wwPDB X-ray Structure Validation Summary Report (i)

Jan 6, 2025 – 12:39 pm GMT

PDB ID	:	8RKY
Title	:	X-ray structure of the drug binding domain of AlbA in complex with the KMR-14-14 compound of the pyrrolobenzodiazepines class
Authors	:	Di Palma, M.; Surani, Y.M.; Rahman, K.M.; Steiner, R.A.
Deposited on	:	2024-01-01
Resolution	:	2.17 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) 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 (i)) were used in the production of this report:

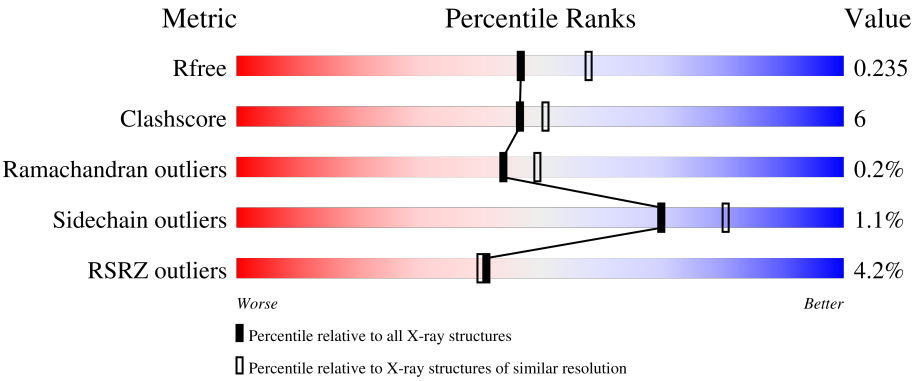
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

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 2.17 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}	164625	8336 (2.20-2.16)
Clashscore	180529	9404 (2.20-2.16)
Ramachandran outliers	177936	9297 (2.20-2.16)
Sidechain outliers	177891	9297 (2.20-2.16)
RSRZ outliers	164620	8337 (2.20-2.16)

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	AAA	224	5% 87% 9% ·
1	BBB	224	2% 88% 8% ·
1	CCC	224	5% 88% 8% ·

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
4	DTV	AAA	304	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 6088 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.

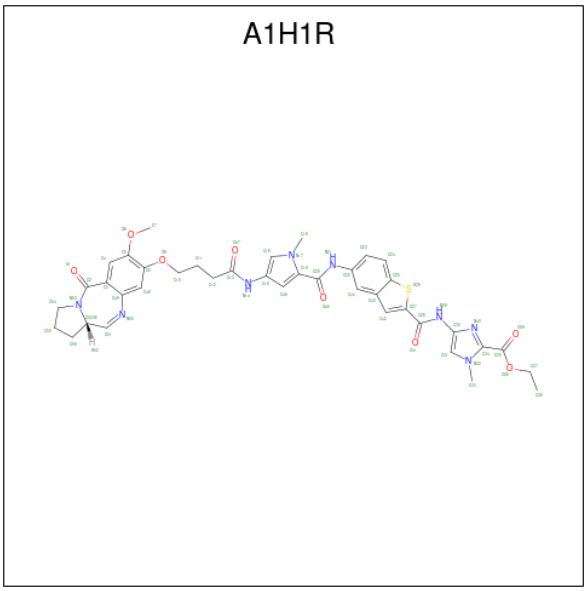
- Molecule 1 is a protein called Albicidin resistance protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	BBB	217	Total	C	N	O	S	0	4	0
			1827	1146	330	336	15			
1	CCC	217	Total	C	N	O	S	0	4	0
			1827	1146	330	336	15			
1	AAA	216	Total	C	N	O	S	0	6	0
			1838	1152	332	339	15			

There are 9 discrepancies between the modelled and reference sequences:

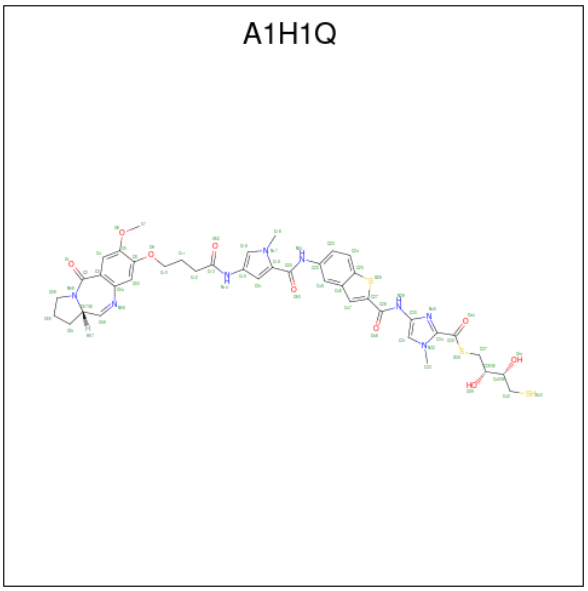
Chain	Residue	Modelled	Actual	Comment	Reference
BBB	0	GLY	-	expression tag	UNP Q8KRS7
BBB	222	GLY	-	expression tag	UNP Q8KRS7
BBB	223	SER	-	expression tag	UNP Q8KRS7
CCC	0	GLY	-	expression tag	UNP Q8KRS7
CCC	222	GLY	-	expression tag	UNP Q8KRS7
CCC	223	SER	-	expression tag	UNP Q8KRS7
AAA	0	GLY	-	expression tag	UNP Q8KRS7
AAA	222	GLY	-	expression tag	UNP Q8KRS7
AAA	223	SER	-	expression tag	UNP Q8KRS7

- Molecule 2 is ethyl 4-[[5-[[4-[4-[[(6 {a} {S})-2-methoxy-11-oxidanylidene-6 {a},7,8,9-tetrahydropyrrolo[2,1-c][1,4]benzodiazepin-3-yl]oxy]butanoylamino]-1-methyl-pyrrol-2-yl]carbonylamino]-1-benzothiophen-2-yl]carbonylamino]-1-methyl-imidazole-2-carboxylate (three-letter code: A1H1R) (formula: $C_{39}H_{40}N_8O_8S$) (labeled as "Ligand of Interest" by depositor).



