



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:09 PM UTC

PDB ID : 7PQ3 / pdb_00007pq3
Title : Crystal Structure of the Ring Nuclease 0811 from *Sulfolobus islandicus* (Sis0811) in complex with its post-catalytic reaction product
Authors : Molina, R.; Jensen, A.L.G.; Marchena-Hurtado, J.; Lopez-Mendez, B.; Stella, S.; Montoya, G.
Deposited on : 2021-09-16
Resolution : 2.85 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

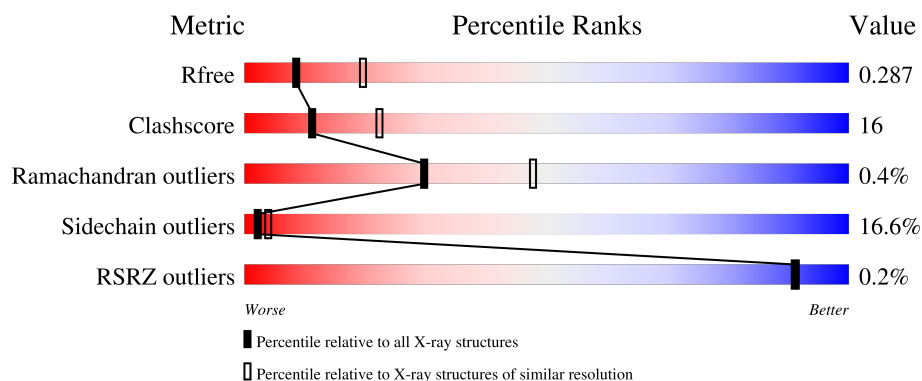
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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	275	
1	BBB	275	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4446 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.

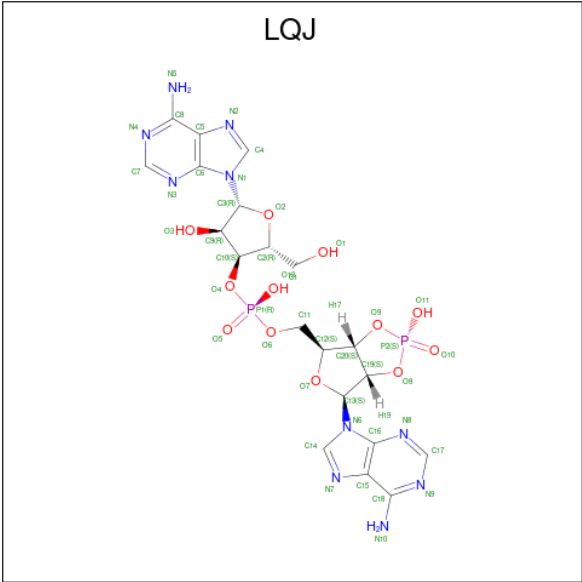
- Molecule 1 is a protein called CRISPR-associated protein, APE2256 family.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	268	Total	C	N	O	S	0	0	0
			2176	1407	351	416	2			
1	BBB	269	Total	C	N	O	S	0	0	0
			2182	1410	352	418	2			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	269	GLY	-	expression tag	UNP F0NH89
AAA	270	SER	-	expression tag	UNP F0NH89
AAA	271	GLU	-	expression tag	UNP F0NH89
AAA	272	PHE	-	expression tag	UNP F0NH89
AAA	273	GLU	-	expression tag	UNP F0NH89
AAA	274	LEU	-	expression tag	UNP F0NH89
AAA	275	GLU	-	expression tag	UNP F0NH89
BBB	269	GLY	-	expression tag	UNP F0NH89
BBB	270	SER	-	expression tag	UNP F0NH89
BBB	271	GLU	-	expression tag	UNP F0NH89
BBB	272	PHE	-	expression tag	UNP F0NH89
BBB	273	GLU	-	expression tag	UNP F0NH89
BBB	274	LEU	-	expression tag	UNP F0NH89
BBB	275	GLU	-	expression tag	UNP F0NH89

- Molecule 2 is 3'-O-[(R)-{[(2S,3aS,4S,6S,6aS)-6-(6-amino-9H-purin-9-yl)-2-hydroxy-2-oxotetrahydro-2H-2lambda 5 -furo[3,4-d][1,3,2]dioxaphosphol-4-yl]methoxy}(hydroxy)phosphoryl]adenosine (CCD ID: LQJ) (formula: C₂₀H₂₄N₁₀O₁₂P₂) (labeled as "Ligand of Interest" by depositor).

