



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 2, 2024 – 04:07 PM EDT

PDB ID : 8UIW
Title : yjdB riboswitch from *R. gouvreauii* in complex with chelerythrine bound to Fab BL3-6 S97N
Authors : Krochmal, D.; Lewicka, A.; Piccirilli, J.A.
Deposited on : 2023-10-10
Resolution : 2.77 Å (reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36.1

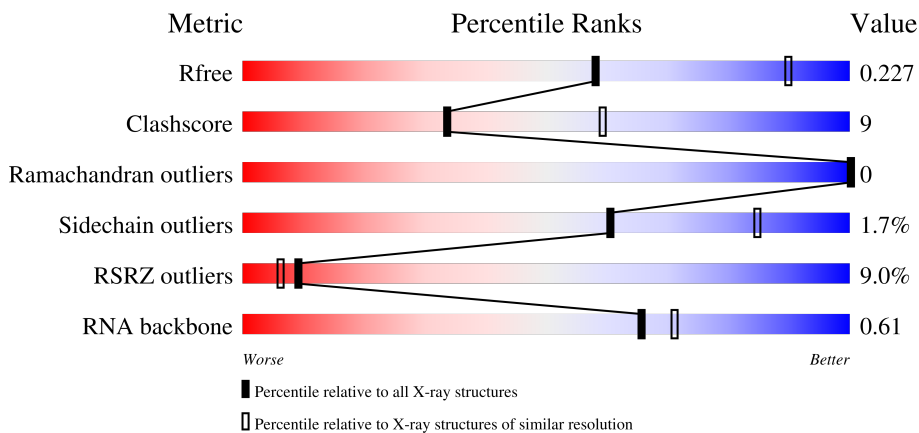
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.77 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	4107 (2.80-2.76)
Clashscore	141614	4575 (2.80-2.76)
Ramachandran outliers	138981	4487 (2.80-2.76)
Sidechain outliers	138945	4489 (2.80-2.76)
RSRZ outliers	127900	4027 (2.80-2.76)
RNA backbone	3102	1092 (3.06-2.50)

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 $\leq 5\%$. 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	N	128	 60% 30% 5% 5%
1	R	128	 61% 32% 7%
2	A	233	 16% 76% 20%
2	H	233	 3% 85% 12%

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Mol	Chain	Length	Quality of chain
3	B	215	
3	L	215	

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	MG	R	204	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 12051 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 RNA chain called yjdB RNA (*R. gausvreauii*).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	N	122	Total 2604	C 1162	N 465	O 853	P 124	0	0	0
1	R	128	Total 2732	C 1220	N 489	O 893	P 130	0	0	0

- Molecule 2 is a protein called Fab BL3-6 S97N heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	A	225	Total 1678	C 1055	N 287	O 330	S 6	0	0	0
2	H	225	Total 1678	C 1055	N 287	O 330	S 6	0	0	0

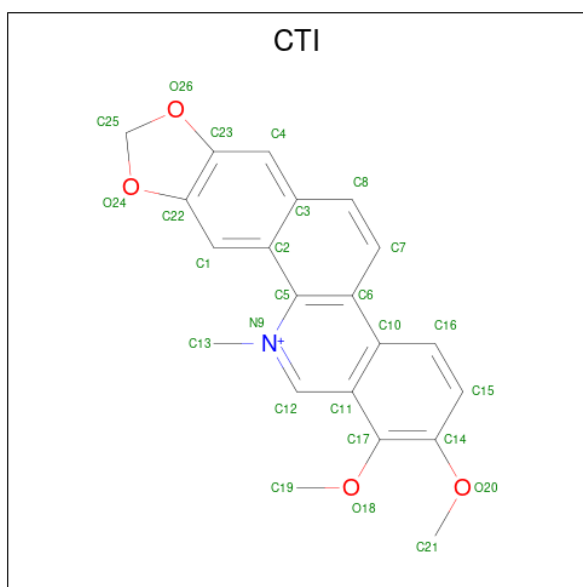
- Molecule 3 is a protein called Fab BL3-6 S97N light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	B	215	Total 1645	C 1026	N 276	O 337	S 6	0	0	0
3	L	215	Total 1645	C 1026	N 276	O 337	S 6	0	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	N	1	Total 1 Mg 1	0	0
4	R	4	Total 4 Mg 4	0	0

- Molecule 5 is 1,2-dimethoxy-12-methyl[1,3]benzodioxolo[5,6-c]phenanthridin-12-ium (three-letter code: CTI) (formula: C₂₁H₁₈NO₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	N	1	Total	C	N	O	0	0
			26	21	1	4		
5	R	1	Total	C	N	O	0	0
			26	21	1	4		

- Molecule 6 is OSMIUM ION (three-letter code: OS) (formula: Os).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	2	Total	Os	0	0
			2	2		
6	L	2	Total	Os	0	0
			2	2		

- Molecule 7 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	L	1	Total	K	0	0
			1	1		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	N	3	Total	O	0	0
			3	3		
8	R	1	Total	O	0	0
			1	1		

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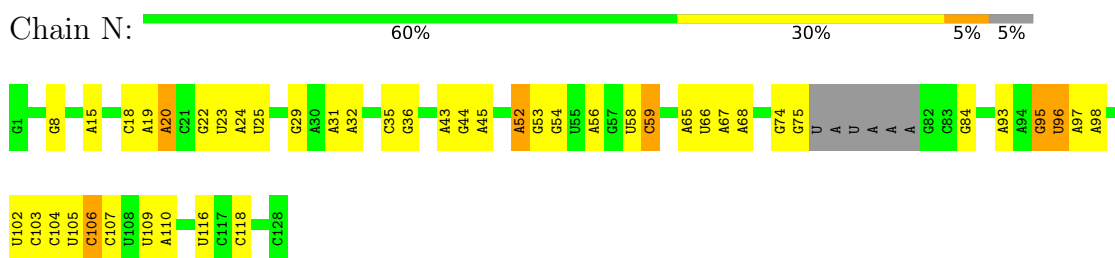
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total O 1 1	0	0
8	H	1	Total O 1 1	0	0
8	L	1	Total O 1 1	0	0