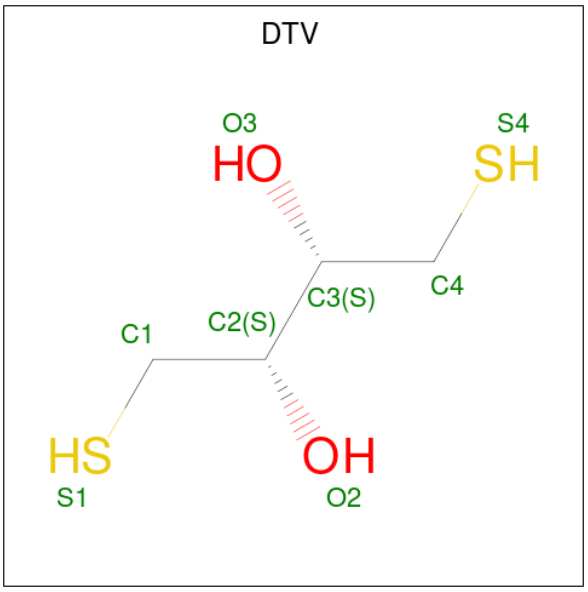
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	BBB	1	Total	C	N	O	S	0	0
			56	39	8	8	1		
2	CCC	1	Total	C	N	O	S	0	0
			56	39	8	8	1		
2	AAA	1	Total	C	N	O	S	0	0
			56	39	8	8	1		
2	AAA	1	Total	C	N	O	S	0	0
			56	39	8	8	1		

- Molecule 3 is {S}-[(2 {S},3 {S})-2,3-bis(oxidanyl)-4-sulfanyl-butyl] 4-[[5-[[4-[4-[[(6 {a} {S})-2-methoxy-11-oxidanylidene-6 {a},7,8,9-tetrahydropyrrolo[2,1-c][1,4]benzodiazepin-3-yl]oxy]butanoylamino]-1-methyl-pyrrol-2-yl]carbonylamino]-1-benzothiophen-2-yl]carbonylamino]-1-methyl-imidazole-2-carbothioate (three-letter code: A1H1Q) (formula: $C_{41}H_{44}N_8O_9S_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	BBB	1	Total	C	N	O	S	0	0
			61	41	8	9	3		
3	CCC	1	Total	C	N	O	S	0	0
			61	41	8	9	3		

- Molecule 4 is (2S,3S)-1,4-DIMERCAPTOBUTANE-2,3-DIOL (three-letter code: DTV) (formula: $C_4H_{10}O_2S_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	BBB	1	Total	C	O	S	0	0
			8	4	2	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	AAA	1	Total C O S 8 4 2 2	0	0
4	AAA	1	Total C O S 8 4 2 2	0	0

- Molecule 5 is water.

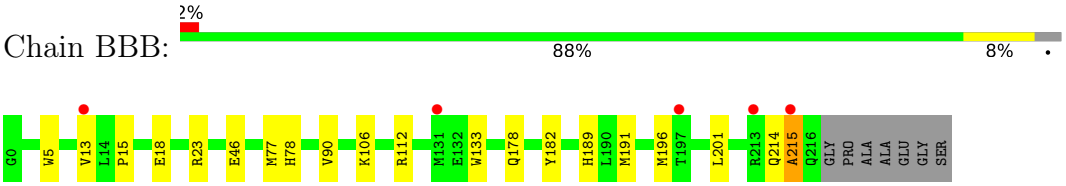
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	BBB	86	Total O 86 86	0	0
5	CCC	54	Total O 54 54	0	0
5	AAA	86	Total O 86 86	0	0

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.

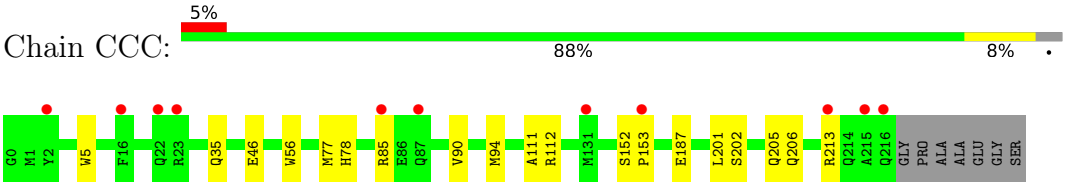
• Molecule 1: Albicidin resistance protein

Chain BBB:



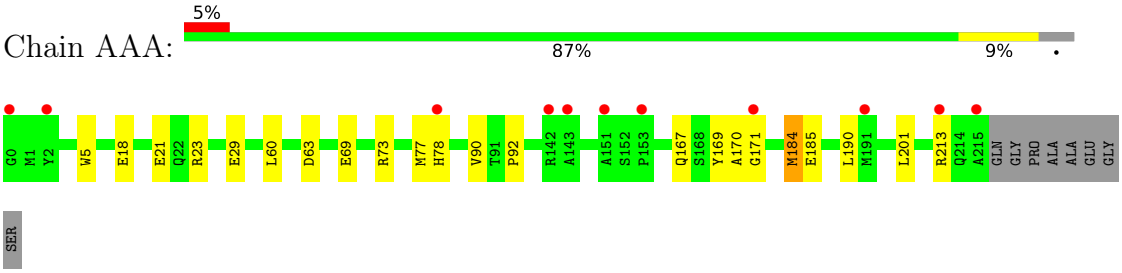
• Molecule 1: Albicidin resistance protein

Chain CCC:



• Molecule 1: Albicidin resistance protein

Chain AAA:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	182.63Å 118.95Å 57.70Å 90.00° 92.07° 90.00°	Depositor
Resolution (Å)	49.49 – 2.17 49.49 – 2.17	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.49-2.17) 99.7 (49.49-2.17)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.54 (at 2.18Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.208 , 0.234 0.212 , 0.235	Depositor DCC
R_{free} test set	3287 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	58.4	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 42.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.016 for -h,-k,l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	6088	wwPDB-VP
Average B, all atoms (Å^2)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.36% 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.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: A1H1Q, DTV, A1H1R

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	AAA	0.63	0/1882	0.73	0/2544
1	BBB	0.63	0/1871	0.69	0/2528
1	CCC	0.63	0/1871	0.71	0/2528
All	All	0.63	0/5624	0.71	0/7600

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

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	AAA	1838	0	1761	27	0
1	BBB	1827	0	1753	19	0
1	CCC	1827	0	1752	15	0
2	AAA	112	0	0	5	0
2	BBB	56	0	0	0	0
2	CCC	56	0	0	2	0
3	BBB	61	0	0	4	0
3	CCC	61	0	0	3	0
4	AAA	16	0	20	4	0
4	BBB	8	0	10	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	AAA	86	0	0	2	0
5	BBB	86	0	0	0	0
5	CCC	54	0	0	0	0
All	All	6088	0	5296	63	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 6.