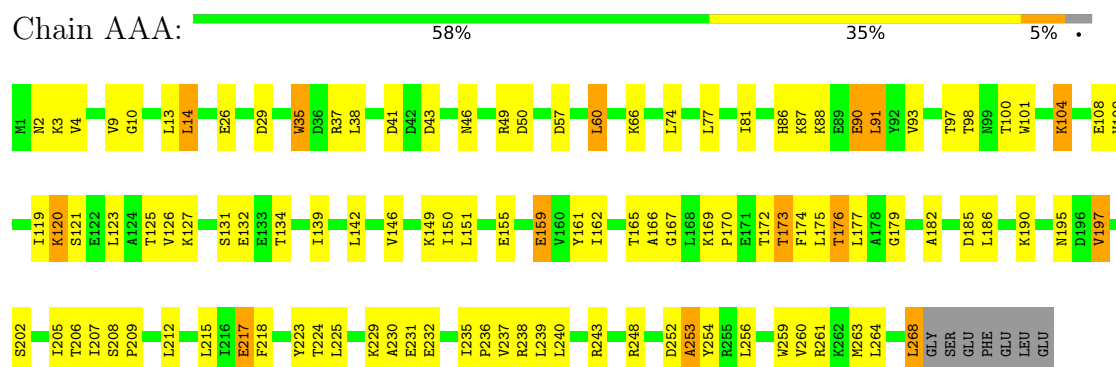


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	AAA	1	Total 44	C 20	N 10	O 12	P 2	0	0
2	BBB	1	Total 44	C 20	N 10	O 12	P 2	0	0

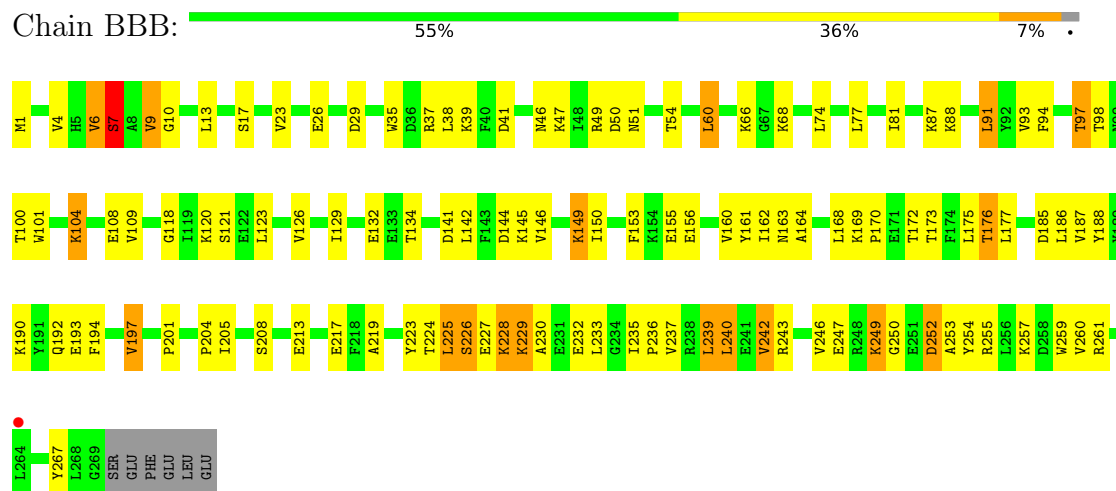
3 Residue-property plots [i](#)

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: CRISPR-associated protein, APE2256 family



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4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	56.73Å 56.73Å 361.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.05 – 2.85 48.05 – 2.85	Depositor EDS
% Data completeness (in resolution range)	99.2 (48.05-2.85) 99.2 (48.05-2.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.48 (at 2.86Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.252 , 0.291 0.250 , 0.287	Depositor DCC
R_{free} test set	740 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	94.8	Xtriage
Anisotropy	0.242	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 91.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4446	wwPDB-VP
Average B, all atoms (Å ²)	125.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.02% 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: LQJ

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	1.01	0/2216	1.52	4/2988 (0.1%)
1	BBB	1.04	1/2222 (0.0%)	1.54	2/2996 (0.1%)
All	All	1.03	1/4438 (0.0%)	1.53	6/5984 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	BBB	7	SER	C-O	-5.75	1.16	1.23

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BBB	192	GLN	CB-CA-C	7.66	124.79	110.63
1	AAA	173	THR	CA-CB-OG1	7.19	120.38	109.60
1	AAA	167	GLY	CA-C-O	-6.72	117.21	122.52
1	AAA	125	THR	CA-CB-OG1	-5.77	100.94	109.60
1	BBB	252	ASP	CA-CB-CG	5.52	118.12	112.60
1	AAA	43	ASP	N-CA-C	-5.11	105.71	111.28

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	2176	0	2212	86	0
1	BBB	2182	0	2220	73	0
2	AAA	44	0	0	3	0
2	BBB	44	0	0	3	0
All	All	4446	0	4432	145	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 16.

