



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:45 PM UTC

PDB ID : 8RKY / pdb_00008rky
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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

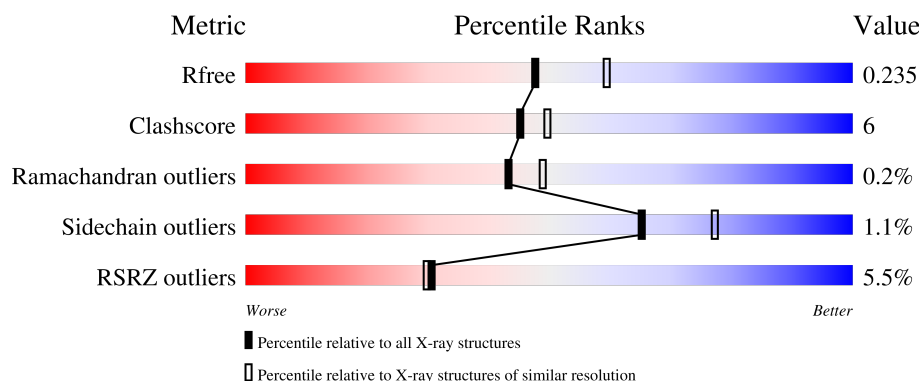
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	8975 (2.20-2.16)
Clashscore	190562	9786 (2.20-2.16)
Ramachandran outliers	187476	9664 (2.20-2.16)
Sidechain outliers	187428	9664 (2.20-2.16)
RSRZ outliers	180081	8979 (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 $\leq 5\%$. 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	AAA	224	7% 87% 9% ••
1	BBB	224	3% 87% 9% •
1	CCC	224	7% 88% 9% •

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

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.

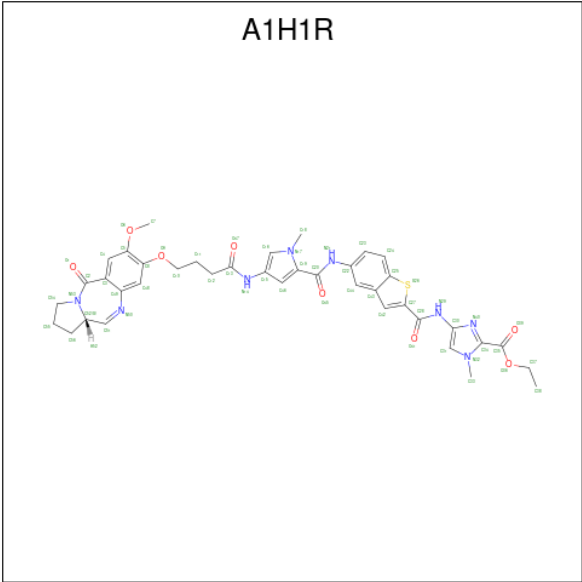
- Molecule 1 is a protein called Albicidin resistance protein.

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:

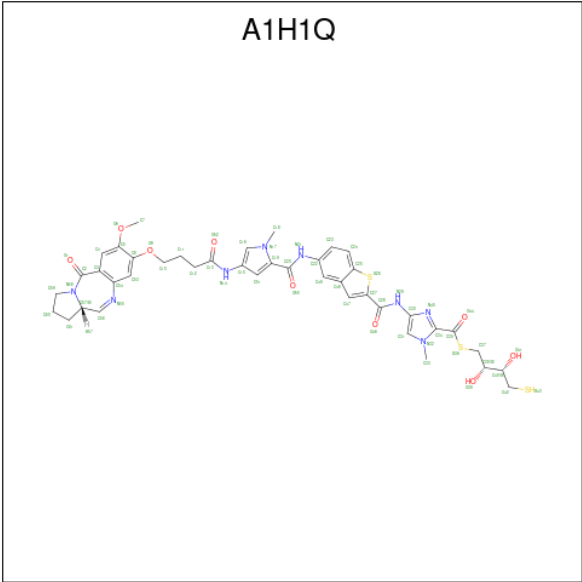
Chain	Residue	Modelled	Actual	Comment	Reference
BBB	0	GLY	-	expression tag	UNP Q8KRS7
BBB	222	GLY	-	expression tag	UNP Q8KRS7
BBB	223	SER	-	expression tag	UNP Q8KRS7
CCC	0	GLY	-	expression tag	UNP Q8KRS7
CCC	222	GLY	-	expression tag	UNP Q8KRS7
CCC	223	SER	-	expression tag	UNP Q8KRS7
AAA	0	GLY	-	expression 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 (CCD ID: A1H1R) (formula: C₃₉H₄₀N₈O₈S) (labeled as "Ligand of Interest" by depositor).



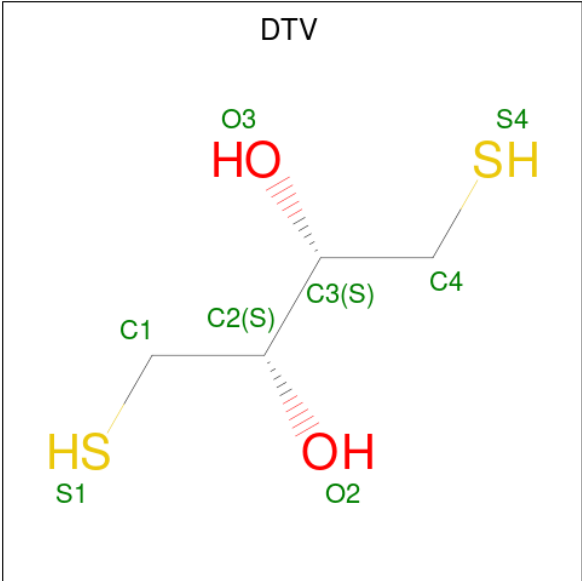
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	BBB	1	Total	C	N	O	S	0	0
			56	39	8	8	1		
2	CCC	1	Total	C	N	O	S	0	0
			56	39	8	8	1		
2	AAA	1	Total	C	N	O	S	0	0
			56	39	8	8	1		
2	AAA	1	Total	C	N	O	S	0	0
			56	39	8	8	1		

- 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 (CCD ID: A1H1Q) (formula: C₄₁H₄₄N₈O₉S₃) (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 (CCD ID: DTV) (formula: C₄H₁₀O₂S₂).



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	0	0
			8	4	2	2		
4	AAA	1	Total	C	O	S	0	0
			8	4	2	2		

- Molecule 5 is water.

