABE7
A	1102	ILE	HIS	engineered mutation	UNP P0ABE7
A	1106	LEU	ARG	engineered mutation	UNP P0ABE7
A	247	ALA	LEU	engineered mutation	UNP P21731
A	324	GLU	-	expression tag	UNP P21731
A	325	PHE	-	expression tag	UNP P21731
A	326	LEU	-	expression tag	UNP P21731
A	327	GLU	-	expression tag	UNP P21731
A	328	VAL	-	expression tag	UNP P21731
A	329	LEU	-	expression tag	UNP P21731
A	330	PHE	-	expression tag	UNP P21731
A	331	GLN	-	expression tag	UNP P21731

- Molecule 2 is 3-[(3R)-3-[(4-fluorophenyl)sulfonylamino]-1,2,3,4-tetrahydrocarbazol-9-yl]prop anoic acid (three-letter code: A8X) (formula: $C_{21}H_{21}FN_2O_4S$).
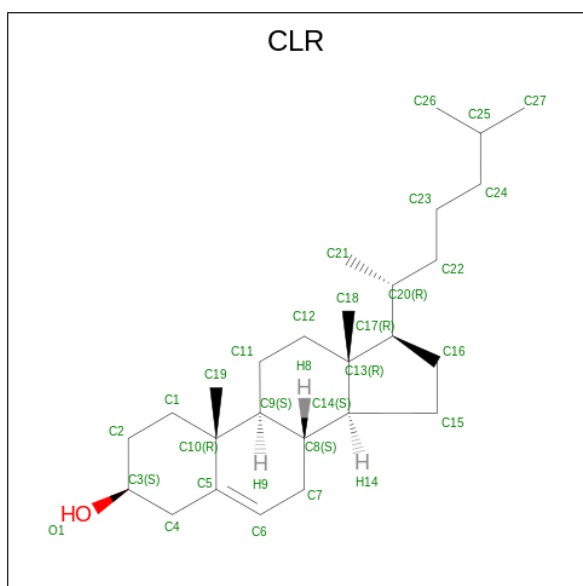
A8X
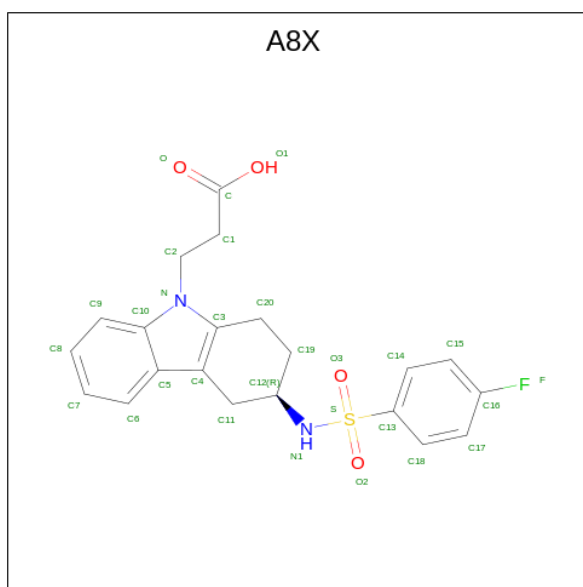
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	S	0	0
			29	21	1	2	4	1		

• Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		

• Molecule 4 is CHOLESTEROL (three-letter code: CLR) (formula: $C_{27}H_{46}O$).

CLR

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 28	C 27	O 1	0	0

- Molecule 5 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (three-letter code: OLC) (formula: $C_{21}H_{40}O_4$).
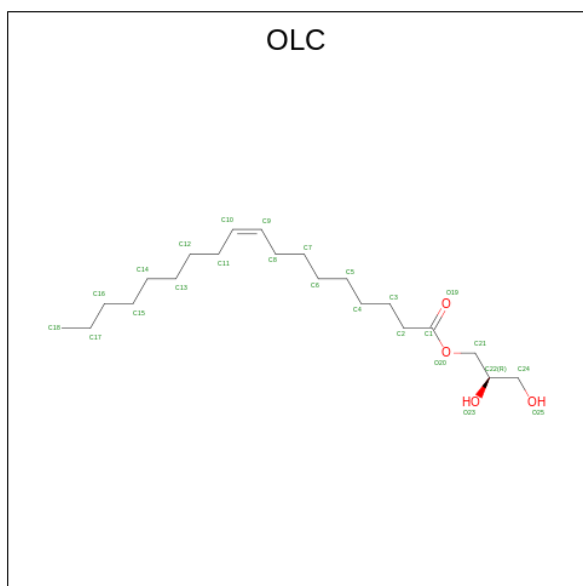
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total 13	C 9	O 4	0	0
5	A	1	Total 19	C 15	O 4	0	0