All (145) 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:AAA:224:THR:CB	1:AAA:254:TYR:HB3	1.91	1.00
1:BBB:236:PRO:HG2	1:BBB:240:LEU:HD23	1.51	0.93
1:AAA:217:GLU:CD	1:AAA:235:ILE:HD11	1.94	0.92
1:AAA:224:THR:CB	1:AAA:254:TYR:CB	2.48	0.91
1:AAA:173:THR:HA	1:BBB:173:THR:HG22	1.56	0.88
1:BBB:144:ASP:OD2	1:BBB:259:TRP:CD1	2.27	0.87
1:AAA:248:ARG:HE	1:AAA:253:ALA:HB2	1.42	0.84
1:AAA:237:VAL:HG21	1:AAA:254:TYR:HE1	1.40	0.84
1:AAA:248:ARG:NE	1:AAA:253:ALA:HB2	1.95	0.82
1:AAA:146:VAL:O	1:AAA:150:ILE:HG12	1.79	0.82
1:BBB:141:ASP:O	1:BBB:145:LYS:HG3	1.88	0.73
1:AAA:91:LEU:HD23	1:AAA:119:ILE:HG23	1.70	0.73
1:BBB:247:GLU:OE2	1:BBB:255:ARG:HD2	1.89	0.73
1:BBB:229:LYS:HA	1:BBB:232:GLU:HG2	1.70	0.72
1:AAA:229:LYS:O	1:AAA:232:GLU:HB2	1.90	0.72
1:AAA:230:ALA:CB	1:AAA:254:TYR:OH	2.39	0.71
1:BBB:7:SER:HB3	1:BBB:163:ASN:HD22	1.57	0.70
1:AAA:237:VAL:HG21	1:AAA:254:TYR:CE1	2.24	0.69
1:AAA:151:LEU:O	1:AAA:155:GLU:HG2	1.94	0.68
1:AAA:225:LEU:O	1:AAA:254:TYR:CE2	2.49	0.66
1:AAA:248:ARG:HG3	1:AAA:253:ALA:HB2	1.77	0.66
1:AAA:207:ILE:HD12	1:AAA:207:ILE:H	1.60	0.65
1:AAA:60:LEU:HD22	1:AAA:109:VAL:HG13	1.77	0.65
1:AAA:224:THR:CB	1:AAA:254:TYR:HB2	2.29	0.62
1:AAA:206:THR:HG23	1:BBB:208:SER:HB3	1.80	0.62
1:BBB:60:LEU:HD22	1:BBB:109:VAL:HG13	1.82	0.62
1:AAA:230:ALA:HB1	1:AAA:254:TYR:OH	1.98	0.62
1:BBB:100:THR:O	1:BBB:104:LYS:HG2	2.00	0.61
1:BBB:88:LYS:HE2	1:BBB:118:GLY:HA3	1.82	0.61
1:AAA:100:THR:O	1:AAA:104:LYS:HG2	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:248:ARG:NE	1:AAA:253:ALA:CB	2.62	0.60
1:BBB:146:VAL:O	1:BBB:150:ILE:HG12	2.02	0.59
1:AAA:209:PRO:HA	1:AAA:212:LEU:HB3	1.85	0.58
1:BBB:225:LEU:HD21	1:BBB:229:LYS:HG2	1.85	0.58
2:AAA:301:LQJ:O10	2:BBB:301:LQJ:O1	2.22	0.57
1:AAA:10:GLY:HA2	2:AAA:301:LQJ:N8	2.19	0.57
1:AAA:224:THR:HA	1:AAA:254:TYR:CG	2.38	0.57
1:BBB:149:LYS:HG3	1:BBB:153:PHE:CE2	2.40	0.57
1:AAA:97:THR:HG22	1:AAA:98:THR:O	2.06	0.56
1:AAA:172:THR:O	1:AAA:176:THR:HG23	2.04	0.56
1:AAA:173:THR:CA	1:BBB:173:THR:HG22	2.34	0.56
1:AAA:224:THR:HA	1:AAA:254:TYR:CD1	2.40	0.56
1:AAA:224:THR:CA	1:AAA:254:TYR:HB3	2.35	0.56
1:BBB:219:ALA:HA	1:BBB:223:TYR:CE1	2.42	0.55
1:AAA:161:TYR:HD1	1:AAA:186:LEU:HB2	1.71	0.55
1:BBB:172:THR:O	1:BBB:176:THR:HG23	2.06	0.55
1:AAA:169:LYS:HB2	1:AAA:170:PRO:HD3	1.89	0.53
1:BBB:225:LEU:HD22	1:BBB:230:ALA:HA	1.90	0.53
1:BBB:77:LEU:O	1:BBB:81:ILE:HG12	2.09	0.52