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

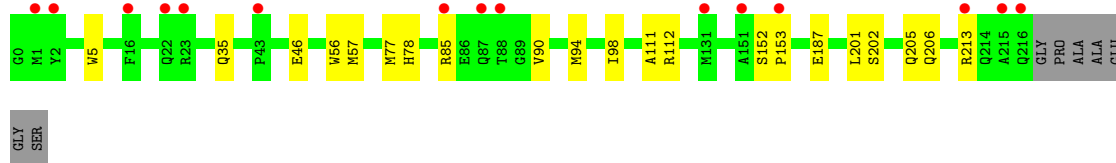
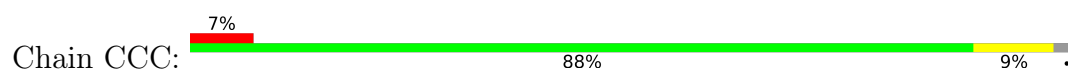
3 Residue-property plots [i](#)

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.

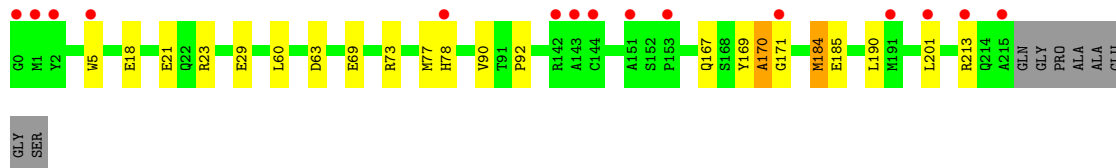
- Molecule 1: Albicidin resistance protein



- Molecule 1: Albicidin resistance protein



- Molecule 1: Albicidin resistance protein



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ 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	3278 reflections (5.04%)	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	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	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.*

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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DTV, A1H1Q, 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	0.94	0/1882	1.44	2/2544 (0.1%)
1	BBB	0.95	0/1871	1.43	2/2528 (0.1%)
1	CCC	0.96	0/1871	1.45	0/2528
All	All	0.95	0/5624	1.44	4/7600 (0.1%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	AAA	170	ALA	CA-C-O	-5.70	115.22	121.89
1	BBB	17	ALA	CA-C-N	5.46	128.46	120.71
1	BBB	17	ALA	C-N-CA	5.46	128.46	120.71
1	AAA	170	ALA	N-CA-C	-5.12	103.17	110.59

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	18	0
2	AAA	112	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	BBB	56	0	0	0	0
2	CCC	56	0	0	3	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
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	66	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.

All (66) 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:BBB:78[B]:HIS:HE2	1:BBB:90:VAL:C	1.83	0.85
1:CCC:90:VAL:HA	1:CCC:94:MET:HE2	1.58	0.85
1:CCC:56:TRP:HH2	1:CCC:94:MET:HE3	1.43	0.84
1:AAA:171:GLY:HA3	5:AAA:444:HOH:O	1.80	0.81
1:BBB:191[B]:MET:HE2	1:BBB:196:MET:HB3	1.64	0.77
1:BBB:191[A]:MET:SD	4:BBB:303:DTV:S1	2.85	0.74
1:AAA:190:LEU:O	4:AAA:304:DTV:O3	2.09	0.68
1:CCC:90:VAL:HA	1:CCC:94:MET:CE	2.25	0.66
1:AAA:69:GLU:O	1:AAA:73[A]:ARG:HG2	1.96	0.66
1:AAA:73[B]:ARG:HG3	1:AAA:73[B]:ARG:HH21	1.61	0.65
1:BBB:212:MET:HA	1:BBB:212:MET:HE2	1.80	0.64
1:BBB:112:ARG:HD3	1:AAA:21:GLU:CB	2.30	0.61
2:AAA:302:A1H1R:C37	2:AAA:302:A1H1R:N40	2.64	0.61
1:AAA:73[B]:ARG:HG3	1:AAA:73[B]:ARG:NH2	2.15	0.60
1:BBB:189:HIS:CD2	1:AAA:29:GLU:OE1	2.59	0.55
1:BBB:106:LYS:HE3	4:BBB:303:DTV:H4C1	1.89	0.55
1:CCC:205:GLN:O	3:CCC:302:A1H1Q:O52	2.25	0.54
1:AAA:73[B]:ARG:HH21	1:AAA:73[B]:ARG:CG	2.20	0.53
1:BBB:112:ARG:HD3	1:AAA:21:GLU:HB2	1.90	0.53
1:AAA:78[B]:HIS:CD2	1:AAA:90:VAL:O	2.61	0.53
3:BBB:302:A1H1Q:C33	3:BBB:302:A1H1Q:S36	2.96	0.53
1:BBB:112:ARG:HD3	1:AAA:21:GLU:HB3	1.91	0.53
1:CCC:56:TRP:CD1	1:CCC:57[A]:MET:HE2	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:184[A]:MET:HE1	1:AAA:201:LEU:HD11	1.91	0.51
1:CCC:112[B]:ARG:NH1	1:CCC:187:GLU:OE2	2.41	0.50
1:BBB:182:TYR:HB2	1:CCC:112[A]:ARG:HD3	1.94	0.49
1:AAA:184[A]:MET:HG3	1:AAA:185:GLU:N	2.21	0.49
1:BBB:178:GLN:HG3	1:CCC:111:ALA:HB1	1.94	0.49
1:BBB:191[B]:MET:HE1	1:BBB:201:LEU:HB2	1.94	0.48
3:CCC:302:A1H1Q:S36	3:CCC:302:A1H1Q:O41	2.71	0.48
1:CCC:57[A]:MET:HE3	1:CCC:98:ILE:HG22	1.94	0.48
1:AAA:184[A]:MET:HE3	1:AAA:184[A]:MET:HB2	1.64	0.48
2:AAA:302:A1H1R:N29	4:AAA:304:DTV:S1	2.87	0.48
1:CCC:56:TRP:CH2	1:CCC:94:MET:HE3	2.34	0.48
1:AAA:169:TYR:OH	4:AAA:304:DTV:S1	2.71	0.47
1:BBB:133:TRP:CG	3:BBB:302:A1H1Q:S36	3.07	0.47
1:CCC:206:GLN:HG2	3:CCC:302:A1H1Q:C8	2.44	0.47
1:AAA:69:GLU:O	1:AAA:73[A]:ARG:CG	2.60	0.47
1:BBB:18:GLU:O	1:BBB:23:ARG:NH2	2.48	0.46
1:AAA:23:ARG:HD2	1:AAA:63:ASP:CG	2.41	0.46
1:AAA:184[A]:MET:HE1	1:AAA:201:LEU:CD1	2.46	0.45
1:CCC:78[B]:HIS:HE1	2:CCC:301:A1H1R:C24	2.30	0.44
1:CCC:201:LEU:O	1:CCC:205:GLN:HG2	2.17	0.44
1:CCC:202:SER:O	1:CCC:206:GLN:HG3	2.18	0.44
1:AAA:18:GLU:O	1:AAA:23:ARG:NH2	2.50	0.44
1:AAA:18:GLU:O	1:AAA:18:GLU:HG2	2.18	0.44
1:AAA:78[B]:HIS:HE1	1:AAA:92:PRO:CA	2.31	0.44
1:BBB:178:GLN:HE22	3:BBB:302:A1H1Q:C18	2.32	0.43
1:AAA:78[B]:HIS:CE1	1:AAA:92:PRO:N	2.86	0.43
1:AAA:171:GLY:CA	5:AAA:444:HOH:O	2.52	0.42
1:CCC:57[A]:MET:HE1	2:CCC:301:A1H1R:C31	2.49	0.42
1:AAA:5:TRP:CD2	1:AAA:77:MET:HG2	2.55	0.42
3:BBB:302:A1H1Q:C37	4:BBB:303:DTV:S4	3.08	0.42
1:CCC:5:TRP:CD2	1:CCC:77:MET:HG2	2.54	0.41
1:BBB:5:TRP:CD2	1:BBB:77:MET:HG2	2.55	0.41
1:AAA:167:GLN:O	1:AAA:170:ALA:O	2.38	0.41
1:CCC:35:GLN:HE22	2:CCC:301:A1H1R:C51	2.33	0.41
1:CCC:152:SER:OG	1:CCC:153:PRO:HD2	2.21	0.41
2:AAA:302:A1H1R:S26	4:AAA:304:DTV:S1	3.08	0.41
1:AAA:73[A]:ARG:HG2	1:AAA:73[A]:ARG:H	1.64	0.41
2:AAA:302:A1H1R:O41	2:AAA:302:A1H1R:C31	2.69	0.41
1:BBB:13:VAL:O	1:BBB:15:PRO:HD3	2.21	0.41
1:AAA:60:LEU:HD12	1:AAA:60:LEU:HA	1.91	0.41
2:AAA:301:A1H1R:O41	2:AAA:301:A1H1R:C31	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:214:GLN:O	1:BBB:215:ALA:HB3	2.21	0.41