The worst 5 of 63 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:BBB:78[B]:HIS:NE2	1:BBB:90:VAL:O	1.89	1.05
1:AAA:171:GLY:HA3	5:AAA:444:HOH:O	1.80	0.81
1:BBB:78[B]:HIS:HE2	1:BBB:90:VAL:C	1.83	0.80
1:BBB:191[A]:MET:SD	4:BBB:303:DTV:S1	2.85	0.74
1:CCC:90:VAL:HA	1:CCC:94:MET:HE1	1.73	0.69

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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	AAA	220/224 (98%)	218 (99%)	2 (1%)	0	100 100
1	BBB	219/224 (98%)	215 (98%)	3 (1%)	1 (0%)	25 26
1	CCC	219/224 (98%)	217 (99%)	2 (1%)	0	100 100
All	All	658/672 (98%)	650 (99%)	7 (1%)	1 (0%)	44 49

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	BBB	215	ALA

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	AAA	187/185 (101%)	184 (98%)	3 (2%)	58	70
1	BBB	186/185 (100%)	185 (100%)	1 (0%)	86	93
1	CCC	186/185 (100%)	183 (98%)	3 (2%)	58	70
All	All	559/555 (101%)	552 (99%)	7 (1%)	70	76

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	CCC	213	ARG
1	AAA	184[A]	MET
1	AAA	213	ARG
1	AAA	184[B]	MET
1	CCC	85	ARG

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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

9 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	A1H1R	CCC	301	-	52,62,62	1.13	3 (5%)	55,89,89	0.78	2 (3%)
2	A1H1R	AAA	302	-	52,62,62	1.05	3 (5%)	55,89,89	0.88	3 (5%)
3	A1H1Q	BBB	302	-	56,67,67	0.97	3 (5%)	57,96,96	0.88	2 (3%)
3	A1H1Q	CCC	302	-	56,67,67	0.87	2 (3%)	57,96,96	0.99	2 (3%)
4	DTV	AAA	304	-	7,7,7	0.47	0	4,8,8	0.48	0
4	DTV	AAA	303	-	7,7,7	0.33	0	4,8,8	0.40	0
2	A1H1R	AAA	301	-	52,62,62	1.34	3 (5%)	55,89,89	0.92	3 (5%)
4	DTV	BBB	303	-	7,7,7	0.31	0	4,8,8	0.31	0
2	A1H1R	BBB	301	-	52,62,62	1.24	3 (5%)	55,89,89	0.89	3 (5%)

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	A1H1R	CCC	301	-	-	1/23/59/59	0/6/7/7
2	A1H1R	AAA	302	-	-	7/23/59/59	0/6/7/7
3	A1H1Q	BBB	302	-	-	15/31/67/67	0/6/7/7
3	A1H1Q	CCC	302	-	-	7/31/67/67	0/6/7/7
4	DTV	AAA	304	-	-	6/8/8/8	-
4	DTV	AAA	303	-	-	6/8/8/8	-
2	A1H1R	AAA	301	-	-	4/23/59/59	0/6/7/7
4	DTV	BBB	303	-	-	4/8/8/8	-
2	A1H1R	BBB	301	-	-	0/23/59/59	0/6/7/7

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	AAA	301	A1H1R	C34-C35	-7.31	1.48	1.53
2	BBB	301	A1H1R	C34-C35	-6.27	1.49	1.53
2	CCC	301	A1H1R	C34-C35	-5.58	1.50	1.53
2	AAA	302	A1H1R	C46-C15	4.65	1.43	1.39
3	CCC	302	A1H1Q	C51-C15	4.56	1.43	1.39

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	CCC	302	A1H1Q	C15-N14-C13	-3.22	121.87	127.50
2	BBB	301	A1H1R	C44-C22-N21	-2.76	113.92	123.13
2	AAA	302	A1H1R	C27-C28-N29	2.72	118.17	113.93
3	CCC	302	A1H1Q	O44-C35-S36	-2.62	116.61	122.58
2	AAA	301	A1H1R	C27-C28-N29	2.54	117.89	113.93

There are no chirality outliers.

5 of 50 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	AAA	301	A1H1R	C10-C11-C12-C13
2	AAA	302	A1H1R	C10-C11-C12-C13
2	AAA	302	A1H1R	C34-C35-O36-C37
3	BBB	302	A1H1Q	C34-C35-S36-C37
3	BBB	302	A1H1Q	O44-C35-S36-C37

There are no ring outliers.