1:BBB:132:GLU:CD	1:BBB:132:GLU:H	2.17	0.52
1:BBB:190:LYS:HB2	1:BBB:197:VAL:HG23	1.90	0.52
1:BBB:227:GLU:HG3	1:BBB:228:LYS:H	1.74	0.52
1:AAA:177:LEU:HD13	1:BBB:177:LEU:HD22	1.90	0.52
1:BBB:161:TYR:HD1	1:BBB:186:LEU:HB2	1.73	0.51
1:AAA:132:GLU:H	1:AAA:132:GLU:CD	2.18	0.51
1:AAA:248:ARG:HA	1:AAA:253:ALA:HA	1.93	0.51
1:AAA:248:ARG:CG	1:AAA:253:ALA:HB2	2.39	0.51
1:BBB:4:VAL:HG11	1:BBB:153:PHE:CE2	2.46	0.51
1:BBB:9:VAL:HG22	1:BBB:97:THR:HA	1.93	0.51
1:AAA:77:LEU:O	1:AAA:81:ILE:HG12	2.11	0.51
1:AAA:252:ASP:O	1:AAA:253:ALA:HB3	2.10	0.51
1:BBB:126:VAL:HG11	1:BBB:142:LEU:HB2	1.93	0.51
1:BBB:10:GLY:HA2	2:BBB:301:LQJ:N8	2.26	0.51
1:BBB:169:LYS:HB2	1:BBB:170:PRO:HD3	1.93	0.50
1:BBB:225:LEU:O	1:BBB:254:TYR:HD2	1.94	0.50
1:BBB:17:SER:HB3	1:BBB:23:VAL:HG11	1.93	0.50
1:AAA:10:GLY:HA2	2:AAA:301:LQJ:C17	2.41	0.50
1:AAA:81:ILE:HD12	1:AAA:91:LEU:HD11	1.93	0.50
1:AAA:243:ARG:HB3	1:BBB:204:PRO:HD3	1.93	0.50
1:BBB:225:LEU:HD23	1:BBB:226:SER:H	1.77	0.49
1:AAA:9:VAL:HG22	1:AAA:97:THR:HA	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:248:ARG:HG3	1:AAA:253:ALA:CB	2.42	0.49
1:AAA:190:LYS:HB2	1:AAA:197:VAL:HG23	1.94	0.49
1:BBB:47:LYS:O	1:BBB:51:ASN:ND2	2.46	0.48
1:BBB:6:VAL:HG21	1:BBB:146:VAL:HG23	1.95	0.48
1:AAA:231:GLU:HG2	1:AAA:235:ILE:O	2.13	0.48
1:AAA:126:VAL:HG11	1:AAA:142:LEU:HB2	1.95	0.48
1:BBB:6:VAL:HG13	1:BBB:162:ILE:HG12	1.95	0.47
1:BBB:10:GLY:HA2	2:BBB:301:LQJ:C17	2.44	0.47
1:AAA:169:LYS:HD3	1:BBB:169:LYS:HD3	1.97	0.47
1:AAA:207:ILE:HD12	1:AAA:207:ILE:N	2.29	0.47
1:BBB:176:THR:HB	1:BBB:187:VAL:HG11	1.96	0.47
1:AAA:91:LEU:CD2	1:AAA:119:ILE:HG23	2.41	0.47
1:AAA:225:LEU:C	1:AAA:254:TYR:CE2	2.93	0.47
1:AAA:86:HIS:HB3	1:AAA:91:LEU:HD12	1.97	0.47
1:AAA:177:LEU:HD13	1:BBB:177:LEU:CD2	2.45	0.47
1:AAA:205:ILE:HG23	1:BBB:205:ILE:HG23	1.97	0.47
1:BBB:239:LEU:O	1:BBB:242:VAL:HG12	2.15	0.47
1:AAA:131:SER:HB2	1:BBB:194:PHE:CE1	2.50	0.46
1:AAA:150:ILE:HB	1:AAA:182:ALA:CB	2.45	0.46
1:BBB:223:TYR:OH	1:BBB:261:ARG:HG3	2.16	0.46
1:BBB:237:VAL:HG13	1:BBB:254:TYR:CE1	2.51	0.45
1:BBB:188:TYR:CD1	1:BBB:197:VAL:HG21	2.51	0.45
1:BBB:150:ILE:HD11	1:BBB:162:ILE:HD11	1.98	0.45
1:BBB:249:LYS:HB2	1:BBB:254:TYR:CD1	2.52	0.45
1:BBB:149:LYS:HG3	1:BBB:153:PHE:HE2	1.80	0.45
1:AAA:268:LEU:HD12	1:AAA:268:LEU:C	2.42	0.45
1:BBB:224:THR:HG23	1:BBB:253:ALA:HB1	1.97	0.45
1:AAA:87:LYS:O	1:AAA:91:LEU:HB2	2.17	0.44