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

GOL

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total 6	C 3	O 3	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	11	Total 11	O 11	0	0

3 Residue-property plots ⓘ

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: Soluble cytochrome b562,Thromboxane A2 receptor,Rubredoxin,Thromboxane A2 receptor
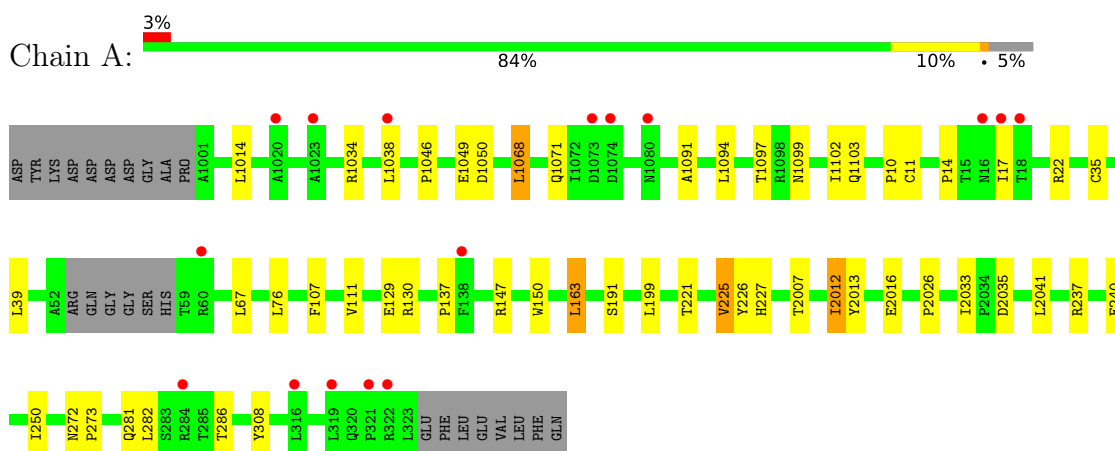
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	81.16Å 155.08Å 128.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.53 – 2.50 41.28 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.6 (41.53-2.50) 97.7 (41.28-2.50)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.36 (at 2.51Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.198 , 0.218 0.215 , 0.245	Depositor DCC
R_{free} test set	1411 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å^2)	60.8	Xtriage
Anisotropy	0.250	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 57.5	EDS
L-test for twinning[2]	$< |L| > = 0.47, < L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	3565	wwPDB-VP
Average B, all atoms (Å^2)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.10% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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.

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: A8X, OLC, ZN, GOL, CLR

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	0.49	0/3537	0.63	0/4831

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	11	CYS	Mainchain

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	3458	0	3402	28	0
2	A	29	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	1	0	0	0	0
4	A	28	0	46	7	0
5	A	32	0	40	1	0
6	A	6	0	8	0	0
7	A	11	0	0	0	0
All	All	3565	0	3496	30	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 (30) 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:150:TRP:HB2	4:A:9003:CLR:H191	1.47	0.95
1:A:150:TRP:CB	4:A:9003:CLR:H191	2.09	0.82
1:A:150:TRP:HB3	4:A:9003:CLR:H182	1.65	0.77
1:A:2016:GLU:O	1:A:2026:PRO:HB3	2.01	0.60
1:A:147:ARG:HA	4:A:9003:CLR:C19	2.33	0.59
1:A:1071:GLN:HE22	1:A:1097:THR:HG21	1.69	0.57
1:A:1099:ASN:HA	1:A:1103:GLN:HB3	1.86	0.57
1:A:107:PHE:HD1	5:A:9004:OLC:H2A	1.69	0.57
1:A:137:PRO:HG2	1:A:2007:THR:HA	1.85	0.56
1:A:237:ARG:HB2	1:A:240:GLU:HG2	1.88	0.55
1:A:147:ARG:HA	4:A:9003:CLR:H192	1.89	0.55
1:A:14:PRO:HG2	1:A:281:GLN:HB2	1.88	0.54
1:A:221:THR:O	1:A:225:VAL:HB	2.10	0.52
1:A:225:VAL:HG12	1:A:226:TYR:CD1	2.48	0.49
1:A:163:LEU:HD11	1:A:199:LEU:HG	1.94	0.49
1:A:129:GLU:OE1	1:A:130:ARG:HD2	2.14	0.47
1:A:2013:TYR:CZ	1:A:2033:ILE:HD11	2.51	0.45
1:A:1068:LEU:HD21	1:A:1102:ILE:HD11	1.99	0.45
4:A:9003:CLR:H162	4:A:9003:CLR:H221	1.77	0.45
1:A:225:VAL:HG12	1:A:226:TYR:HD1	1.81	0.44
1:A:67:LEU:HD21	1:A:308:TYR:CD1	2.54	0.43
1:A:17:ILE:HG12	1:A:22:ARG:HG3	2.01	0.43
1:A:35:CYS:O	1:A:39:LEU:HG	2.20	0.42
1:A:1091:ALA:HA	1:A:1094:LEU:HD12	2.02	0.41
4:A:9003:CLR:H183	4:A:9003:CLR:H20	1.93	0.41
1:A:282:LEU:HD22	1:A:286:THR:HG21	2.01	0.41
1:A:272:ASN:CB	1:A:273:PRO:HD3	2.50	0.41
1:A:2012:ILE:O	1:A:2012:ILE:HG13	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1046:PRO:HA	1:A:1049:GLU:HG3	2.03	0.41
1:A:1034:ARG:NH1	1:A:1038:LEU:HD11	2.36	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	456/484 (94%)	444 (97%)	12 (3%)	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	357/398 (90%)	343 (96%)	14 (4%)	32	57