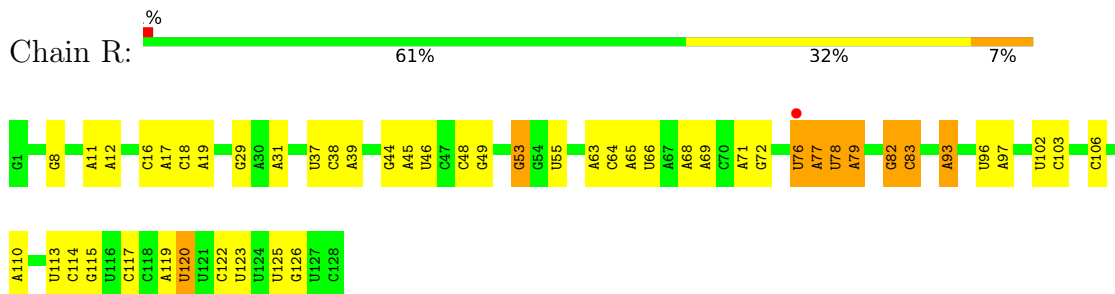
3 Residue-property plots [i](#)

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.

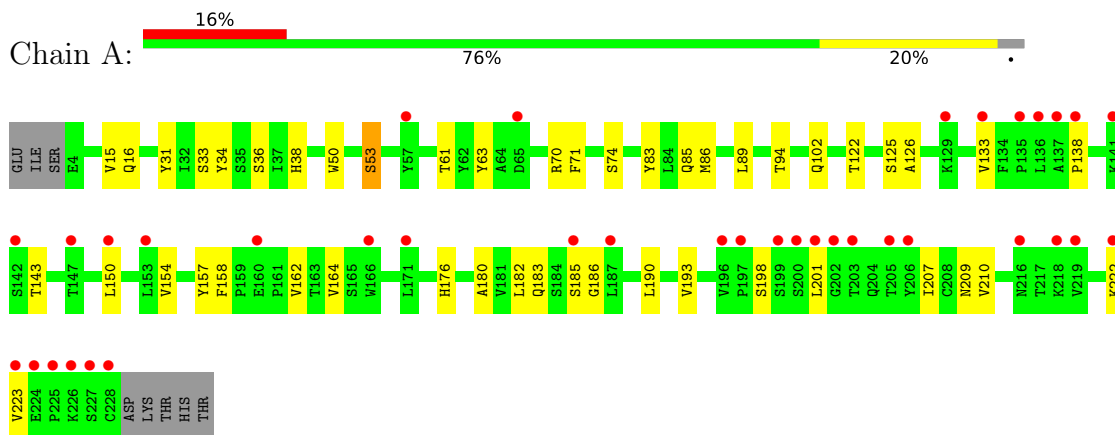
- Molecule 1: yjdF RNA (R. gauvreauii)



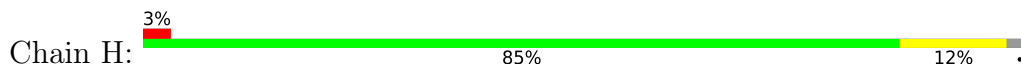
- Molecule 1: yjdF RNA (R. gauvreauii)

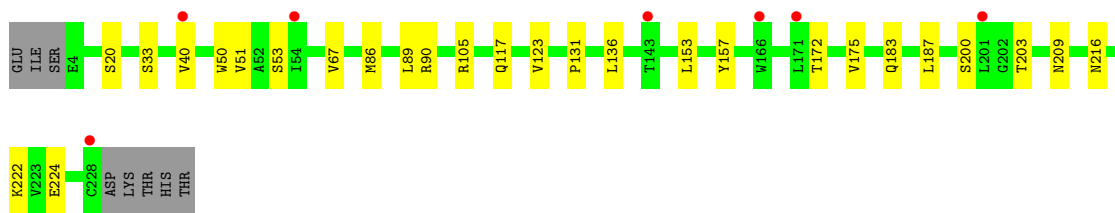


- Molecule 2: Fab BL3-6 S97N heavy chain

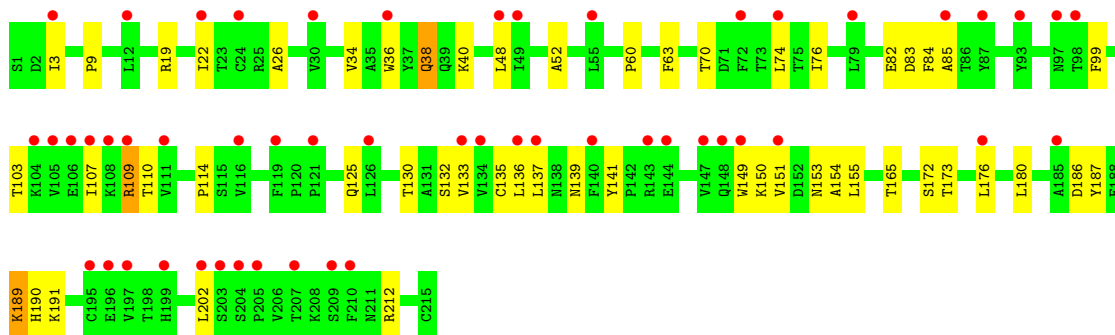
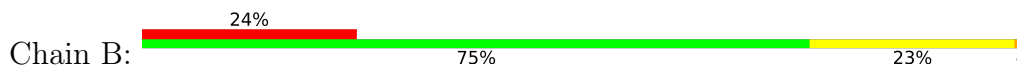