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%)	24	25
1	CCC	219/224 (98%)	217 (99%)	2 (1%)	0	100	100
All	All	658/672 (98%)	650 (99%)	7 (1%)	1 (0%)	43	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%)	55	68
1	BBB	186/185 (100%)	185 (100%)	1 (0%)	81	89

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	CCC	186/185 (100%)	183 (98%)	3 (2%)	55	68
All	All	559/555 (101%)	552 (99%)	7 (1%)	65	74

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	BBB	46	GLU
1	CCC	46	GLU
1	CCC	85	ARG
1	CCC	213	ARG
1	AAA	184[A]	MET
1	AAA	184[B]	MET
1	AAA	213	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	-	58,62,62	0.26	0	71,89,89	0.61	2 (2%)
3	A1H1Q	CCC	302	-	60,67,67	0.31	0	70,96,96	0.77	1 (1%)
4	DTV	AAA	304	-	7,7,7	0.48	0	4,8,8	0.50	0
4	DTV	BBB	303	-	7,7,7	0.31	0	4,8,8	0.31	0
2	A1H1R	BBB	301	-	58,62,62	0.24	0	71,89,89	0.64	2 (2%)
3	A1H1Q	BBB	302	-	60,67,67	0.27	0	70,96,96	0.93	3 (4%)
2	A1H1R	AAA	302	-	58,62,62	0.37	0	71,89,89	0.98	4 (5%)
2	A1H1R	AAA	301	-	58,62,62	0.25	0	71,89,89	0.68	2 (2%)
4	DTV	AAA	303	-	7,7,7	0.34	0	4,8,8	0.39	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
2	A1H1R	CCC	301	-	-	3/36/59/59	0/6/7/7
3	A1H1Q	CCC	302	-	-	10/41/67/67	0/6/7/7
4	DTV	AAA	304	-	-	6/8/8/8	-
4	DTV	BBB	303	-	-	4/8/8/8	-
2	A1H1R	BBB	301	-	-	2/36/59/59	0/6/7/7
3	A1H1Q	BBB	302	-	-	17/41/67/67	0/6/7/7
2	A1H1R	AAA	302	-	-	9/36/59/59	0/6/7/7
2	A1H1R	AAA	301	-	-	6/36/59/59	0/6/7/7
4	DTV	AAA	303	-	-	6/8/8/8	-

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	BBB	302	A1H1Q	C20-C19-N17	4.78	127.97	122.78
2	AAA	302	A1H1R	N29-C30-N40	3.85	128.12	118.64
3	CCC	302	A1H1Q	C20-C19-N17	3.73	126.83	122.78
2	AAA	302	A1H1R	C37-O36-C35	3.02	121.71	116.49
3	BBB	302	A1H1Q	N29-C30-N45	2.65	125.17	118.64
2	CCC	301	A1H1R	N29-C30-N40	2.57	124.97	118.64
2	AAA	302	A1H1R	C27-C28-N29	2.55	118.17	115.55
2	AAA	301	A1H1R	N29-C30-N40	2.39	124.52	118.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AAA	302	A1H1R	C28-C27-S26	2.32	119.14	116.08
2	AAA	301	A1H1R	C27-C28-N29	2.27	117.89	115.55
2	CCC	301	A1H1R	C27-C28-N29	2.08	117.69	115.55
3	BBB	302	A1H1Q	C51-C19-C20	-2.08	124.23	129.54
2	BBB	301	A1H1R	C28-C27-S26	2.02	118.74	116.08
2	BBB	301	A1H1R	C27-C28-N29	2.02	117.63	115.55

There are no chirality outliers.