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

Mol	Chain	Res	Type
1	A	1014	LEU
1	A	1050	ASP
1	A	1068	LEU
1	A	10	PRO

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Mol	Chain	Res	Type
1	A	76	LEU
1	A	111	VAL
1	A	163	LEU
1	A	191	SER
1	A	225	VAL
1	A	227	HIS
1	A	2012	ILE
1	A	2035	ASP
1	A	2041	LEU
1	A	250	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1080	ASN
1	A	1099	ASN
1	A	146	GLN
1	A	227	HIS
1	A	2022	ASN

5.3.3   RNA ⓘ

There are no RNA molecules in this entry.

5.4   Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5   Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6   Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 1 is monoatomic - leaving 5 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
5	OLC	A	9004	-	12,12,24	0.67	0	13,13,25	0.57	0
6	GOL	A	9006	-	5,5,5	0.24	0	5,5,5	0.81	0
4	CLR	A	9003	-	31,31,31	0.74	0	48,48,48	1.81	12 (25%)
2	A8X	A	9001	-	27,32,32	2.36	8 (29%)	34,47,47	1.98	9 (26%)
5	OLC	A	9005	-	18,18,24	1.18	1 (5%)	18,19,25	0.79	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
5	OLC	A	9004	-	-	5/12/12/24	-
6	GOL	A	9006	-	-	1/4/4/4	-
4	CLR	A	9003	-	-	9/10/68/68	0/4/4/4
2	A8X	A	9001	-	-	3/16/25/25	0/4/4/4
5	OLC	A	9005	-	-	8/18/18/24	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	9001	A8X	C13-S	-7.39	1.65	1.76
2	A	9001	A8X	C11-C12	5.61	1.56	1.52
5	A	9005	OLC	C9-C10	4.11	1.55	1.31
2	A	9001	A8X	C17-C16	3.42	1.43	1.37
2	A	9001	A8X	C14-C13	3.00	1.43	1.38
2	A	9001	A8X	C12-N1	-2.21	1.44	1.47
2	A	9001	A8X	C8-C9	2.16	1.41	1.36
2	A	9001	A8X	C18-C13	2.08	1.42	1.38
2	A	9001	A8X	S-N1	2.02	1.65	1.61

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	9001	A8X	C2-N-C3	-6.28	114.20	124.72
2	A	9001	A8X	C4-C11-C12	-4.29	106.77	112.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	9003	CLR	C21-C20-C17	-3.58	107.44	112.92
4	A	9003	CLR	C21-C20-C22	3.55	115.92	110.36
2	A	9001	A8X	O3-S-C13	3.42	112.19	107.97
4	A	9003	CLR	C12-C11-C9	3.36	118.93	113.11
4	A	9003	CLR	C9-C10-C5	3.33	114.87	109.65
2	A	9001	A8X	C4-C3-N	3.32	111.09	107.01
2	A	9001	A8X	O1-C-O	-3.32	115.03	123.30
4	A	9003	CLR	C7-C8-C14	3.27	115.65	110.91
4	A	9003	CLR	C16-C17-C20	3.22	117.13	112.15
4	A	9003	CLR	C1-C2-C3	3.22	114.59	110.47
2	A	9001	A8X	C15-C14-C13	2.89	122.44	119.45
4	A	9003	CLR	C22-C20-C17	2.86	116.20	110.28
2	A	9001	A8X	C13-S-N1	-2.82	103.87	107.78
4	A	9003	CLR	C1-C10-C5	-2.80	103.63	108.75
4	A	9003	CLR	C4-C5-C10	2.79	120.12	116.42
4	A	9003	CLR	C17-C13-C14	2.26	102.75	100.07
2	A	9001	A8X	C12-N1-S	2.20	125.89	122.08
2	A	9001	A8X	C19-C12-C11	2.17	111.72	110.12
4	A	9003	CLR	C8-C7-C6	-2.01	109.84	112.73