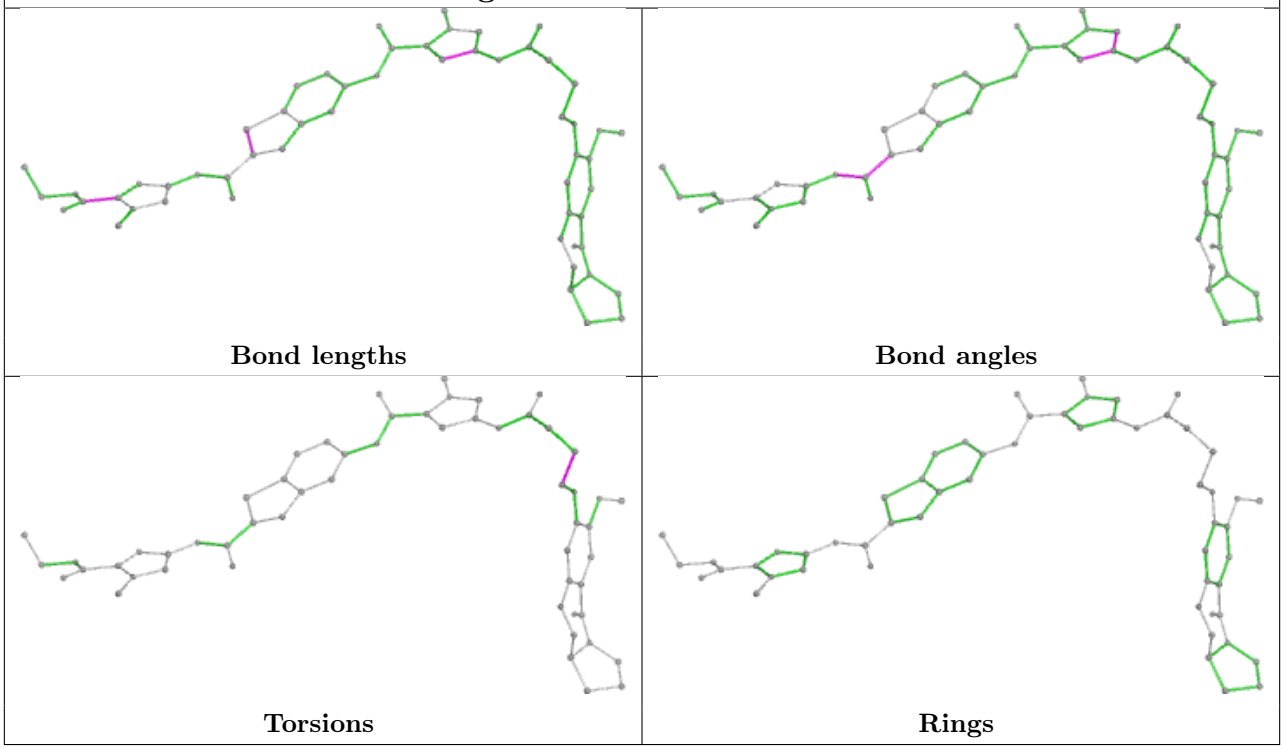
7 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	CCC	301	A1H1R	2	0
2	AAA	302	A1H1R	4	0
3	BBB	302	A1H1Q	4	0
3	CCC	302	A1H1Q	3	0
4	AAA	304	DTV	4	0
2	AAA	301	A1H1R	1	0
4	BBB	303	DTV	3	0

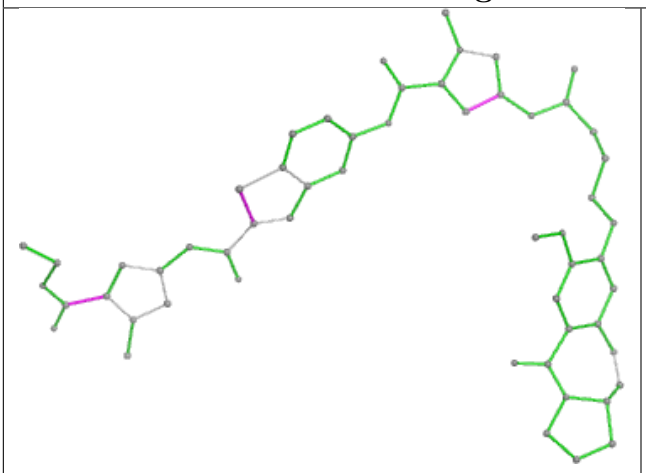
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