All (63) 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
3	BBB	302	A1H1Q	S36-C37-C38-C40
3	BBB	302	A1H1Q	C37-C38-C40-O41
3	BBB	302	A1H1Q	O39-C38-C40-C42
3	BBB	302	A1H1Q	C38-C40-C42-S43
3	BBB	302	A1H1Q	O41-C40-C42-S43
3	CCC	302	A1H1Q	C16-C15-N14-C13
3	CCC	302	A1H1Q	C51-C15-N14-C13
3	CCC	302	A1H1Q	C34-C35-S36-C37
3	CCC	302	A1H1Q	O44-C35-S36-C37
3	CCC	302	A1H1Q	O39-C38-C40-C42
4	BBB	303	DTV	S1-C1-C2-O2
4	BBB	303	DTV	S1-C1-C2-C3
4	BBB	303	DTV	C2-C3-C4-S4
4	BBB	303	DTV	O3-C3-C4-S4
4	AAA	303	DTV	C1-C2-C3-O3
4	AAA	303	DTV	C1-C2-C3-C4
4	AAA	303	DTV	O2-C2-C3-C4
4	AAA	304	DTV	C1-C2-C3-O3
4	AAA	304	DTV	C1-C2-C3-C4
4	AAA	304	DTV	O2-C2-C3-C4
4	AAA	304	DTV	C2-C3-C4-S4
4	AAA	304	DTV	O3-C3-C4-S4
2	AAA	302	A1H1R	O39-C35-O36-C37
3	CCC	302	A1H1Q	O9-C10-C11-C12
2	CCC	301	A1H1R	O9-C10-C11-C12
3	BBB	302	A1H1Q	O9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
3	BBB	302	A1H1Q	C11-C10-O9-C8
2	AAA	301	A1H1R	C5-C8-O9-C10
3	BBB	302	A1H1Q	C53-C8-O9-C10
3	BBB	302	A1H1Q	O39-C38-C40-O41
3	CCC	302	A1H1Q	O39-C38-C40-O41
4	AAA	303	DTV	O2-C2-C3-O3
4	AAA	304	DTV	O2-C2-C3-O3
3	BBB	302	A1H1Q	C5-C8-O9-C10
3	BBB	302	A1H1Q	C10-C11-C12-C13
2	AAA	302	A1H1R	C48-C8-O9-C10
2	AAA	301	A1H1R	C48-C8-O9-C10
3	BBB	302	A1H1Q	S26-C27-C28-N29
3	BBB	302	A1H1Q	C37-C38-C40-C42
2	BBB	301	A1H1R	S26-C27-C28-N29
3	BBB	302	A1H1Q	S36-C37-C38-O39
4	AAA	303	DTV	S1-C1-C2-O2
2	AAA	301	A1H1R	C42-C27-C28-N29
3	CCC	302	A1H1Q	C47-C27-C28-N29
2	AAA	302	A1H1R	C42-C27-C28-N29
4	AAA	303	DTV	S1-C1-C2-C3
3	CCC	302	A1H1Q	N32-C34-C35-O44
2	AAA	302	A1H1R	C11-C12-C13-O47
2	CCC	301	A1H1R	S26-C27-C28-N29
2	AAA	301	A1H1R	S26-C27-C28-N29
3	CCC	302	A1H1Q	S26-C27-C28-N29
2	AAA	302	A1H1R	C5-C8-O9-C10
2	BBB	301	A1H1R	C42-C27-C28-N29
2	CCC	301	A1H1R	C42-C27-C28-N29
3	BBB	302	A1H1Q	C47-C27-C28-N29
2	AAA	302	A1H1R	S26-C27-C28-N29
2	AAA	302	A1H1R	C11-C12-C13-N14
2	AAA	301	A1H1R	C11-C10-O9-C8

There are no ring outliers.

7 monomers are involved in 19 short contacts:

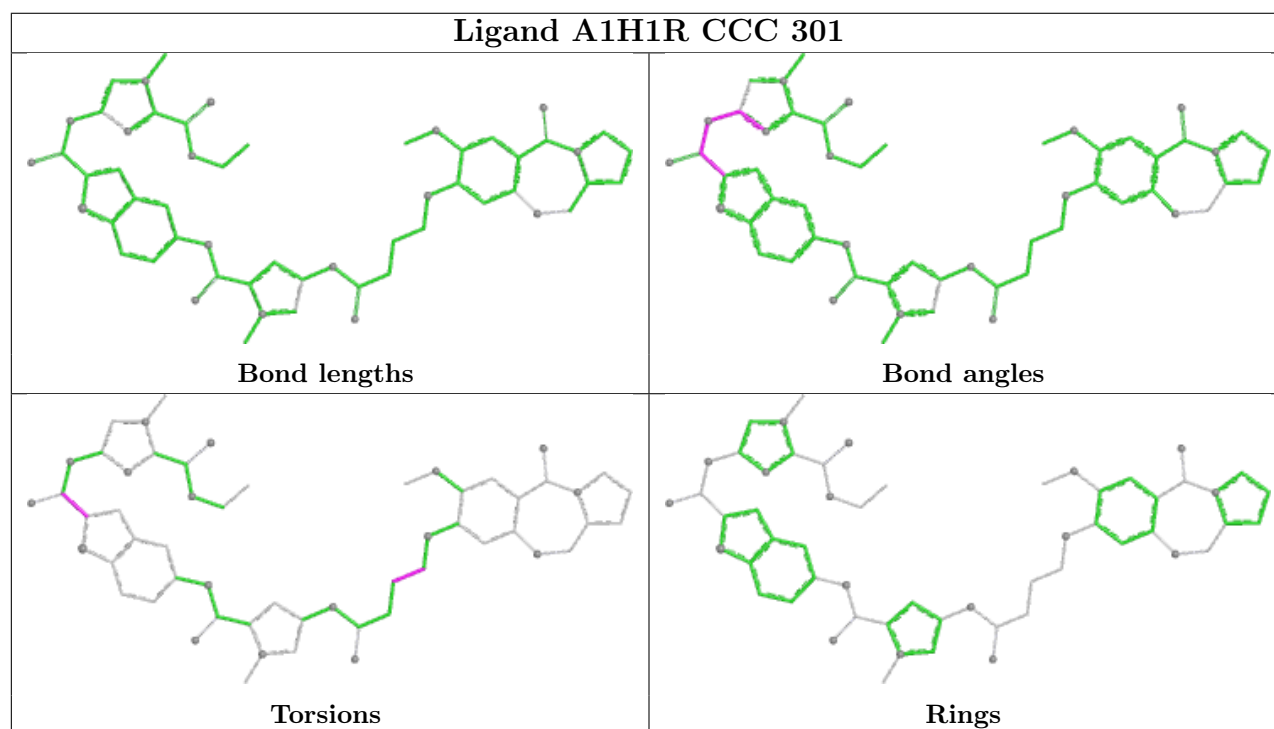
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	CCC	301	A1H1R	3	0
3	CCC	302	A1H1Q	3	0
4	AAA	304	DTV	4	0
4	BBB	303	DTV	3	0
3	BBB	302	A1H1Q	4	0