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	9003	CLR	C13-C17-C20-C21
4	A	9003	CLR	C16-C17-C20-C21
5	A	9005	OLC	C9-C10-C11-C12
4	A	9003	CLR	C13-C17-C20-C22
4	A	9003	CLR	C21-C20-C22-C23
4	A	9003	CLR	C16-C17-C20-C22
2	A	9001	A8X	O-C-C1-C2
5	A	9004	OLC	C2-C1-O20-C21
4	A	9003	CLR	C17-C20-C22-C23
5	A	9004	OLC	O19-C1-O20-C21
4	A	9003	CLR	C20-C22-C23-C24
2	A	9001	A8X	O1-C-C1-C2
5	A	9005	OLC	C2-C1-O20-C21
5	A	9005	OLC	C1-C2-C3-C4
5	A	9005	OLC	C6-C7-C8-C9
5	A	9004	OLC	C2-C3-C4-C5
5	A	9005	OLC	O19-C1-O20-C21
5	A	9004	OLC	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
5	A	9005	OLC	C4-C5-C6-C7
5	A	9005	OLC	C5-C6-C7-C8
2	A	9001	A8X	C-C1-C2-N
4	A	9003	CLR	C22-C23-C24-C25
5	A	9004	OLC	C3-C4-C5-C6
5	A	9005	OLC	C3-C4-C5-C6
6	A	9006	GOL	O1-C1-C2-O2
4	A	9003	CLR	C23-C24-C25-C26

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	9004	OLC	1	0
4	A	9003	CLR	7	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 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 OLC A 9004