- Molecule 2: Fab BL3-6 S97N heavy chain

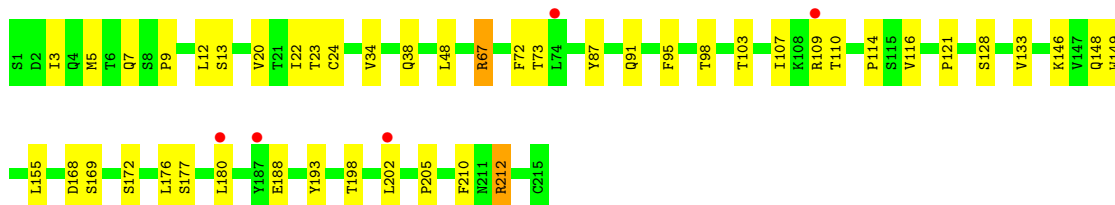
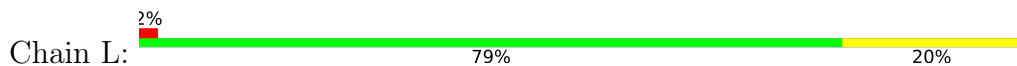




● Molecule 3: Fab BL3-6 S97N light chain



● Molecule 3: Fab BL3-6 S97N light chain



4 Data and refinement statistics i

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	65.79Å 77.44Å 95.85Å 87.19° 88.43° 88.05°	Depositor
Resolution (Å)	95.70 – 2.77 95.70 – 2.77	Depositor EDS
% Data completeness (in resolution range)	90.2 (95.70-2.77) 89.6 (95.70-2.77)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.30 (at 2.77Å)	Xtrriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.211 , 0.231 0.209 , 0.227	Depositor DCC
R_{free} test set	2003 reflections (4.46%)	wwPDB-VP
Wilson B-factor (Å ²)	90.2	Xtrriage
Anisotropy	0.347	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 70.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.018 for h,-k,-l	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12051	wwPDB-VP
Average B, all atoms (Å ²)	131.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.89% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: OS, MG, K, GTP, CTI

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	N	0.45	0/2875	1.00	0/4473
1	R	0.44	0/3020	0.96	0/4701
2	A	0.49	0/1719	0.74	0/2339
2	H	0.32	0/1719	0.57	0/2339
3	B	0.52	0/1680	0.73	0/2280
3	L	0.40	0/1680	0.63	0/2280
All	All	0.44	0/12693	0.84	0/18412

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	N	2604	0	1315	24	0
1	R	2732	0	1378	35	0
2	A	1678	0	1637	28	0
2	H	1678	0	1637	16	0
3	B	1645	0	1595	48	0
3	L	1645	0	1594	30	0
4	N	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	R	4	0	0	0	0
5	N	26	0	18	4	0
5	R	26	0	18	5	0
6	B	2	0	0	0	0
6	L	2	0	0	0	0
7	L	1	0	0	0	0
8	A	1	0	0	0	0
8	H	1	0	0	0	0
8	L	1	0	0	1	0
8	N	3	0	0	1	0
8	R	1	0	0	0	0
All	All	12051	0	9192	181	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 9.