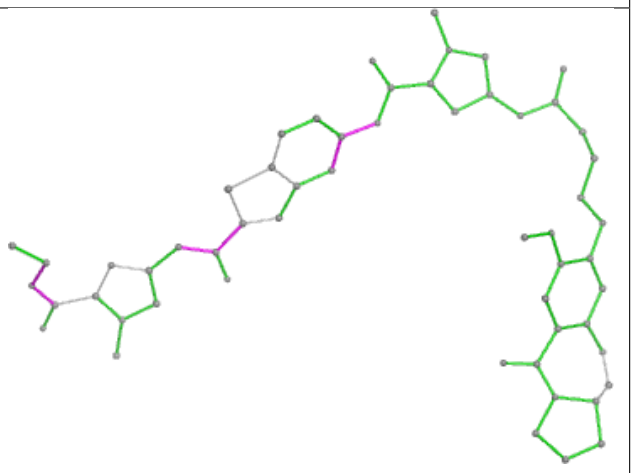
Ligand A1H1R CCC 301



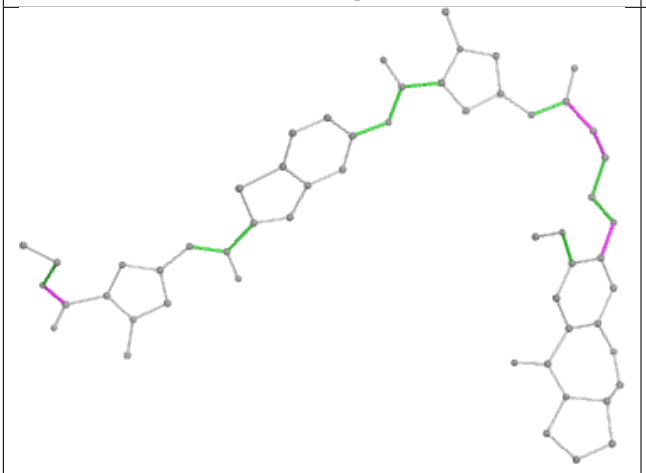
Ligand A1H1R AAA 302



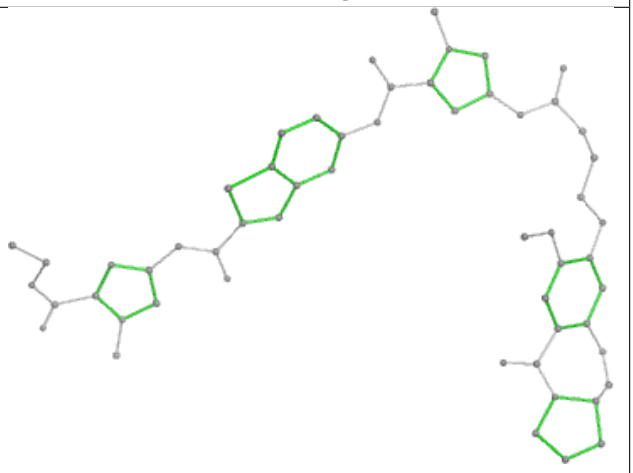
Bond lengths



Bond angles

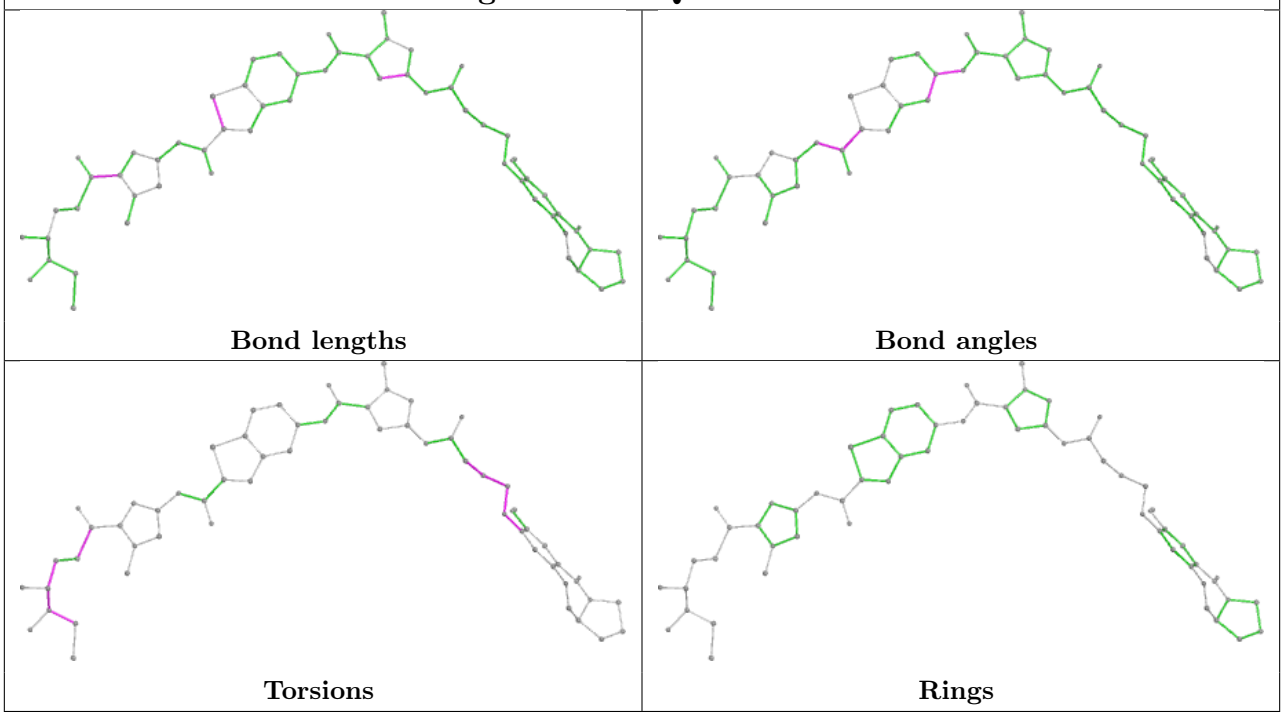


Torsions

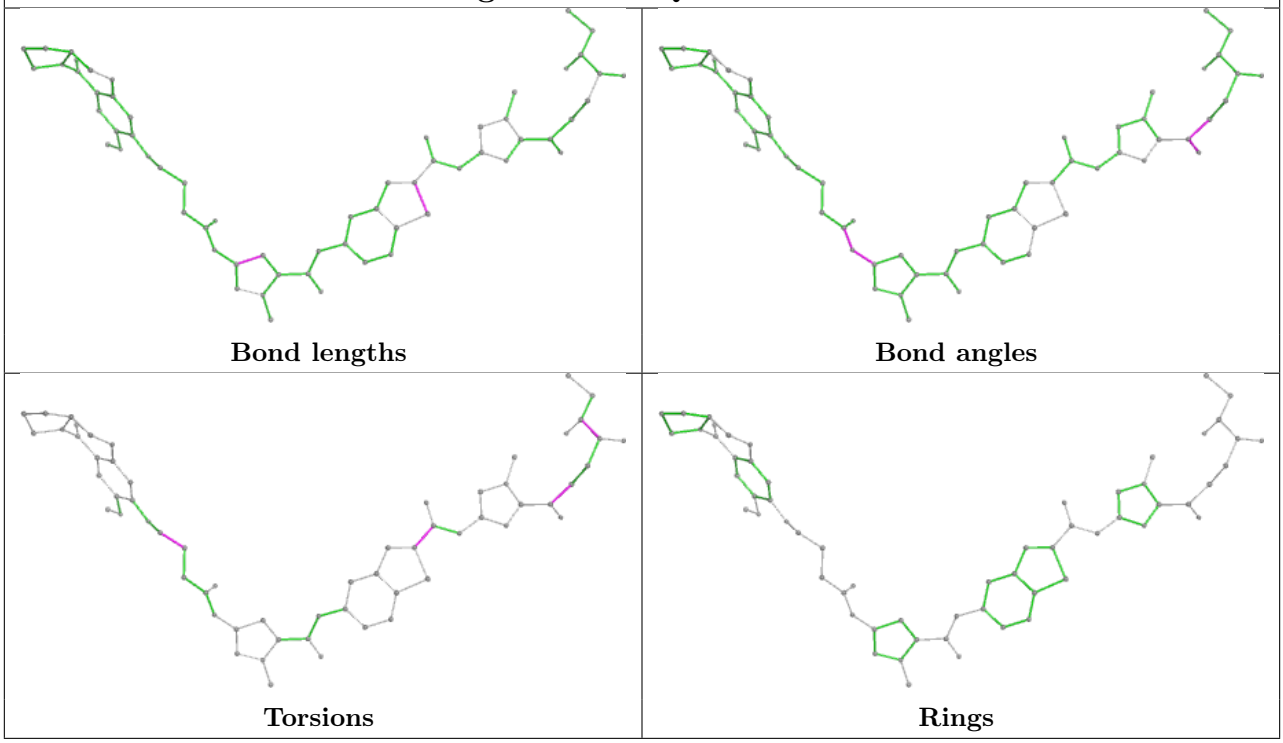


Rings

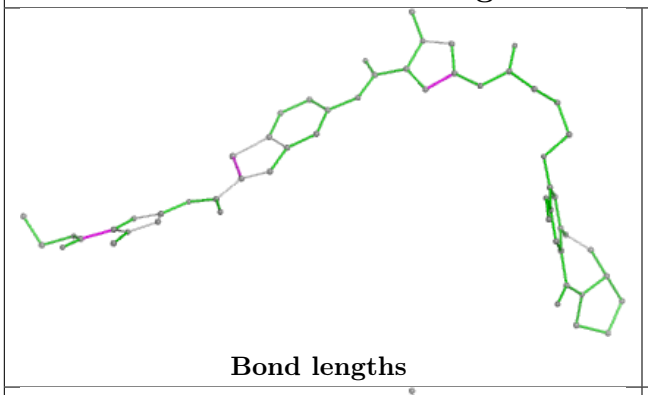
Ligand A1H1Q BBB 302



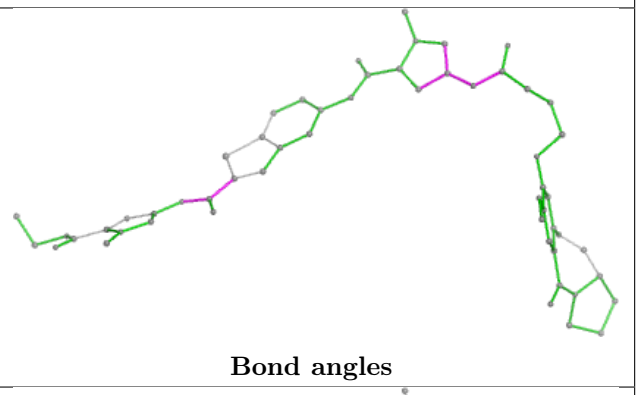
Ligand A1H1Q CCC 302



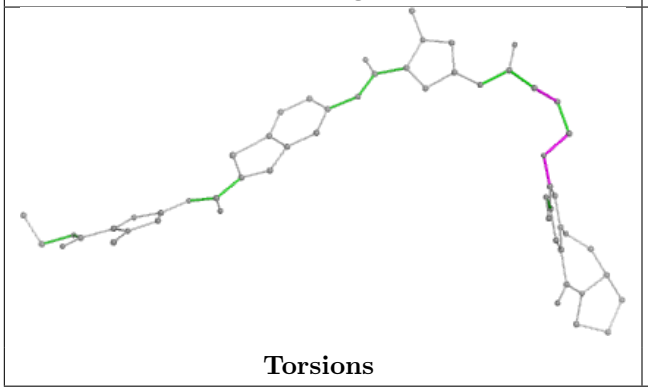
Ligand A1H1R AAA 301



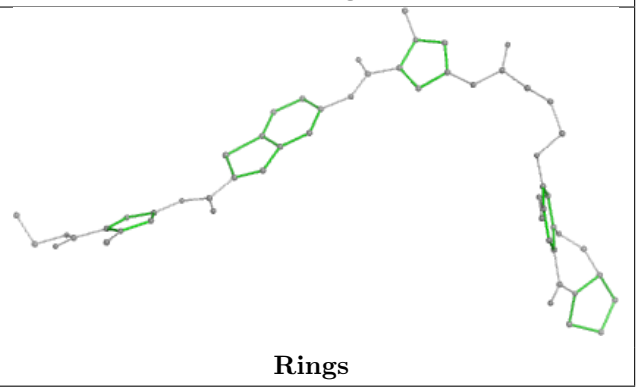
Bond lengths



Bond angles

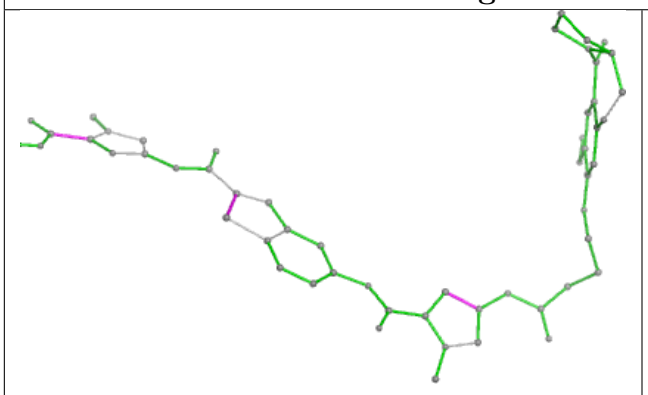


Torsions

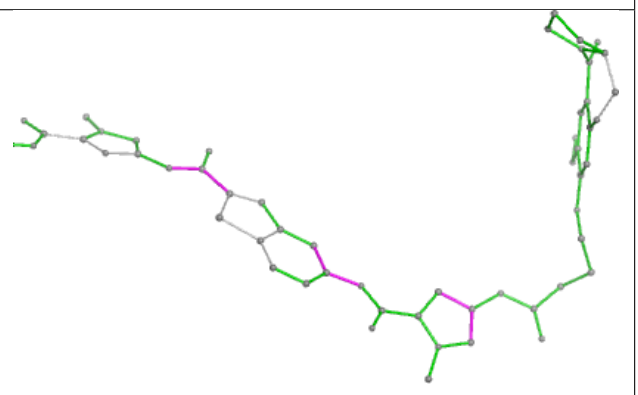


Rings

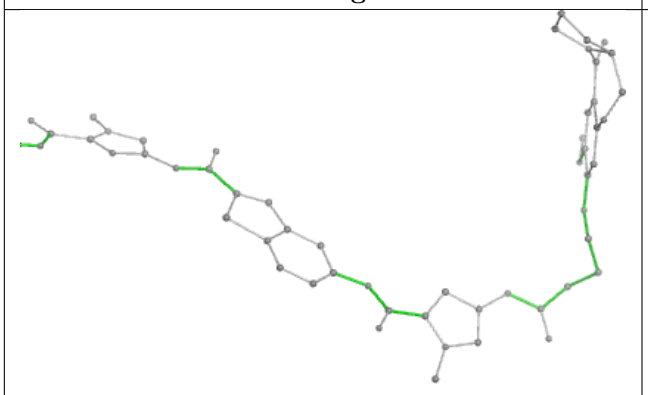
Ligand A1H1R BBB 301



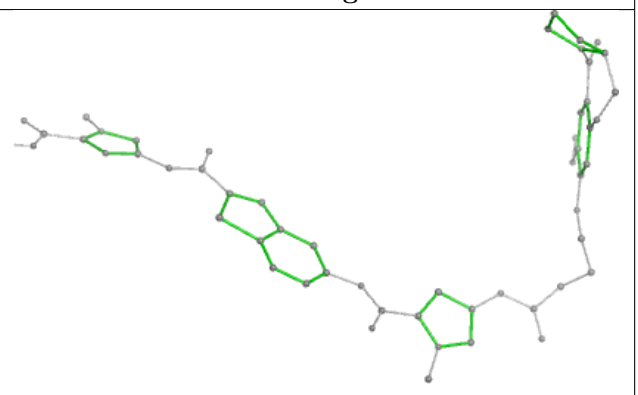
Bond lengths