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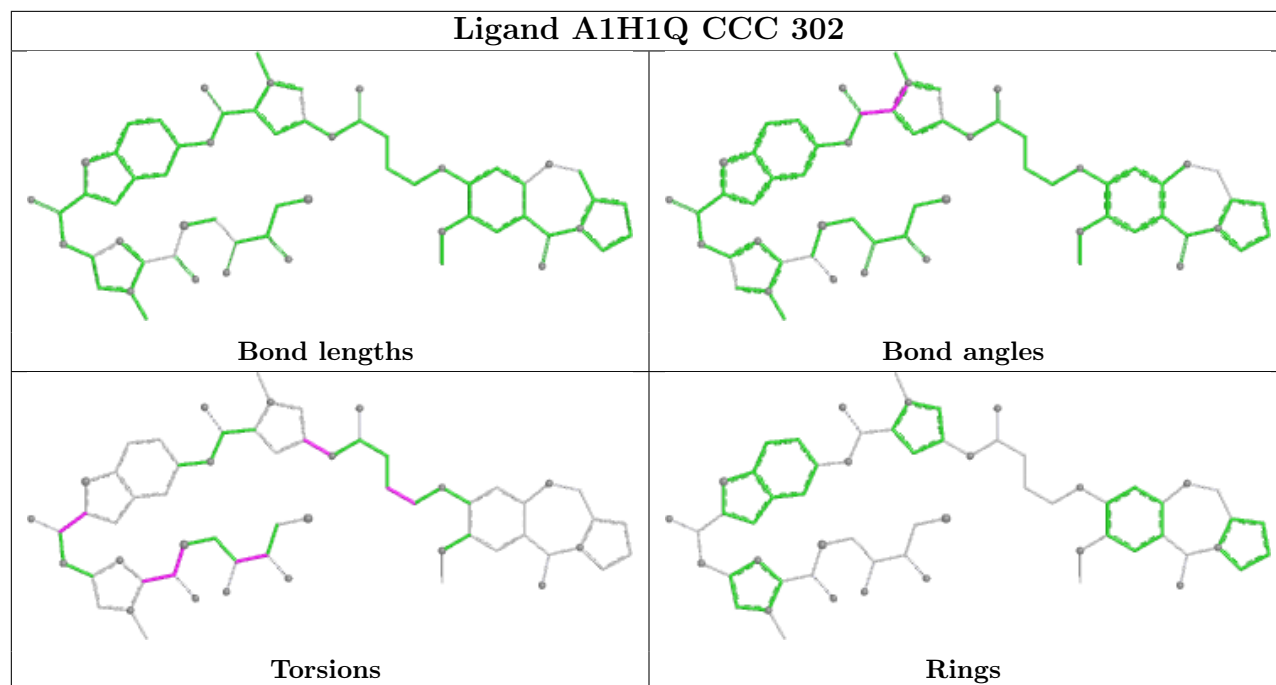
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	AAA	302	A1H1R	4	0
2	AAA	301	A1H1R	1	0

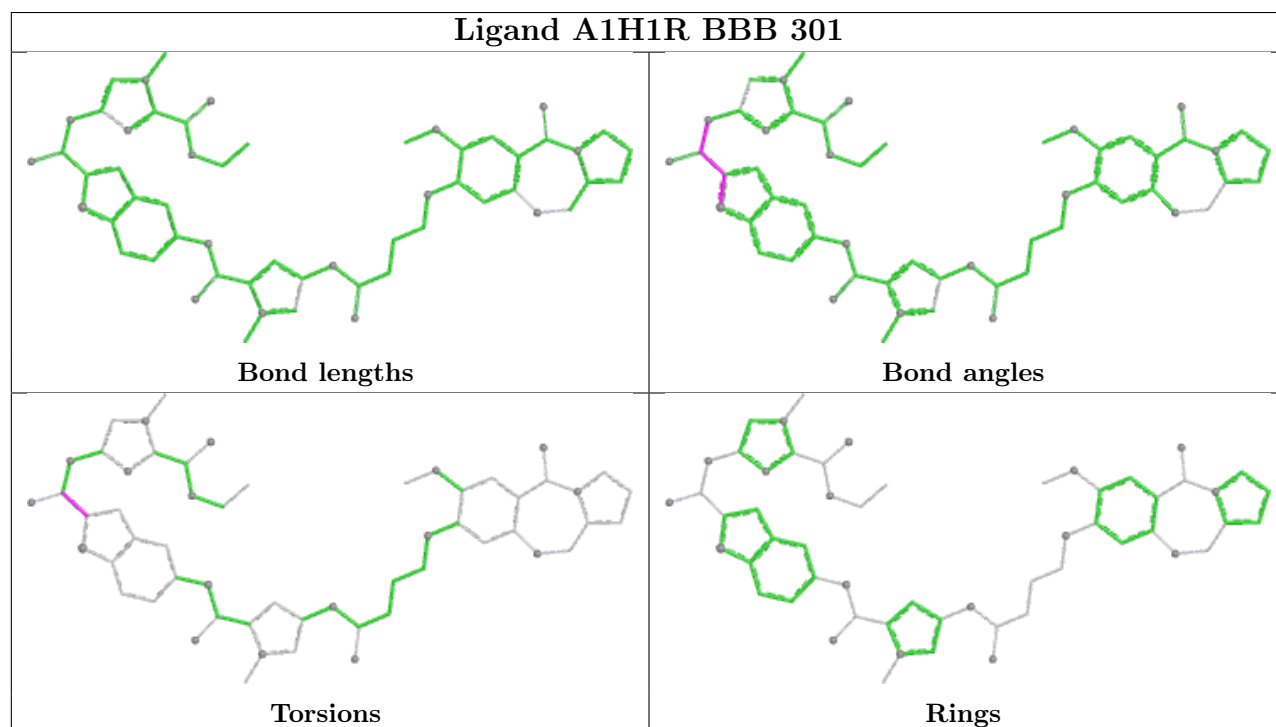
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