All (181) 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)
5:R:205:CTI:H1	5:R:205:CTI:C13	2.13	0.79
3:B:109:ARG:HG3	3:B:141:TYR:CD2	2.18	0.78
2:A:126:ALA:HB3	2:A:158:PHE:CE2	2.24	0.73
2:A:50:TRP:HB2	3:B:99:PHE:HE1	1.55	0.71
3:B:107:ILE:HD12	3:B:107:ILE:H	1.57	0.70
2:H:117:GLN:N	2:H:117:GLN:OE1	2.23	0.68
1:R:29:G:H2'	1:R:31:A:H62	1.59	0.67
2:A:133:VAL:HG22	2:A:154:VAL:HG12	1.80	0.64
1:N:29:G:H2'	1:N:31:A:H62	1.62	0.63
3:B:186:ASP:HA	3:B:189:LYS:HD3	1.80	0.63
5:N:202:CTI:H1	5:N:202:CTI:C13	2.28	0.62
3:B:38:GLN:HB3	3:B:48:LEU:HD11	1.80	0.62
2:H:222:LYS:NZ	2:H:224:GLU:OE1	2.32	0.62
3:B:149:TRP:CB	3:B:180:LEU:HD11	2.29	0.62
2:A:150:LEU:HD13	2:A:223:VAL:HG21	1.80	0.61
2:H:40:VAL:HG22	2:H:50:TRP:HA	1.81	0.61
2:A:16:GLN:OE1	2:A:125:SER:HA	2.00	0.61
3:L:198:THR:HG22	3:L:205:PRO:HB3	1.83	0.61
5:R:205:CTI:H1	5:R:205:CTI:H13B	1.81	0.61
2:A:50:TRP:HZ2	2:A:53:SER:HB3	1.67	0.60
5:R:205:CTI:H1	5:R:205:CTI:H13A	1.84	0.59
1:R:55:U:H3'	5:R:205:CTI:H21B	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:136:LEU:HD11	2:H:153:LEU:HB2	1.84	0.59
3:B:135:CYS:HB2	3:B:149:TRP:CZ2	2.37	0.59
1:N:23:U:H2'	1:N:24:A:H8	1.69	0.58
2:H:183:GLN:HG2	2:H:187:LEU:O	2.04	0.57
3:B:34:VAL:HG22	3:B:52:ALA:HB2	1.85	0.57
3:L:133:VAL:HG22	3:L:180:LEU:HB3	1.85	0.57
3:B:26:ALA:HB3	3:B:70:THR:HB	1.85	0.57
3:L:146:LYS:HB3	3:L:198:THR:OG1	2.04	0.57
2:A:154:VAL:HG11	2:A:210:VAL:HG11	1.87	0.57
3:B:22:ILE:HD11	3:B:103:THR:HG21	1.85	0.57
3:L:114:PRO:HD2	3:L:202:LEU:HD13	1.85	0.56
3:L:38:GLN:HB2	3:L:48:LEU:HD11	1.87	0.56
1:R:16:C:H2'	1:R:17:A:C8	2.41	0.56
3:L:67:ARG:HG3	3:L:72:PHE:CE1	2.41	0.55
1:R:38:C:H2'	1:R:39:A:H8	1.70	0.55
2:A:94:THR:HG23	2:A:122:THR:HA	1.89	0.55
5:R:205:CTI:C13	5:R:205:CTI:C1	2.84	0.55
1:N:104:C:H2'	1:N:105:U:C6	2.43	0.54
3:B:139:ASN:OD1	3:B:173:THR:HG21	2.07	0.54
3:B:137:LEU:HD22	3:B:176:LEU:HD23	1.90	0.54
1:R:114:C:H2'	1:R:115:G:C8	2.43	0.54
1:N:29:G:OP2	2:H:105:ARG:NH2	2.41	0.54
1:R:113:U:H2'	1:R:114:C:C6	2.43	0.54
1:N:67:A:H2'	1:N:68:A:C8	2.42	0.54
2:H:200:SER:HA	2:H:203:THR:HG22	1.90	0.53
3:L:23:THR:HG22	3:L:73:THR:HG22	1.89	0.53
1:N:67:A:H2'	1:N:68:A:H8	1.74	0.52
1:N:18:C:H5''	1:N:19:A:H5'	1.91	0.52
5:N:202:CTI:H1	5:N:202:CTI:H13A	1.91	0.52
1:N:52:A:H3'	1:N:52:A:OP2	2.10	0.52
3:B:189:LYS:HG3	3:B:190:HIS:ND1	2.25	0.52
1:N:23:U:H2'	1:N:24:A:C8	2.45	0.52
3:B:109:ARG:NH1	3:B:110:THR:OG1	2.43	0.51
1:R:38:C:H2'	1:R:39:A:C8	2.46	0.51
1:R:114:C:H2'	1:R:115:G:H8	1.76	0.51
3:B:151:VAL:O	3:B:154:ALA:HB3	2.11	0.51
3:L:3:ILE:O	3:L:98:THR:HG21	2.10	0.51
3:B:150:LYS:HE2	3:B:155:LEU:HB2	1.92	0.51
3:B:151:VAL:HG12	3:B:190:HIS:HB3	1.93	0.51
3:L:168:ASP:OD1	3:L:169:SER:N	2.43	0.51
1:R:113:U:H2'	1:R:114:C:H6	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:22:ILE:HG22	3:B:74:LEU:HB3	1.91	0.50
3:B:109:ARG:HD2	3:B:141:TYR:HB2	1.93	0.50
3:L:109:ARG:HD2	3:L:172:SER:O	2.12	0.50
3:L:109:ARG:HG2	3:L:110:THR:N	2.26	0.50
1:R:18:C:H5''	1:R:19:A:H5'	1.94	0.49
1:R:82:G:H2'	1:R:83:C:C6	2.48	0.49
3:L:133:VAL:HG23	3:L:149:TRP:CH2	2.47	0.49
1:R:65:A:H2'	1:R:66:U:C6	2.48	0.49
2:A:164:VAL:HG12	2:A:210:VAL:HG13	1.94	0.49
3:B:109:ARG:HD3	3:B:110:THR:O	2.12	0.49
1:R:53:G:OP2	1:R:53:G:H3'	2.11	0.49
3:L:121:PRO:HD3	3:L:133:VAL:HG12	1.94	0.49
3:B:133:VAL:HG13	3:B:149:TRP:CZ3	2.48	0.49
3:B:149:TRP:CD1	3:B:180:LEU:HD21	2.48	0.48
3:B:136:LEU:HD12	3:B:137:LEU:N	2.28	0.48
1:N:102:U:H2'	1:N:103:C:C6	2.49	0.48
3:L:188:GLU:HA	3:L:212:ARG:NH1	2.28	0.48
3:B:187:TYR:CE2	3:B:212:ARG:HD2	2.49	0.48
1:N:56:A:C8	5:N:202:CTI:H19B	2.49	0.47
2:A:15:VAL:HG11	2:A:89:LEU:HD13	1.94	0.47
3:L:12:LEU:HD21	3:L:20:VAL:HG13	1.97	0.47
2:H:216:ASN:O	2:H:216:ASN:OD1	2.32	0.47
3:B:149:TRP:CG	3:B:180:LEU:HD11	2.48	0.47
3:L:9:PRO:O	3:L:103:THR:OG1	2.20	0.47
1:N:59:C:H5''	1:N:96:U:H5''	1.96	0.47