1:BBB:49:ARG:HB3	1:BBB:101:TRP:CD2	2.53	0.44
1:AAA:217:GLU:OE1	1:AAA:235:ILE:HD11	2.17	0.44
1:BBB:257:LYS:O	1:BBB:260:VAL:HG22	2.18	0.44
1:BBB:37:ARG:O	1:BBB:37:ARG:HG3	2.17	0.44
1:BBB:164:ALA:HB2	1:BBB:176:THR:HG22	2.00	0.44
1:AAA:37:ARG:NH1	1:BBB:193:GLU:OE1	2.51	0.43
1:AAA:225:LEU:O	1:AAA:254:TYR:HE2	2.01	0.43
1:AAA:256:LEU:HD23	1:AAA:261:ARG:HE	1.82	0.43
1:AAA:165:THR:O	1:BBB:169:LYS:NZ	2.51	0.43
1:AAA:202:SER:HB2	1:BBB:243:ARG:HH21	1.82	0.43
1:AAA:46:ASN:HA	1:AAA:49:ARG:HG2	1.99	0.43
1:AAA:93:VAL:O	1:AAA:121:SER:HA	2.18	0.43
1:AAA:215:LEU:HB3	1:AAA:264:LEU:HD11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:139:ILE:HB	1:AAA:174:PHE:HD2	1.83	0.43
1:AAA:195:ASN:HD21	1:BBB:39:LYS:NZ	2.16	0.43
1:AAA:237:VAL:HG11	1:AAA:254:TYR:CE1	2.54	0.43
1:BBB:87:LYS:HA	1:BBB:87:LYS:HD3	1.85	0.43
1:BBB:240:LEU:HD13	1:BBB:240:LEU:HA	1.86	0.43
1:AAA:139:ILE:CD1	1:BBB:201:PRO:HD2	2.49	0.42
1:AAA:2:ASN:H	1:AAA:90:GLU:HG3	1.84	0.42
1:BBB:46:ASN:HA	1:BBB:49:ARG:HG2	2.01	0.42
1:AAA:235:ILE:HG22	1:AAA:237:VAL:HG23	2.02	0.42
1:AAA:14:LEU:HD12	1:AAA:35:TRP:CH2	2.54	0.42
1:AAA:218:PHE:HE1	1:AAA:223:TYR:HB2	1.85	0.42
1:AAA:248:ARG:CG	1:AAA:253:ALA:CB	2.98	0.42
1:AAA:248:ARG:HE	1:AAA:253:ALA:CB	2.21	0.42
1:AAA:49:ARG:HB3	1:AAA:101:TRP:CD2	2.55	0.42
1:AAA:3:LYS:HD3	1:AAA:159:GLU:HB2	2.01	0.42
1:AAA:162:ILE:CD1	1:AAA:179:GLY:HA3	2.50	0.42
1:BBB:98:THR:HB	1:BBB:129:ILE:HG21	2.00	0.42
1:AAA:120:LYS:HE3	1:AAA:120:LYS:HA	2.02	0.41
1:AAA:208:SER:HA	1:AAA:209:PRO:HD3	1.94	0.41
1:AAA:259:TRP:CE2	1:AAA:260:VAL:HG23	2.55	0.41
1:BBB:88:LYS:HA	1:BBB:91:LEU:HD23	2.02	0.41
1:AAA:139:ILE:HB	1:AAA:174:PHE:CD2	2.55	0.41
1:BBB:225:LEU:O	1:BBB:254:TYR:CD2	2.74	0.41
1:BBB:225:LEU:HD22	1:BBB:230:ALA:CA	2.49	0.41
1:BBB:237:VAL:HG13	1:BBB:254:TYR:CD1	2.55	0.41
1:BBB:246:VAL:HG13	1:BBB:255:ARG:O	2.21	0.41
1:AAA:206:THR:HG23	1:BBB:208:SER:CB	2.49	0.41
1:AAA:236:PRO:HB2	1:AAA:239:LEU:HB3	2.03	0.41
1:BBB:247:GLU:HB3	1:BBB:257:LYS:CE	2.51	0.41
1:BBB:170:PRO:HA	1:BBB:173:THR:OG1	2.21	0.40
1:BBB:249:LYS:HG2	1:BBB:250:GLY:N	2.36	0.40
1:AAA:166:ALA:O	1:AAA:172:THR:HG22	2.20	0.40
1:BBB:93:VAL:O	1:BBB:121:SER:HA	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AAA	266/275 (97%)	245 (92%)	20 (8%)	1 (0%)	30	48
1	BBB	267/275 (97%)	247 (92%)	19 (7%)	1 (0%)	30	48
All	All	533/550 (97%)	492 (92%)	39 (7%)	2 (0%)	30	48