Bond angles



Torsions



Rings

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, 95^{th} 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	AAA	216/224 (96%)	0.54	11 (5%)	34	34	27, 63, 106, 133	6 (2%)
1	BBB	217/224 (96%)	0.43	5 (2%)	61	59	26, 64, 97, 128	4 (1%)
1	CCC	217/224 (96%)	0.58	11 (5%)	34	34	28, 71, 115, 135	4 (1%)
All	All	650/672 (96%)	0.52	27 (4%)	41	40	26, 67, 109, 135	14 (2%)

The worst 5 of 27 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	215	ALA	3.5
1	BBB	215	ALA	3.4
1	AAA	0	GLY	3.2
1	AAA	191	MET	3.2
1	AAA	143	ALA	3.0

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

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

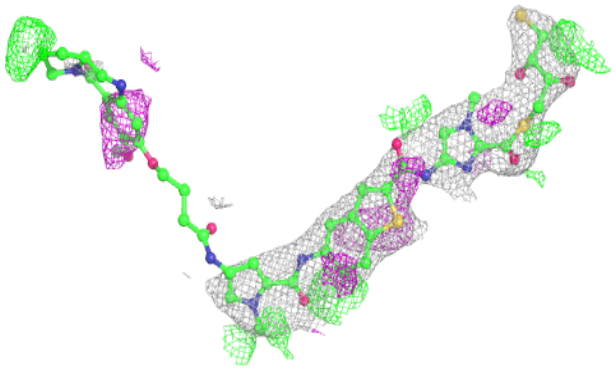
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