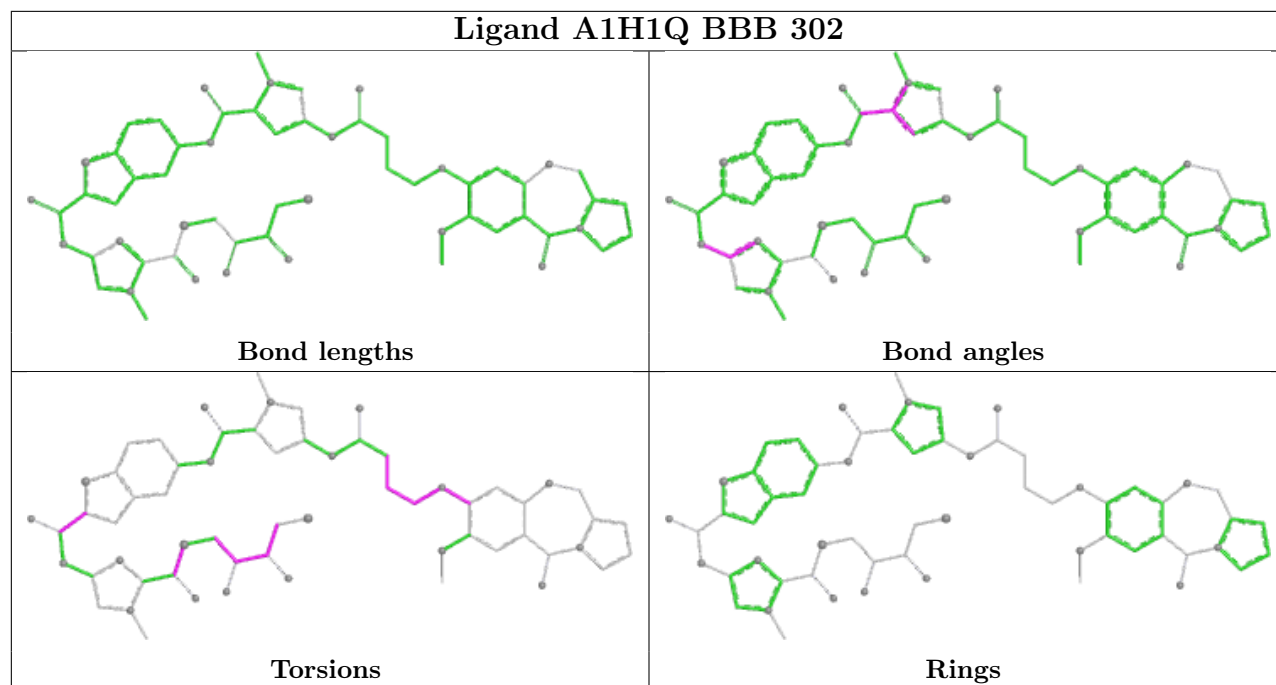
Ligand A1H1Q CCC 302



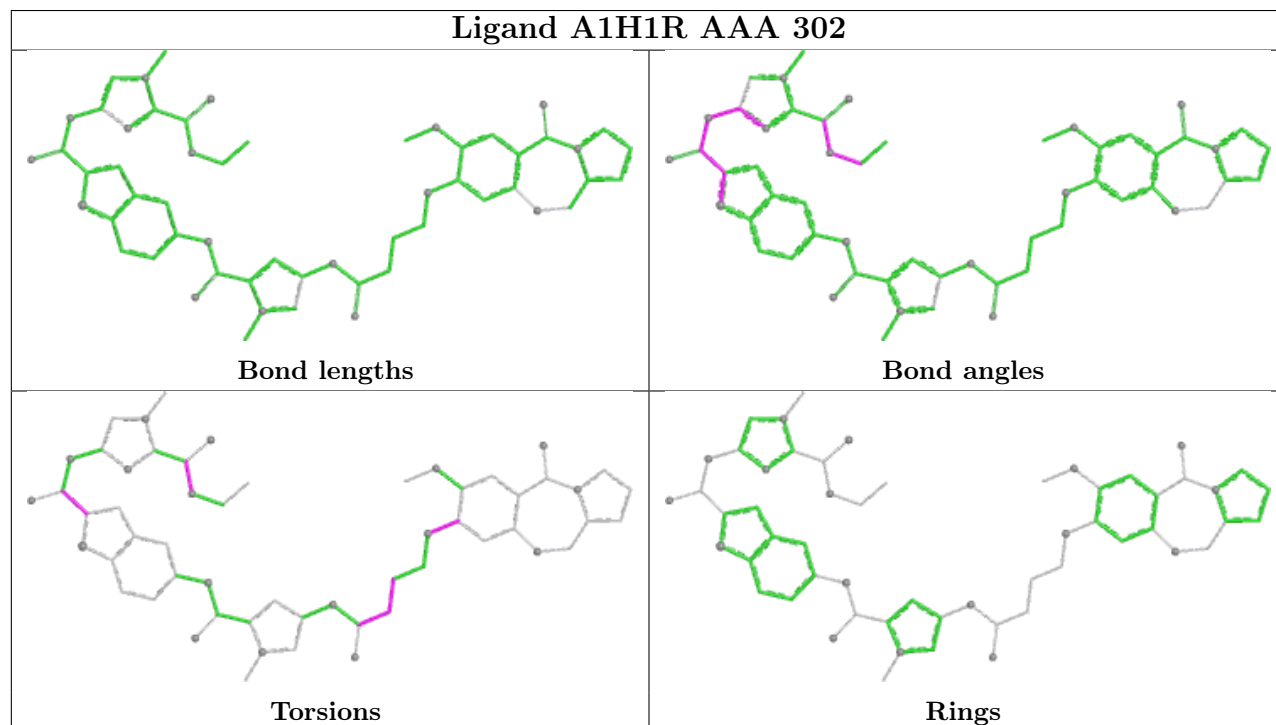
Ligand A1H1R BBB 301

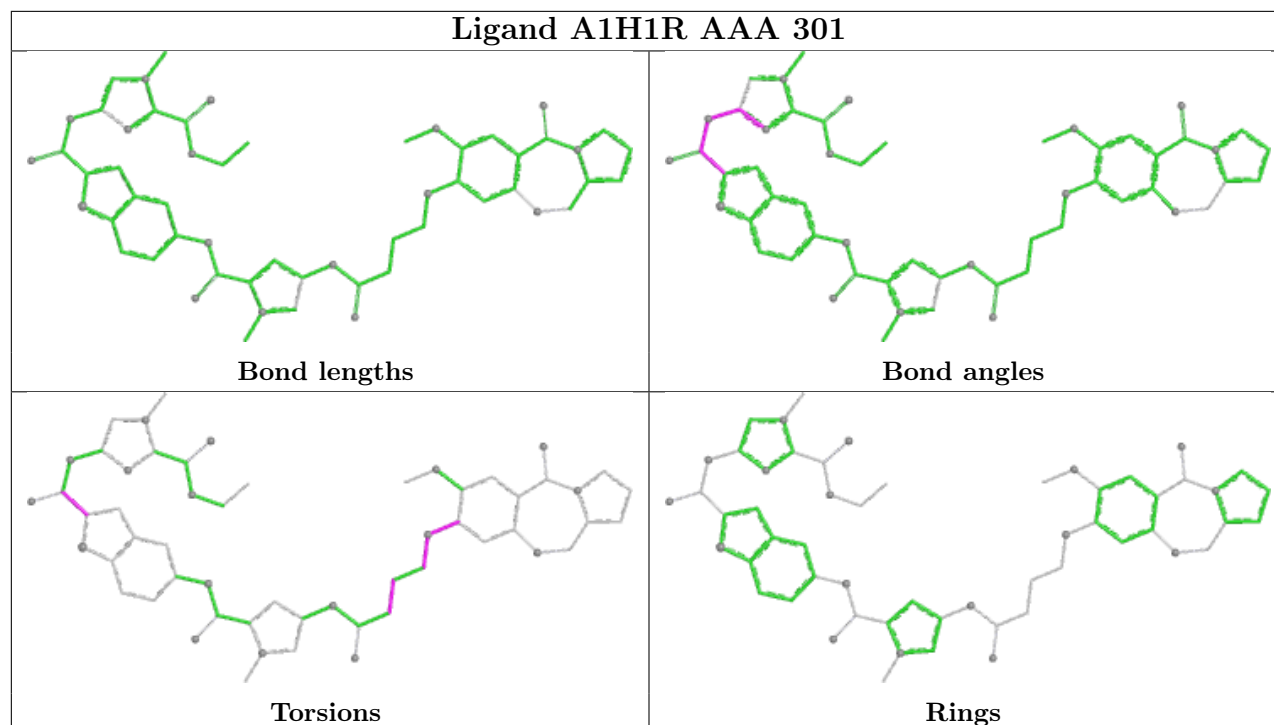


Ligand A1H1Q BBB 302



Ligand A1H1R AAA 302





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	AAA	216/224 (96%)	0.65	15 (6%) 23 22	27, 63, 106, 133	6 (2%)
1	BBB	217/224 (96%)	0.53	6 (2%) 55 54	26, 64, 97, 128	4 (1%)
1	CCC	217/224 (96%)	0.69	15 (6%) 23 22	28, 71, 115, 135	4 (1%)
All	All	650/672 (96%)	0.62	36 (5%) 30 30	26, 67, 109, 135	14 (2%)

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	215	ALA	3.7
1	BBB	215	ALA	3.6
1	AAA	0	GLY	3.4
1	AAA	191	MET	3.3
1	AAA	143	ALA	3.2
1	CCC	215	ALA	2.9
1	CCC	131	MET	2.8
1	BBB	13	VAL	2.8
1	CCC	216	GLN	2.8
1	CCC	16	PHE	2.7
1	AAA	151	ALA	2.7