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AAA	253	ALA
1	BBB	68	LYS

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AAA	238/245 (97%)	205 (86%)	33 (14%)	3	6
1	BBB	239/245 (98%)	193 (81%)	46 (19%)	1	2
All	All	477/490 (97%)	398 (83%)	79 (17%)	2	4

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	4	VAL
1	AAA	13	LEU
1	AAA	14	LEU
1	AAA	26	GLU

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Mol	Chain	Res	Type
1	AAA	29	ASP
1	AAA	35	TRP
1	AAA	38	LEU
1	AAA	41	ASP
1	AAA	50	ASP
1	AAA	57	ASP
1	AAA	60	LEU
1	AAA	66	LYS
1	AAA	74	LEU
1	AAA	88	LYS
1	AAA	90	GLU
1	AAA	91	LEU
1	AAA	104	LYS
1	AAA	108	GLU
1	AAA	120	LYS
1	AAA	123	LEU
1	AAA	127	LYS
1	AAA	134	THR
1	AAA	149	LYS
1	AAA	159	GLU
1	AAA	175	LEU
1	AAA	176	THR
1	AAA	185	ASP
1	AAA	197	VAL
1	AAA	217	GLU
1	AAA	238	ARG
1	AAA	240	LEU
1	AAA	263	MET
1	AAA	268	LEU
1	BBB	1	MET
1	BBB	6	VAL
1	BBB	7	SER
1	BBB	9	VAL
1	BBB	13	LEU
1	BBB	26	GLU
1	BBB	29	ASP
1	BBB	35	TRP
1	BBB	38	LEU
1	BBB	41	ASP
1	BBB	50	ASP
1	BBB	54	THR
1	BBB	60	LEU

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Mol	Chain	Res	Type
1	BBB	66	LYS
1	BBB	74	LEU
1	BBB	91	LEU
1	BBB	94	PHE
1	BBB	97	THR
1	BBB	104	LYS
1	BBB	108	GLU
1	BBB	120	LYS
1	BBB	123	LEU
1	BBB	134	THR
1	BBB	149	LYS
1	BBB	155	GLU
1	BBB	156	GLU
1	BBB	160	VAL
1	BBB	168	LEU
1	BBB	175	LEU
1	BBB	176	THR
1	BBB	185	ASP
1	BBB	197	VAL
1	BBB	213	GLU
1	BBB	217	GLU
1	BBB	225	LEU
1	BBB	226	SER
1	BBB	228	LYS
1	BBB	229	LYS
1	BBB	233	LEU
1	BBB	235	ILE
1	BBB	239	LEU
1	BBB	240	LEU
1	BBB	242	VAL
1	BBB	249	LYS
1	BBB	252	ASP
1	BBB	267	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

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](#)

2 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	LQJ	BBB	301	-	48,50,50	0.40	0	70,78,78	0.99	5 (7%)
2	LQJ	AAA	301	-	48,50,50	0.44	0	70,78,78	1.10	4 (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	LQJ	BBB	301	-	-	9/21/63/63	0/7/7/7
2	LQJ	AAA	301	-	-	8/21/63/63	0/7/7/7

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AAA	301	LQJ	C19-C13-N6	5.33	122.52	113.75
2	BBB	301	LQJ	C19-C13-N6	4.85	121.73	113.75
2	AAA	301	LQJ	O7-C13-C19	-3.53	100.50	106.59
2	AAA	301	LQJ	C9-C3-N1	2.66	119.91	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AAA	301	LQJ	O11-P2-O10	-2.63	101.42	109.89
2	BBB	301	LQJ	O11-P2-O10	-2.44	102.02	109.89
2	BBB	301	LQJ	C12-O7-C13	-2.40	104.18	109.47
2	BBB	301	LQJ	O7-C12-C20	-2.35	99.95	104.92
2	BBB	301	LQJ	P1-O6-C11	-2.24	108.49	121.35