1:R:16:C:O2	1:R:97:A:N6	2.47	0.47
3:B:109:ARG:HD2	3:B:141:TYR:CB	2.45	0.47
2:A:193:VAL:HG21	3:B:136:LEU:HD22	1.96	0.47
3:B:125:GLN:O	3:B:130:THR:O	2.33	0.47
3:L:7:GLN:HG3	3:L:24:CYS:SG	2.55	0.47
2:A:198:SER:HA	2:A:201:LEU:HB2	1.97	0.47
3:B:60:PRO:O	3:B:63:PHE:HD1	1.97	0.47
1:N:24:A:H2'	1:N:25:U:C6	2.51	0.46
2:H:172:THR:O	2:H:175:VAL:HG12	2.15	0.46
1:N:74:G:C2	1:N:84:G:C2	3.03	0.46
2:A:183:GLN:HE21	2:A:185:SER:HB3	1.79	0.46
2:A:193:VAL:HG11	3:B:136:LEU:CD2	2.45	0.46
3:B:82:GLU:HG3	3:B:83:ASP:OD1	2.15	0.46
1:R:71:A:H2'	1:R:72:G:C8	2.51	0.46
3:B:114:PRO:HD2	3:B:202:LEU:HG	1.98	0.46
3:B:189:LYS:CG	3:B:190:HIS:ND1	2.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:120:U:H6	1:R:120:U:O5'	1.98	0.46
2:A:38:HIS:ND1	2:A:53:SER:HB2	2.31	0.46
1:N:56:A:H5'	5:N:202:CTI:H19	1.99	0.45
3:B:109:ARG:HG2	3:B:172:SER:O	2.16	0.45
1:R:64:C:H2'	1:R:65:A:C8	2.52	0.45
1:R:76:U:H4'	1:R:77:A:OP1	2.17	0.45
2:A:183:GLN:HG3	2:A:185:SER:H	1.81	0.45
3:B:191:LYS:HA	3:B:212:ARG:HG3	1.98	0.45
3:L:193:TYR:HB2	3:L:210:PHE:CE1	2.52	0.45
3:L:148:GLN:HG2	3:L:155:LEU:CD1	2.47	0.45
2:A:157:TYR:CE2	2:A:162:VAL:HG13	2.52	0.44
3:L:5:MET:SD	3:L:91:GLN:HB3	2.57	0.44
3:L:22:ILE:HG12	3:L:103:THR:HG21	1.99	0.44
1:R:18:C:H4'	1:R:93:A:N6	2.32	0.44
1:R:71:A:H2'	1:R:72:G:H8	1.82	0.44
2:H:131:PRO:HB3	2:H:157:TYR:HB3	1.98	0.44
1:N:65:A:H2'	1:N:66:U:C6	2.53	0.44
1:R:37:U:H2'	1:R:38:C:C6	2.52	0.44
3:B:189:LYS:HG2	3:B:190:HIS:N	2.32	0.44
3:L:176:LEU:C	3:L:176:LEU:HD23	2.38	0.44
2:H:90:ARG:C	2:H:123:VAL:HG11	2.38	0.44
2:A:61:THR:HB	2:A:63:TYR:CE1	2.54	0.43
1:N:20:A:O2'	1:N:22:G:O6	2.31	0.43
3:B:3:ILE:HD12	3:B:3:ILE:N	2.33	0.43
3:L:109:ARG:HG2	3:L:110:THR:H	1.84	0.43
1:N:29:G:H2'	1:N:31:A:N6	2.32	0.43
1:R:29:G:H2'	1:R:31:A:N6	2.29	0.43
1:R:78:U:O2	1:R:79:A:N6	2.52	0.43
3:L:12:LEU:HD12	3:L:13:SER:N	2.34	0.43
2:A:138:PRO:HG3	2:A:150:LEU:HB3	2.01	0.43
1:R:79:A:N3	1:R:79:A:H2'	2.33	0.43
3:B:84:PHE:CE2	3:B:107:ILE:HG13	2.54	0.42
3:L:176:LEU:HD23	3:L:177:SER:N	2.33	0.42
3:B:40:LYS:HG2	3:B:85:ALA:HB2	2.01	0.42
1:R:102:U:H2'	1:R:103:C:C6	2.53	0.42
1:R:113:U:C2	1:R:114:C:C5	3.07	0.42
1:R:122:C:H2'	1:R:123:U:H6	1.84	0.42
3:B:19:ARG:HA	3:B:76:ILE:O	2.18	0.42
3:B:84:PHE:CD2	3:B:107:ILE:HG13	2.55	0.42
1:N:54:G:N2	1:N:118:C:C2	2.88	0.42
1:R:11:A:H2'	1:R:12:A:C8	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:34:VAL:HG21	3:L:72:PHE:CE2	2.54	0.42
1:N:15:A:C2	1:N:98:A:N1	2.87	0.42
3:L:38:GLN:HG3	3:L:87:TYR:CE2	2.55	0.42
3:L:107:ILE:H	3:L:107:ILE:HG13	1.54	0.42
2:H:20:SER:HA	2:H:86:MET:O	2.20	0.42
1:N:95:G:O4'	1:N:97:A:C8	2.73	0.41
2:A:36:SER:HB2	2:A:102:GLN:HB3	2.01	0.41
2:A:180:ALA:HB2	2:A:190:LEU:HD23	2.01	0.41
3:B:36:TRP:CG	3:B:74:LEU:HD13	2.55	0.41
1:R:125:U:H2'	1:R:126:G:H8	1.85	0.41
1:R:125:U:H2'	1:R:126:G:C8	2.56	0.41
2:A:176:HIS:HB3	3:B:165:THR:HG21	2.02	0.41
1:R:53:G:H3'	1:R:53:G:P	2.60	0.41
2:H:51:VAL:HG13	2:H:67:VAL:HG11	2.01	0.41
3:B:150:LYS:CG	3:B:153:ASN:HA	2.50	0.41
3:B:26:ALA:N	3:B:70:THR:O	2.54	0.41
3:L:116:VAL:O	8:L:401:HOH:O	2.22	0.41
1:N:32:A:C6	3:L:95:PHE:CZ	3.09	0.41
2:A:31:TYR:HD2	2:A:34:TYR:CE2	2.38	0.41
2:A:74:SER:OG	2:A:83:TYR:HB2	2.20	0.41
1:N:35:C:H2'	1:N:36:G:C8	2.56	0.41
1:R:63:A:H2'	1:R:64:C:O4'	2.21	0.41
1:R:64:C:H2'	1:R:65:A:H8	1.86	0.41
1:R:68:A:H2'	1:R:69:A:H8	1.86	0.41
2:A:182:LEU:HD11	2:A:186:GLY:HA2	2.03	0.41
2:A:207:ILE:HD13	2:A:222:LYS:HA	2.02	0.41
2:A:71:PHE:HA	2:A:85:GLN:O	2.20	0.41
2:A:71:PHE:CE1	2:A:86:MET:HG2	2.56	0.40
3:B:132:SER:HA	3:B:180:LEU:O	2.22	0.40
3:B:9:PRO:HD2	3:B:22:ILE:HD12	2.03	0.40
3:B:149:TRP:HB3	3:B:180:LEU:HD11	2.02	0.40
2:H:50:TRP:HZ2	2:H:53:SER:HB3	1.86	0.40
1:N:106:C:O2'	8:N:301:HOH:O	2.22	0.40
1:R:48:C:H2'	1:R:49:G:C8	2.57	0.40
2:H:89:LEU:HB3	2:H:123:VAL:HG21	2.04	0.40
2:H:216:ASN:O	2:H:216:ASN:CG	2.59	0.40