1	AAA	171	GLY	2.7
1	CCC	2	TYR	2.6
1	BBB	213	ARG	2.5
1	BBB	197	THR	2.4
1	BBB	131	MET	2.4
1	AAA	213	ARG	2.4
1	CCC	153	PRO	2.4
1	CCC	87	GLN	2.3
1	AAA	78[A]	HIS	2.2
1	CCC	23	ARG	2.2
1	CCC	85	ARG	2.2
1	AAA	2	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	CCC	213	ARG	2.2
1	AAA	5	TRP	2.2
1	AAA	153	PRO	2.1
1	CCC	22	GLN	2.1
1	AAA	142	ARG	2.1
1	AAA	201	LEU	2.1
1	CCC	151	ALA	2.1
1	AAA	144	CYS	2.1
1	BBB	145	ARG	2.1
1	CCC	88	THR	2.1
1	CCC	43	PRO	2.0
1	CCC	1	MET	2.0
1	AAA	1	MET	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

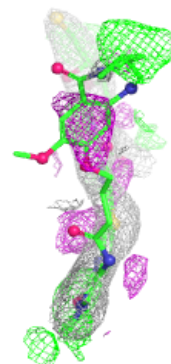
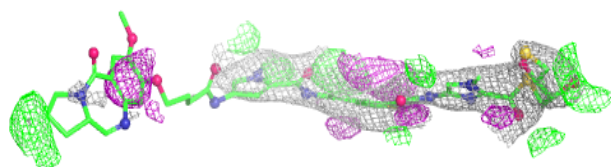
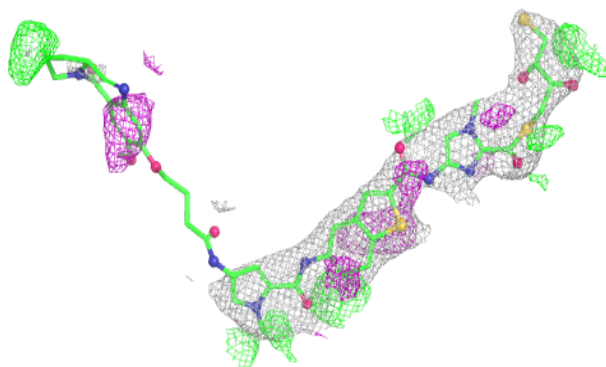
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	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.