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	AAA	301	LQJ	C11-O6-P1-O4
2	AAA	301	LQJ	C11-O6-P1-O5
2	AAA	301	LQJ	C11-O6-P1-O12
2	AAA	301	LQJ	O1-C1-C2-C10
2	BBB	301	LQJ	C11-O6-P1-O4
2	BBB	301	LQJ	C19-C13-N6-C16
2	BBB	301	LQJ	O6-C11-C12-O7
2	BBB	301	LQJ	O6-C11-C12-C20
2	AAA	301	LQJ	O1-C1-C2-O2
2	BBB	301	LQJ	O1-C1-C2-C10
2	BBB	301	LQJ	O1-C1-C2-O2
2	BBB	301	LQJ	C19-C13-N6-C14
2	AAA	301	LQJ	C19-C13-N6-C16
2	BBB	301	LQJ	C11-O6-P1-O5
2	AAA	301	LQJ	C19-C13-N6-C14
2	AAA	301	LQJ	O2-C3-N1-C4
2	BBB	301	LQJ	O2-C3-N1-C4

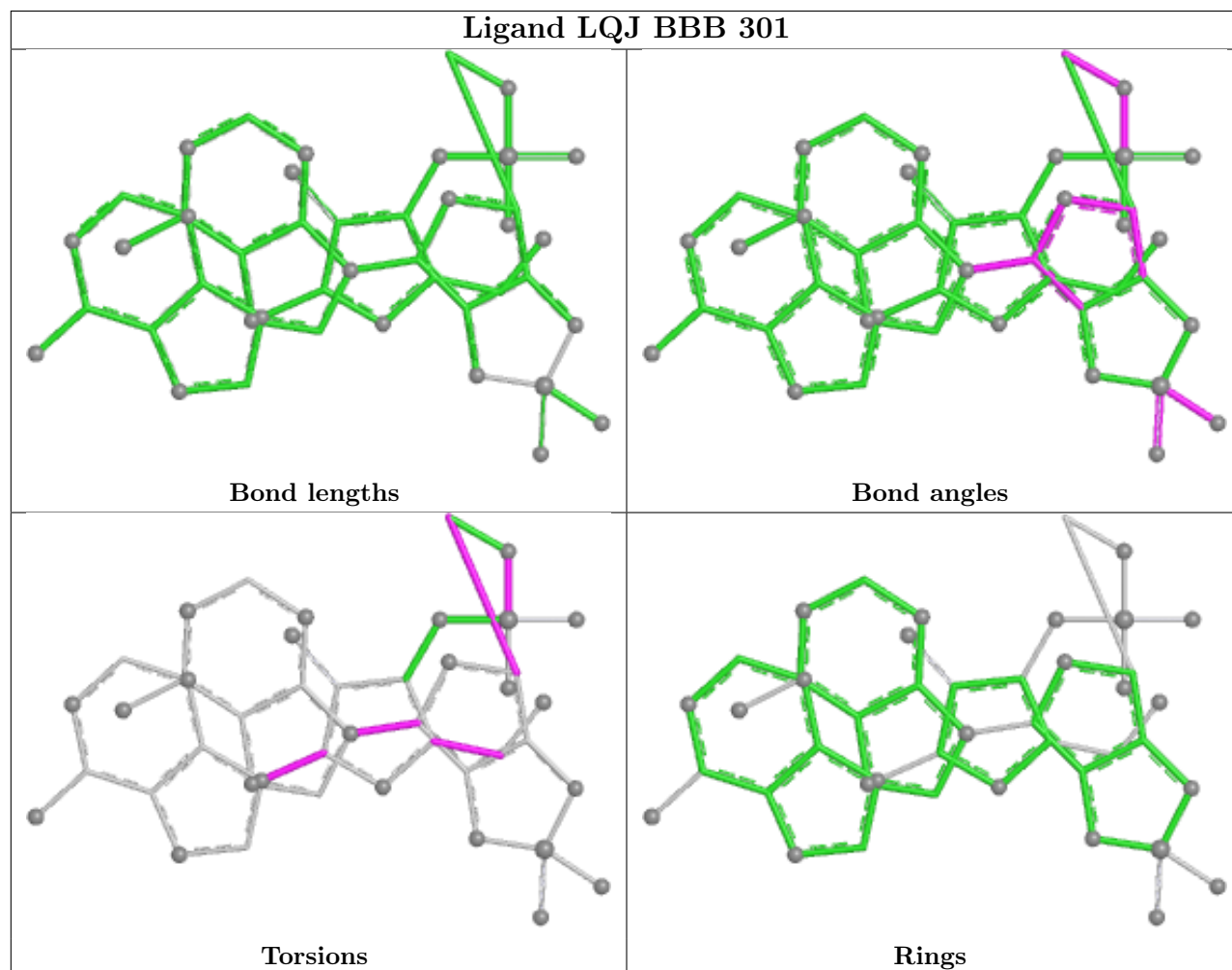
There are no ring outliers.