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	
2	A	223/233 (96%)	222 (100%)	1 (0%)	0	100	100
2	H	223/233 (96%)	223 (100%)	0	0	100	100
3	B	213/215 (99%)	207 (97%)	6 (3%)	0	100	100
3	L	213/215 (99%)	213 (100%)	0	0	100	100
All	All	872/896 (97%)	865 (99%)	7 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	
2	A	186/194 (96%)	181 (97%)	5 (3%)	44	75
2	H	186/194 (96%)	184 (99%)	2 (1%)	73	90
3	B	190/190 (100%)	187 (98%)	3 (2%)	62	86
3	L	190/190 (100%)	187 (98%)	3 (2%)	62	86
All	All	752/768 (98%)	739 (98%)	13 (2%)	60	85

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	33	SER
2	A	53	SER

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Mol	Chain	Res	Type
2	A	70	ARG
2	A	143	THR
2	A	209	ASN
2	H	33	SER
2	H	209	ASN
3	B	38	GLN
3	B	109	ARG
3	B	189	LYS
3	L	67	ARG
3	L	128	SER
3	L	212	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
3	B	90	GLN
3	B	97	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	N	119/128 (92%)	15 (12%)	6 (5%)
1	R	126/128 (98%)	16 (12%)	4 (3%)
All	All	245/256 (95%)	31 (12%)	10 (4%)

All (31) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	N	8	G
1	N	20	A
1	N	44	G
1	N	45	A
1	N	52	A
1	N	53	G
1	N	58	U
1	N	59	C
1	N	75	G
1	N	93	A
1	N	95	G
1	N	96	U

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Mol	Chain	Res	Type
1	N	106	C
1	N	109	U
1	N	110	A
1	R	8	G
1	R	44	G
1	R	45	A
1	R	46	U
1	R	53	G
1	R	76	U
1	R	77	A
1	R	78	U
1	R	79	A
1	R	83	C
1	R	93	A
1	R	96	U
1	R	106	C
1	R	110	A
1	R	117	C
1	R	120	U

All (10) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	N	43	A
1	N	44	G
1	N	52	A
1	N	58	U
1	N	107	C
1	N	116	U
1	R	76	U
1	R	77	A
1	R	82	G
1	R	119	A

5.4 Non-standard residues in protein, DNA, RNA chains [\(i\)](#)

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

5.5 Carbohydrates [\(i\)](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 12 ligands modelled in this entry, 10 are monoatomic - leaving 2 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	CTI	N	202	-	28,30,30	1.23	2 (7%)	41,45,45	1.18	4 (9%)
5	CTI	R	205	-	28,30,30	1.06	2 (7%)	41,45,45	1.00	3 (7%)

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	CTI	N	202	-	-	0/4/10/10	0/5/5/5
5	CTI	R	205	-	-	0/4/10/10	0/5/5/5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	N	202	CTI	C2-C5	5.62	1.50	1.40
5	R	205	CTI	C2-C5	4.39	1.48	1.40
5	N	202	CTI	C6-C5	2.44	1.44	1.40
5	R	205	CTI	C6-C5	2.26	1.44	1.40

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	N	202	CTI	C13-N9-C12	-3.08	113.87	118.53
5	N	202	CTI	C8-C3-C4	-2.80	117.08	122.02
5	N	202	CTI	C7-C6-C5	2.61	120.64	117.86
5	R	205	CTI	C7-C6-C5	2.52	120.55	117.86
5	R	205	CTI	C13-N9-C12	-2.18	115.23	118.53
5	N	202	CTI	C4-C3-C2	2.11	122.19	119.77
5	R	205	CTI	C8-C3-C4	-2.00	118.49	122.02

There are no chirality outliers.

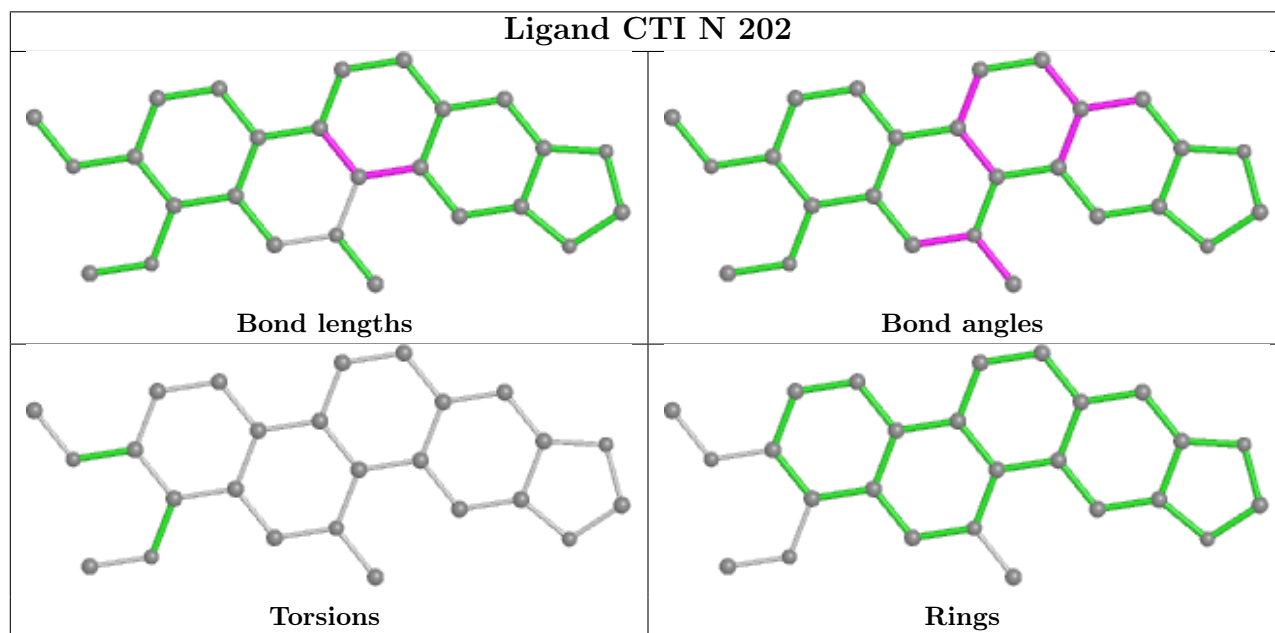
There are no torsion outliers.