Bond lengths   Bond angles

Torsions   Rings

Ligand CLR A 9003

Bond lengths

Bond angles

Torsions

Rings

Ligand A8X A 9001

Bond lengths

Bond angles

Torsions

Rings

Ligand OLC A 9005

Bond lengths

Bond angles

Torsions

Rings
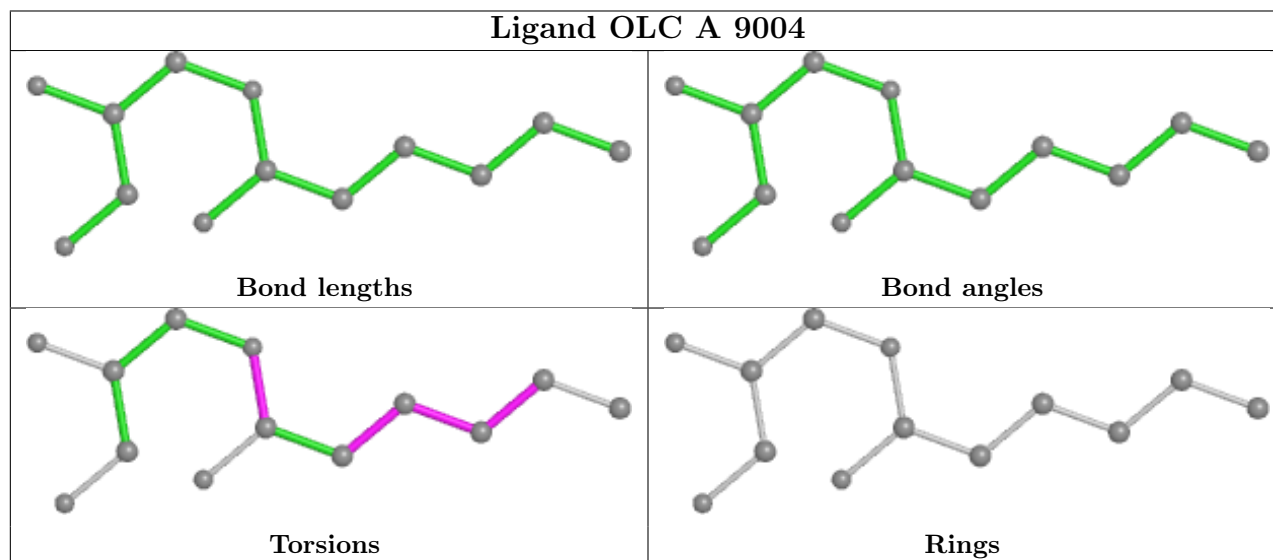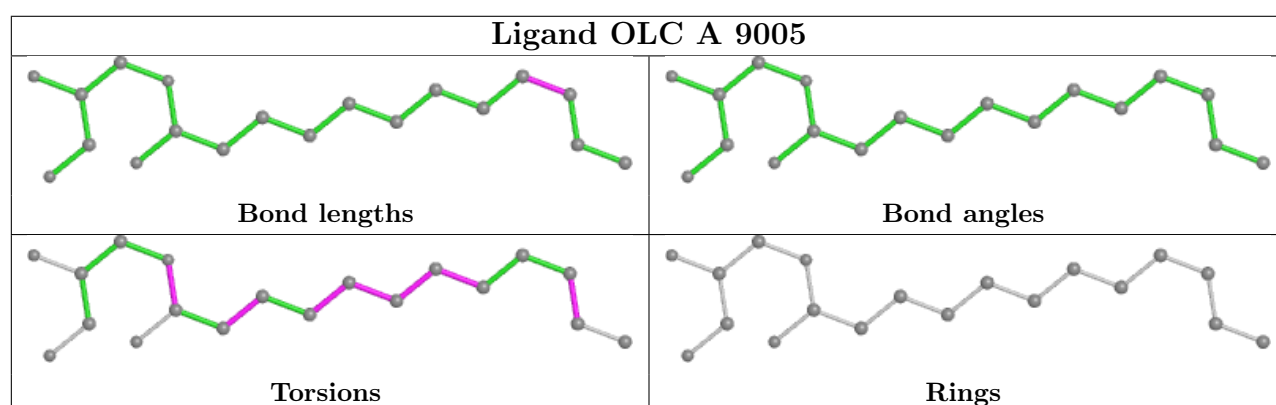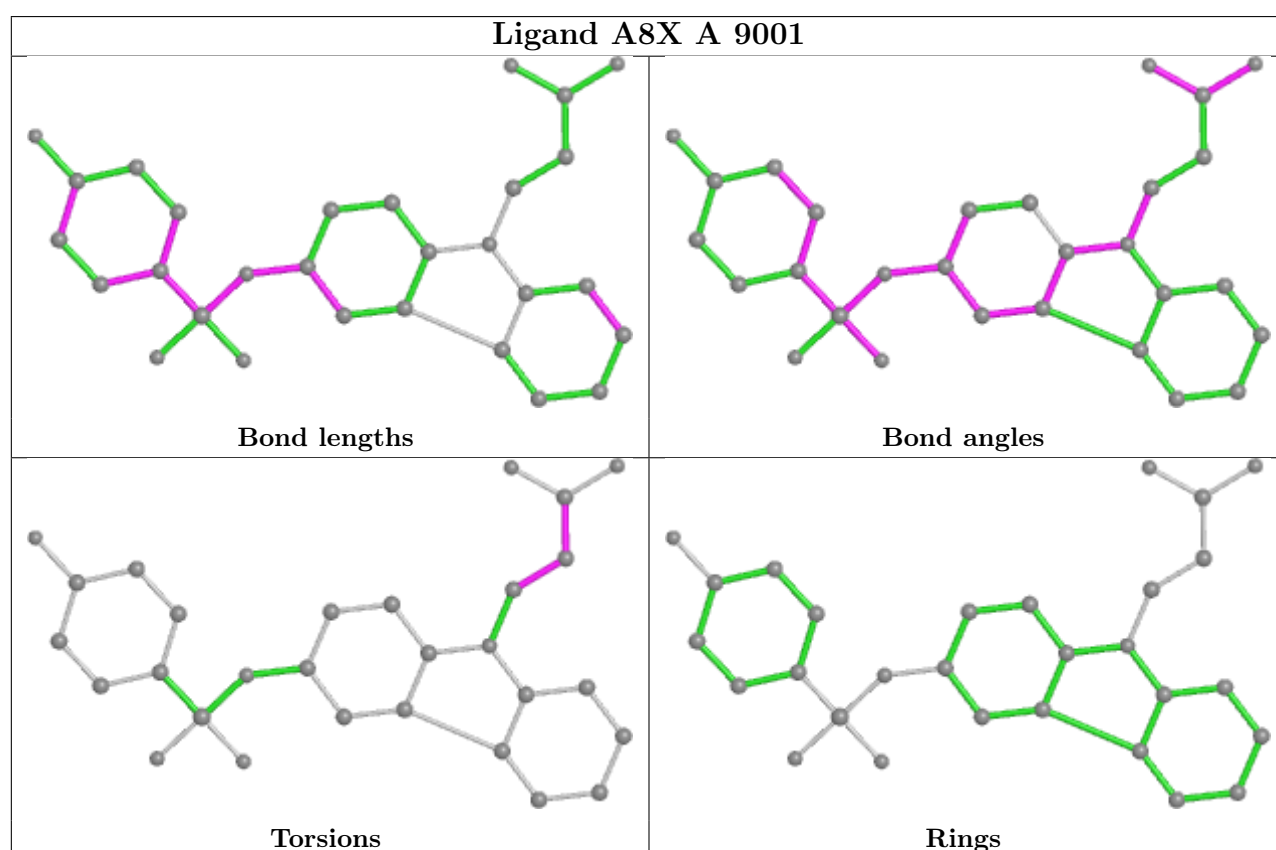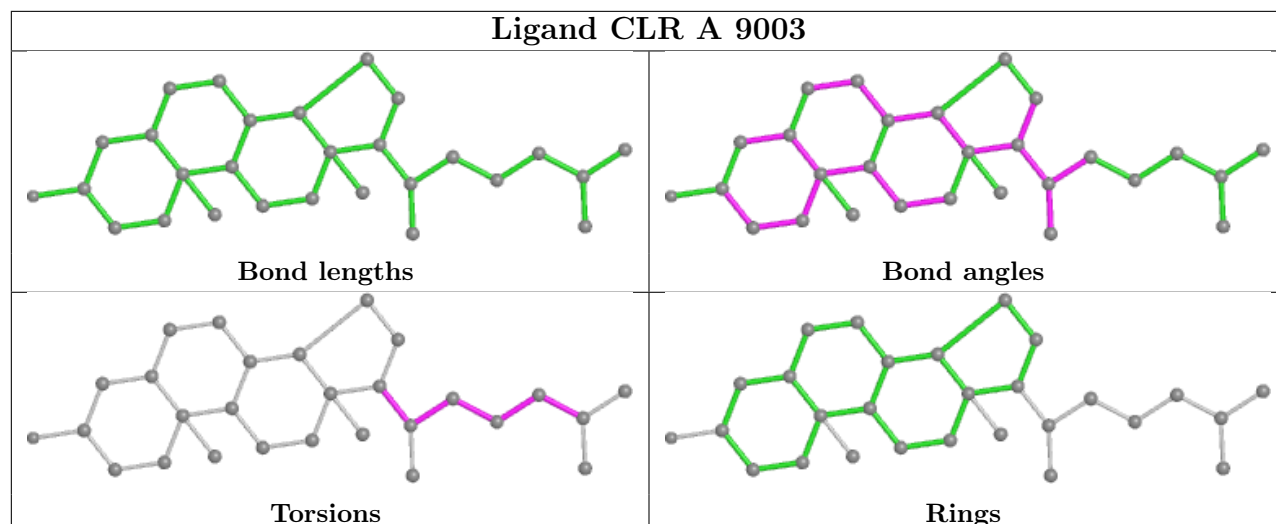
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	460/484 (95%)	0.17	16 (3%)	44	47	46, 71, 114, 181	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	321	PRO	3.7
1	A	319	LEU	3.1
1	A	284	ARG	3.0
1	A	1080	ASN	3.0
1	A	322	ARG	2.9
1	A	138	PHE	2.8
1	A	1073	ASP	2.7
1	A	60	ARG	2.4
1	A	1038	LEU	2.4
1	A	1023	ALA	2.2
1	A	1020	ALA	2.2
1	A	18	THR	2.2
1	A	316	LEU	2.2
1	A	1074	ASP	2.2
1	A	17	ILE	2.2
1	A	16	ASN	2.1