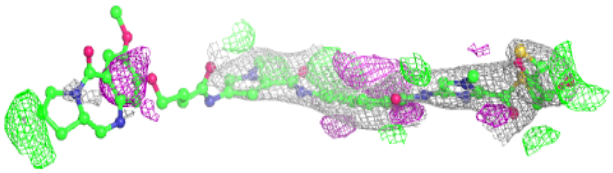
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	DTV	AAA	304	8/8	0.74	0.27	105,118,125,126	0
3	A1H1Q	CCC	302	61/61	0.76	0.25	90,119,205,209	0
2	A1H1R	CCC	301	56/56	0.86	0.20	67,124,137,146	0
2	A1H1R	BBB	301	56/56	0.87	0.18	66,94,173,174	0
2	A1H1R	AAA	302	56/56	0.87	0.21	62,81,188,190	0
3	A1H1Q	BBB	302	61/61	0.89	0.17	60,97,147,149	0
4	DTV	BBB	303	8/8	0.90	0.19	116,120,125,136	0
4	DTV	AAA	303	8/8	0.93	0.19	112,117,123,123	0
2	A1H1R	AAA	301	56/56	0.95	0.09	49,61,69,70	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 A1H1Q CCC 302:

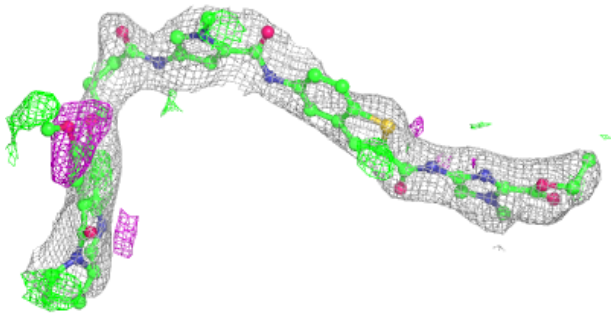
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

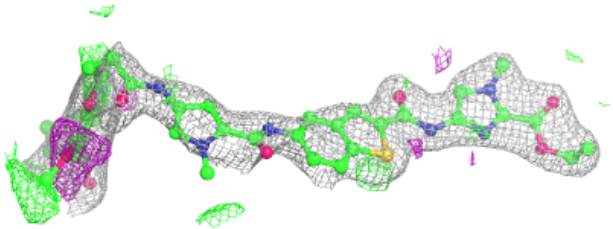


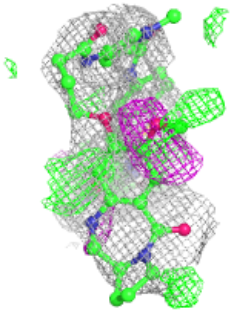


Electron density around A1H1R CCC 301:

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

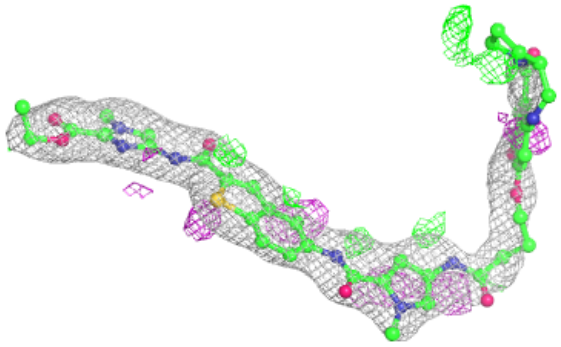


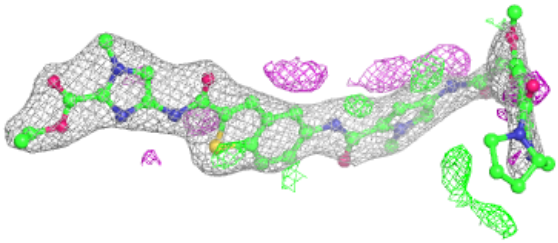


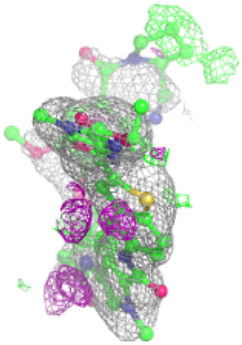


Electron density around A1H1R BBB 301:

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

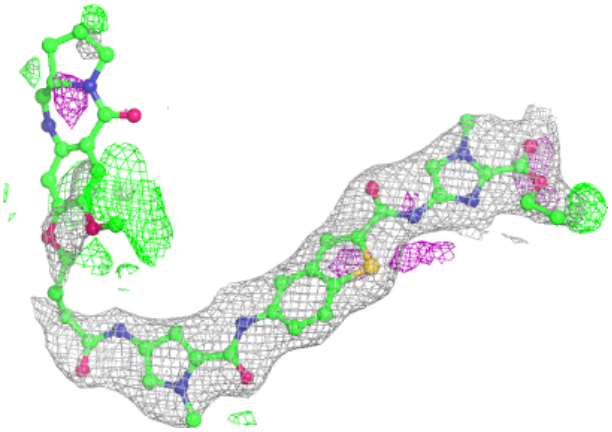


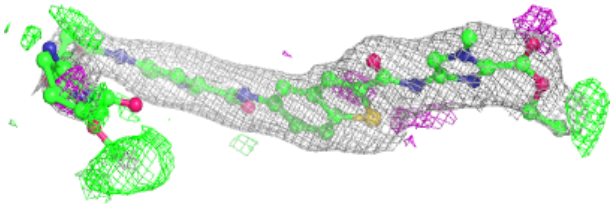


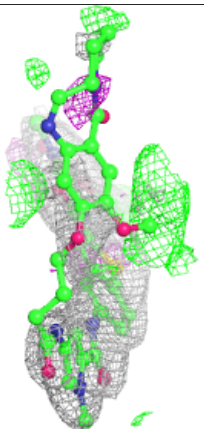


Electron density around A1H1R AAA 302:

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

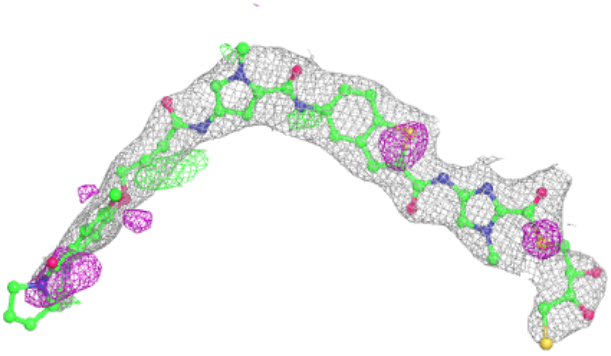


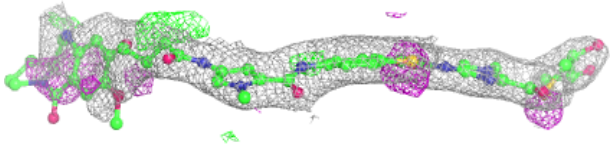


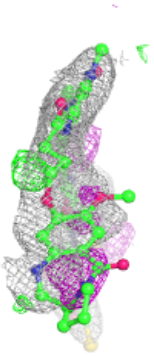


Electron density around A1H1Q BBB 302:

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

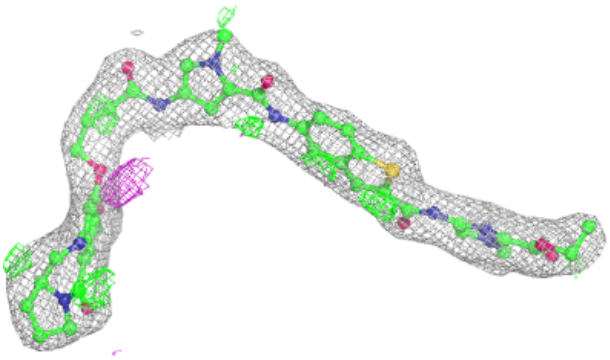


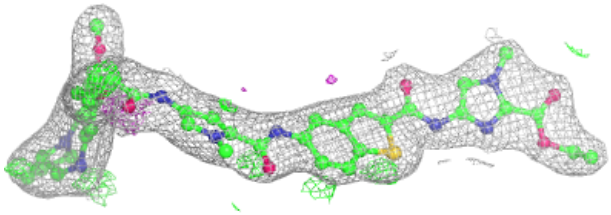


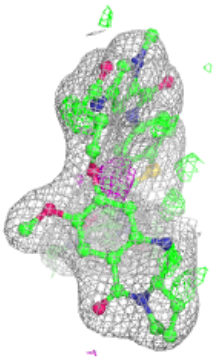


Electron density around A1H1R AAA 301:

$2mF_o$-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

There are no such residues in this entry.