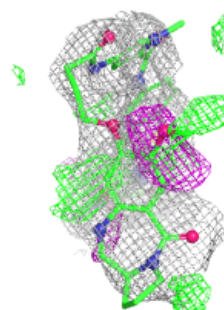
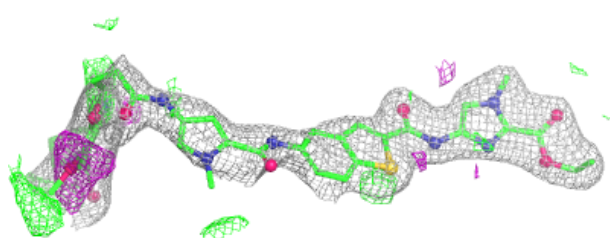
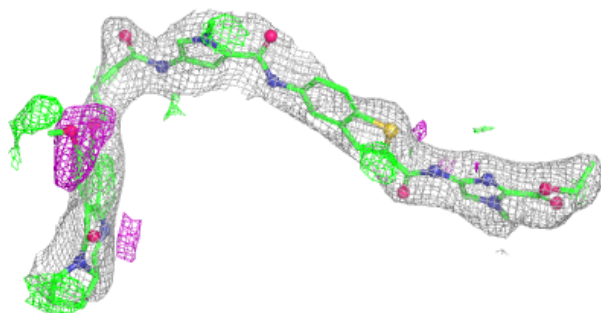
Electron density around A1H1Q CCC 302:

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

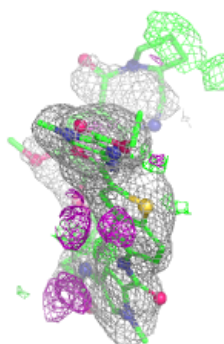
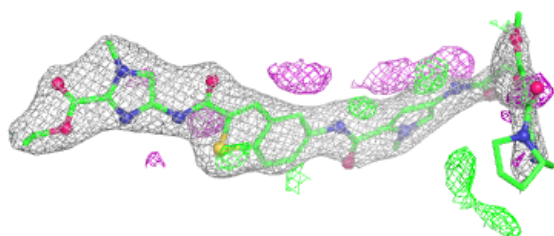
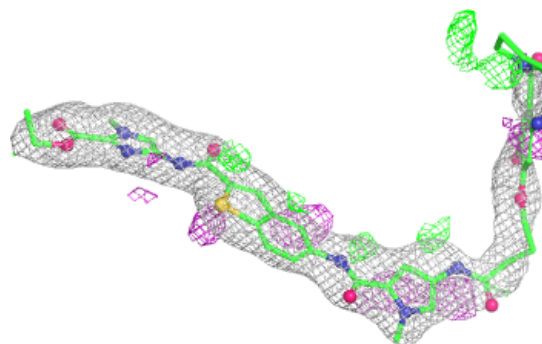


Electron density around A1H1R CCC 301:

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

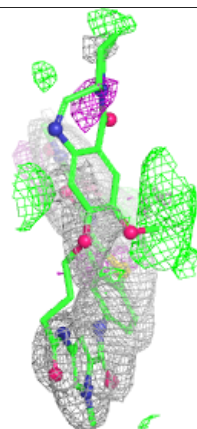
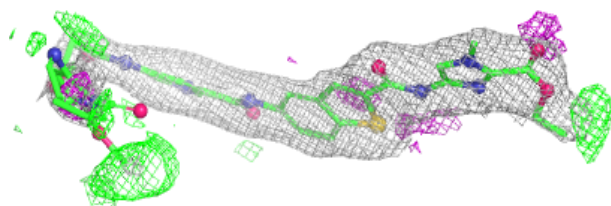
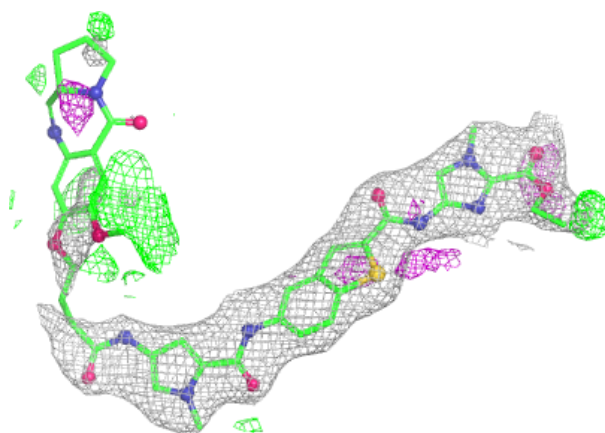
**Electron density around A1H1R BBB 301:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

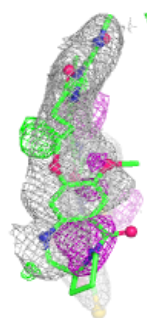
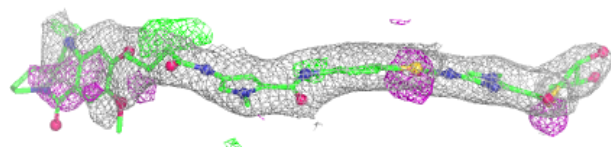
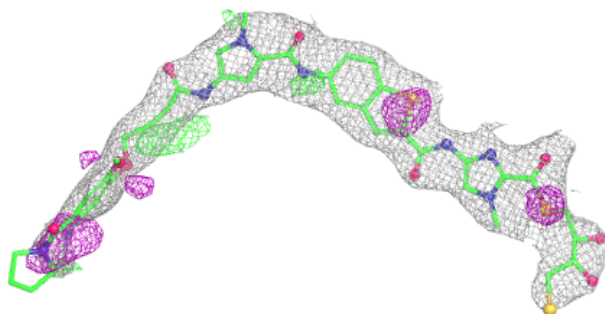


Electron density around A1H1R AAA 302:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

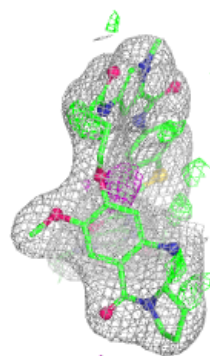
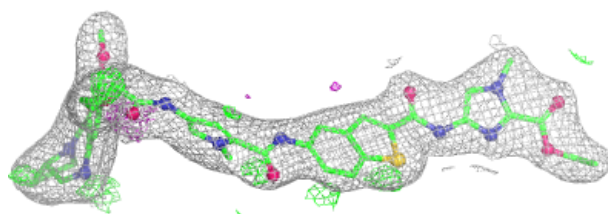
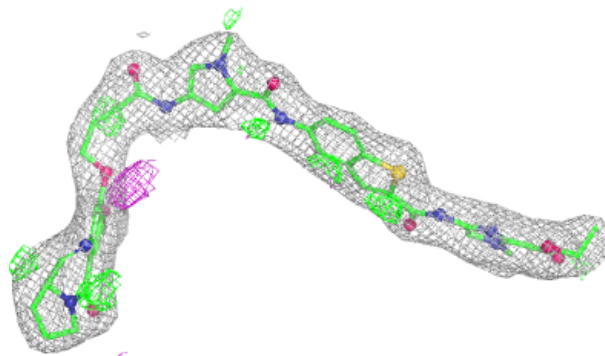
**Electron density around A1H1Q BBB 302:**

$2mF_o-DF_c$ (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.