6.2　Non-standard residues in protein, DNA, RNA chains ⓘ

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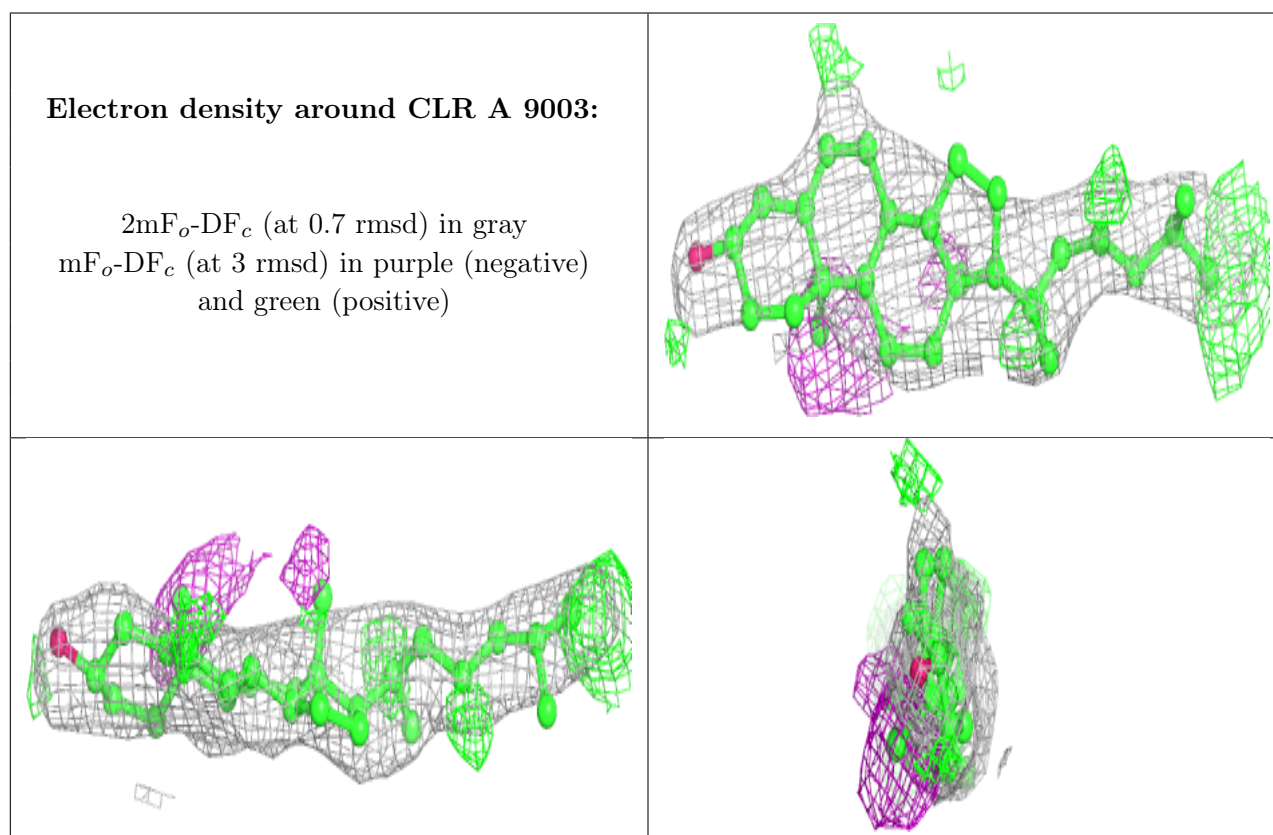
6.3　Carbohydrates ⓘ

There are no 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
4	CLR	A	9003	28/28	0.76	0.31	84,101,108,110	0
6	GOL	A	9006	6/6	0.79	0.32	54,70,71,73	0
5	OLC	A	9005	19/25	0.80	0.25	85,88,100,101	0
5	OLC	A	9004	13/25	0.88	0.25	88,92,95,96	0
2	A8X	A	9001	29/29	0.98	0.16	47,56,68,74	0
3	ZN	A	9002	1/1	0.99	0.11	71,71,71,71	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 CLR A 9003:

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

Electron density around OLC A 9005:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
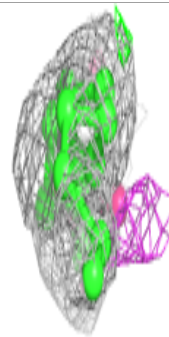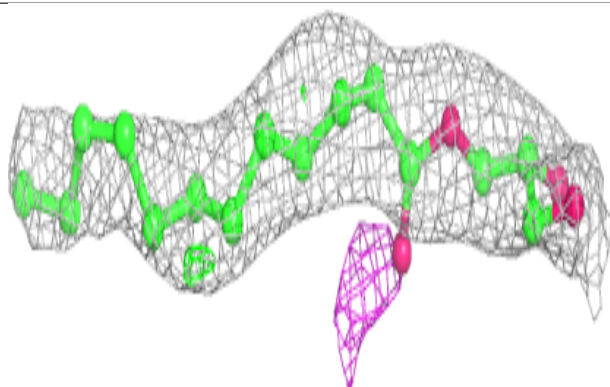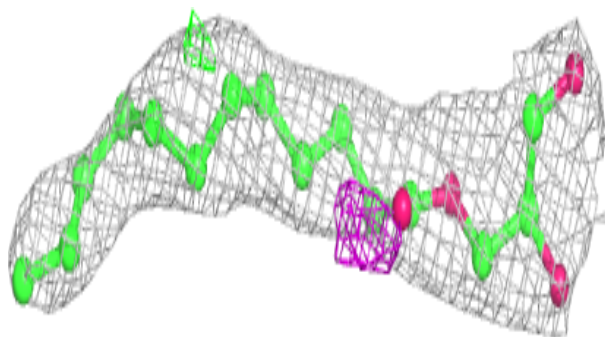
Electron density around OLC A 9004:

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

Electron density around A8X A 9001:

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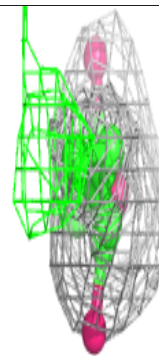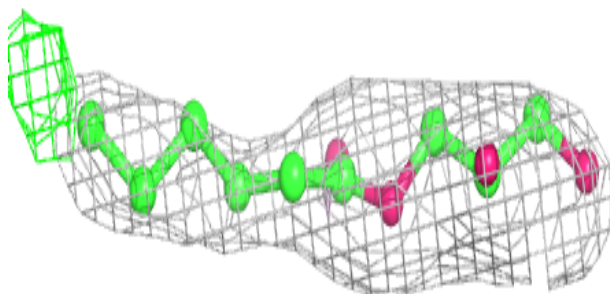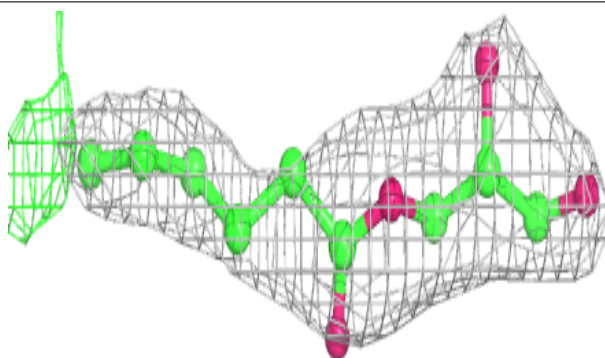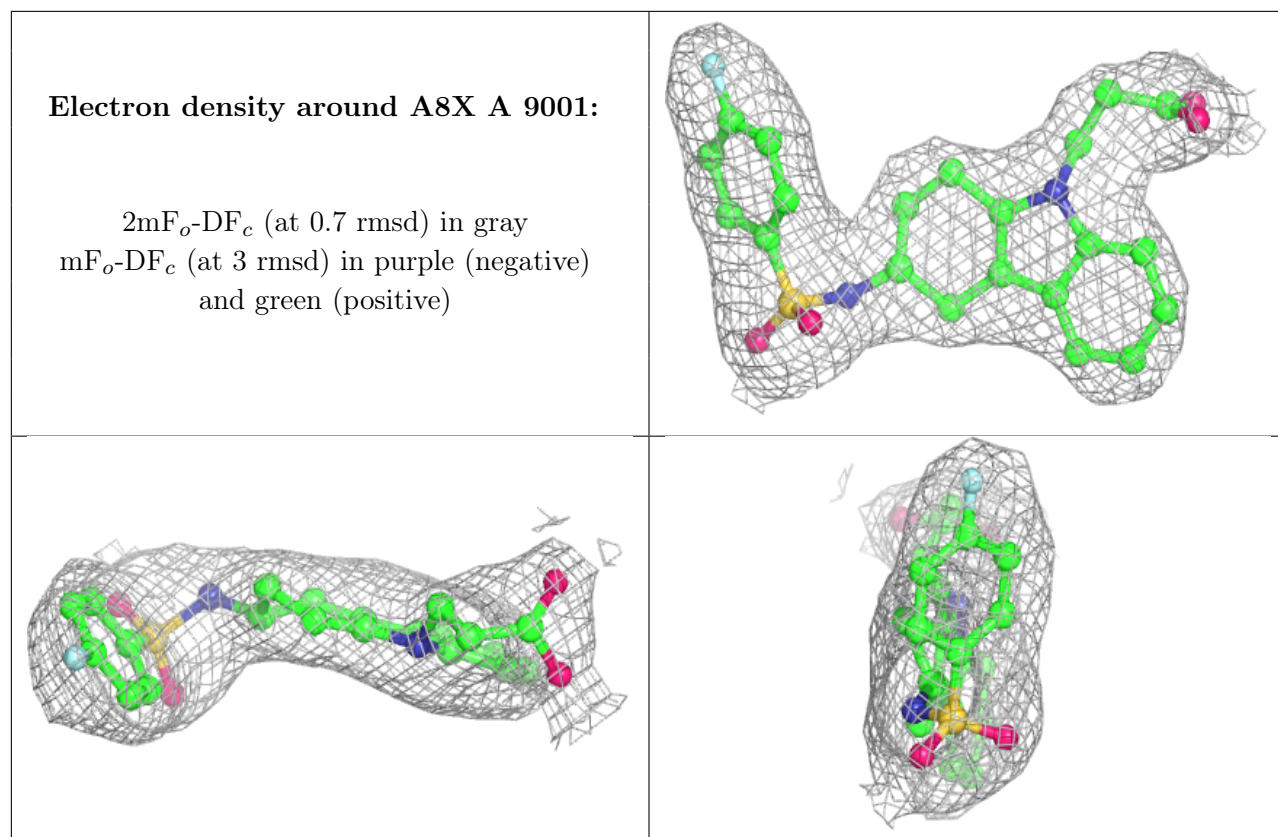
6.5 Other polymers (i)

There are no such residues in this entry.