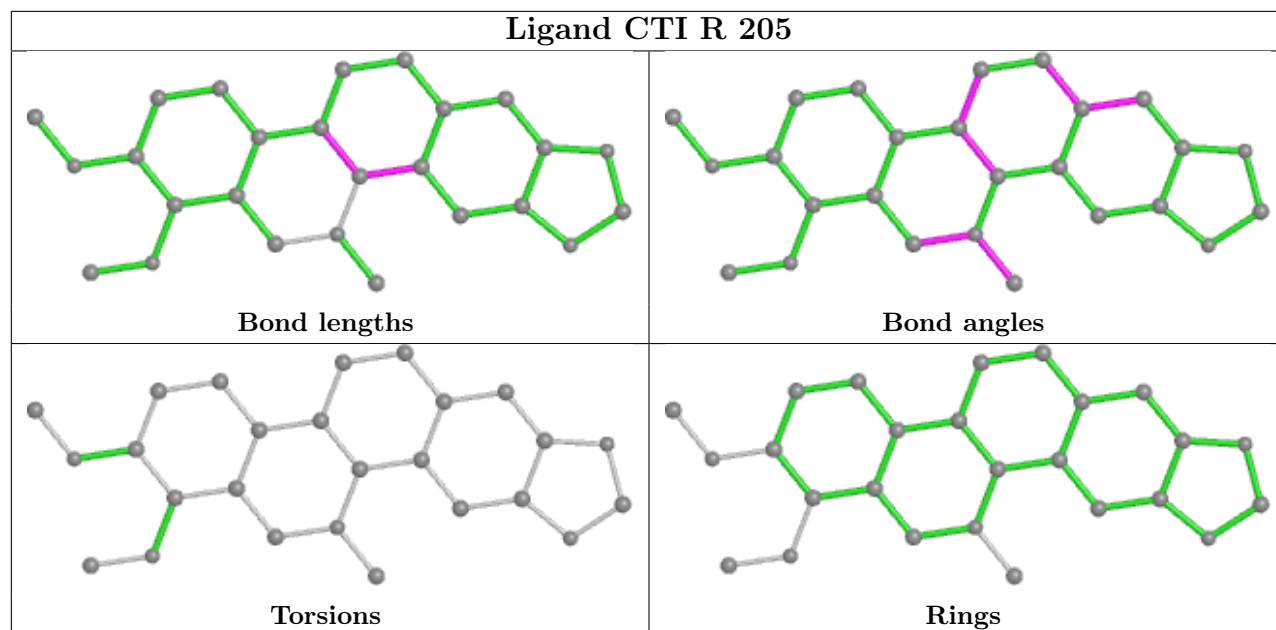
There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	N	202	CTI	4	0
5	R	205	CTI	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	N	121/128 (94%)	-0.75	0 100 100	90, 129, 191, 218	0
1	R	127/128 (99%)	-0.66	1 (0%) 86 84	88, 143, 233, 332	0
2	A	225/233 (96%)	1.01	37 (16%) 1 1	70, 114, 198, 239	0
2	H	225/233 (96%)	0.18	7 (3%) 49 44	67, 89, 125, 195	0
3	B	215/215 (100%)	1.10	52 (24%) 0 0	102, 159, 206, 234	0
3	L	215/215 (100%)	0.33	5 (2%) 60 55	67, 101, 144, 171	0
All	All	1128/1152 (97%)	0.36	102 (9%) 9 6	67, 118, 196, 332	0

All (102) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	205	THR	11.7
2	A	201	LEU	8.0
3	B	202	LEU	7.6
2	A	202	GLY	7.3
2	A	227	SER	7.2
3	B	207	THR	7.0
3	B	107	ILE	6.5
2	A	228	CYS	5.9
3	B	105	VAL	5.5
2	A	199	SER	5.3
2	A	200	SER	5.1
2	H	228	CYS	5.1
3	B	30	VAL	4.8
2	A	218	LYS	4.6
2	A	196	VAL	4.6
2	A	150	LEU	4.6
2	A	223	VAL	4.4
2	A	206	TYR	4.3
3	B	49	ILE	4.1

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Mol	Chain	Res	Type	RSRZ
3	B	147	VAL	4.0
3	B	134	VAL	3.9
3	B	148	GLN	3.9
2	A	147	THR	3.8
1	R	76	U	3.8
2	A	197	PRO	3.8
3	B	93	TYR	3.7
2	A	219	VAL	3.6
2	A	203	THR	3.6
3	B	119	PHE	3.5
3	B	36	TRP	3.5
2	A	138	PRO	3.4
2	A	133	VAL	3.4
3	B	196	GLU	3.3
2	A	185	SER	3.2
2	A	65	ASP	3.2
3	B	205	PRO	3.2
3	B	126	LEU	3.1
2	A	142	SER	3.1
2	A	129	LYS	3.0
2	A	225	PRO	3.0
3	L	202	LEU	2.9
3	B	140	PHE	2.9
3	B	210	PHE	2.9
3	B	197	VAL	2.9
3	B	104	LYS	2.8
3	B	151	VAL	2.8
3	B	74	LEU	2.8
3	B	24	CYS	2.8
3	B	209	SER	2.8
3	B	85	ALA	2.7
3	B	203	SER	2.7
3	B	149	TRP	2.7
3	B	185	ALA	2.6
3	B	87	TYR	2.6
3	L	74	LEU	2.6
2	A	224	GLU	2.6
2	H	143	THR	2.6
3	B	116	VAL	2.6
3	B	143	ARG	2.6
3	B	79	LEU	2.5
2	A	135	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
3	B	199	HIS	2.4
2	A	57	TYR	2.4
3	L	187	TYR	2.4
3	B	48	LEU	2.4
2	A	153	LEU	2.4
3	B	121	PRO	2.3
3	B	136	LEU	2.3
2	A	141	LYS	2.3
2	A	226	LYS	2.3
3	B	111	VAL	2.3
3	B	106	GLU	2.3
3	B	144	GLU	2.3
2	A	187	LEU	2.3
3	L	109	ARG	2.3
2	A	216	ASN	2.3
2	H	40	VAL	2.2
2	H	54	ILE	2.2
3	B	195	CYS	2.2
3	B	176	LEU	2.2
2	H	171	LEU	2.2
3	B	12	LEU	2.1
3	B	98	THR	2.1
3	B	108	LYS	2.1
2	A	171	LEU	2.1
2	A	166	TRP	2.1
2	H	166	TRP	2.1
3	B	133	VAL	2.1
3	B	109	ARG	2.1
3	B	204	SER	2.1
3	B	97	ASN	2.1
2	A	160	GLU	2.1
3	B	72	PHE	2.1
3	B	22	ILE	2.0
2	H	201	LEU	2.0
3	B	55	LEU	2.0
3	B	3	ILE	2.0
2	A	137	ALA	2.0
2	A	136	LEU	2.0
3	B	137	LEU	2.0
3	L	180	LEU	2.0
2	A	222	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

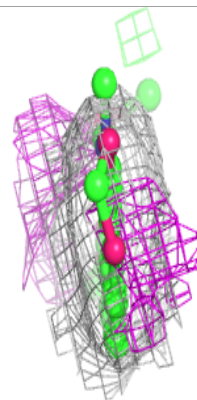
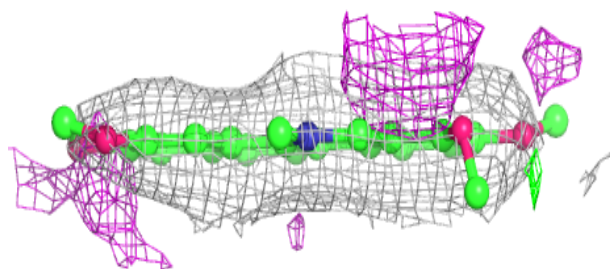
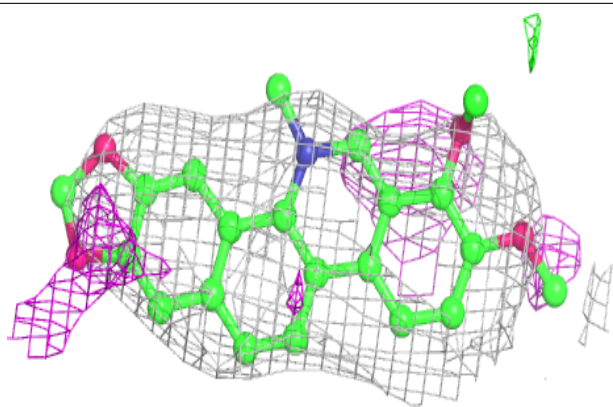
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	MG	R	204	1/1	0.72	0.67	145,145,145,145	0
6	OS	B	302	1/1	0.76	0.10	175,175,175,175	1
4	MG	R	202	1/1	0.85	0.58	127,127,127,127	0
5	CTI	R	205	26/26	0.88	0.28	99,107,126,137	0
4	MG	R	203	1/1	0.89	0.48	123,123,123,123	0
5	CTI	N	202	26/26	0.90	0.24	82,100,112,120	0
4	MG	R	201	1/1	0.91	0.44	106,106,106,106	0
7	K	L	301	1/1	0.91	0.14	171,171,171,171	0
6	OS	L	302	1/1	0.92	0.13	144,144,144,144	1
6	OS	B	301	1/1	0.92	0.21	176,176,176,176	1
4	MG	N	201	1/1	0.96	0.39	109,109,109,109	0
6	OS	L	303	1/1	0.97	0.07	162,162,162,162	1

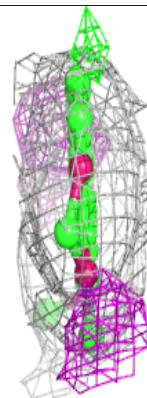
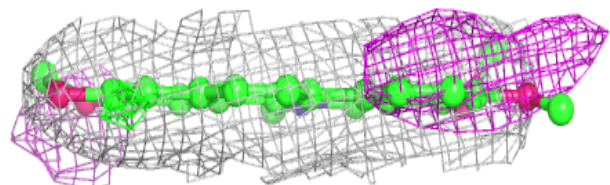
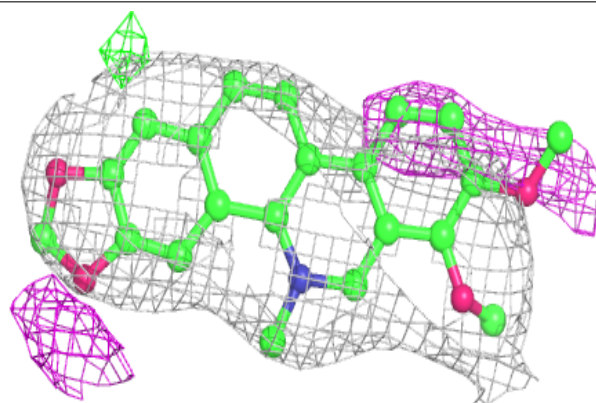
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around CTI R 205:

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

**Electron density around CTI N 202:**

$2mF_o-DF_c$ (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.