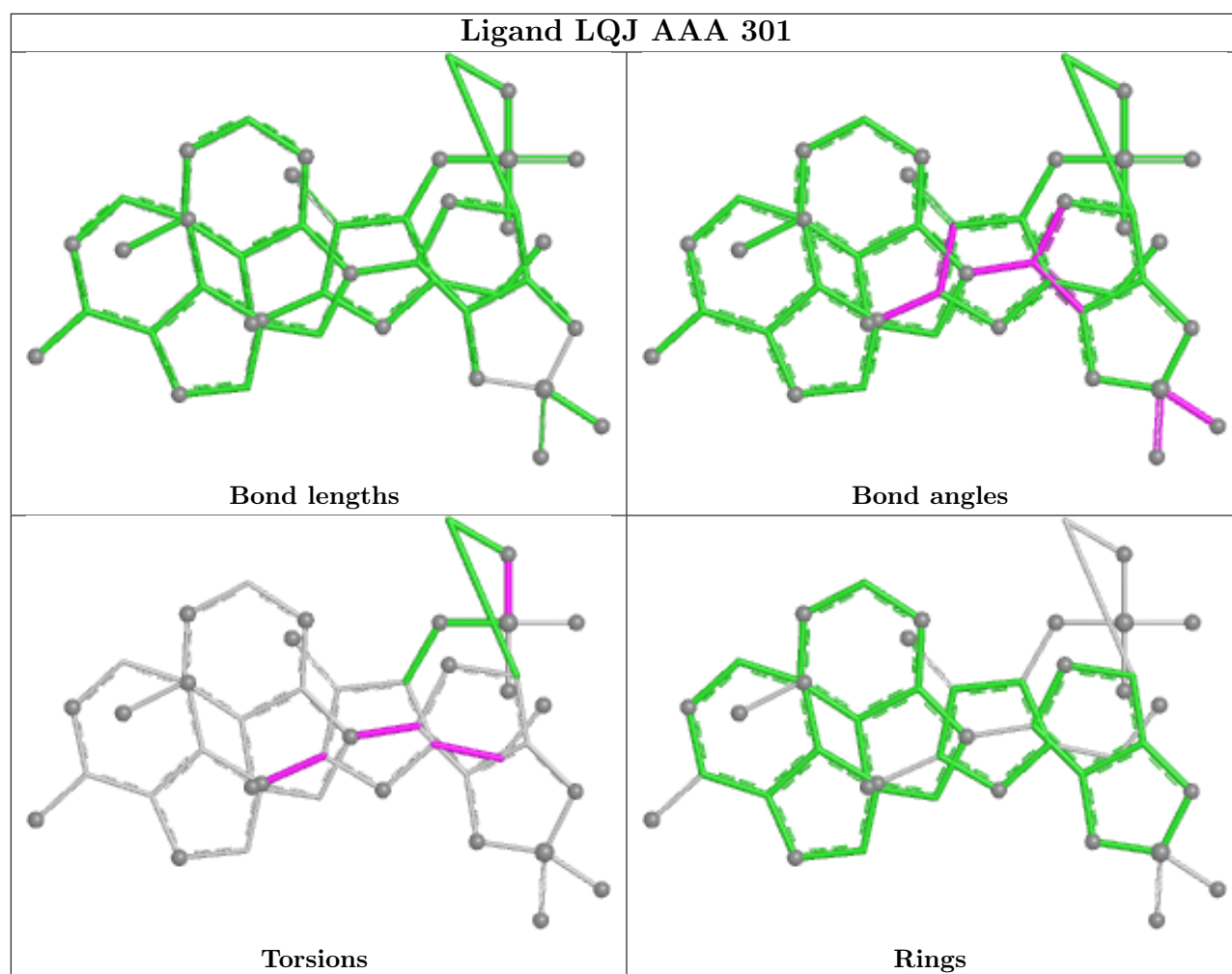
2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	BBB	301	LQJ	3	0
2	AAA	301	LQJ	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 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	268/275 (97%)	-0.23	0	100 100	70, 114, 199, 230	0
1	BBB	269/275 (97%)	-0.05	1 (0%)	88 87	78, 121, 210, 245	0
All	All	537/550 (97%)	-0.14	1 (0%)	91 91	70, 116, 209, 245	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BBB	264	LEU	2.2

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 oligosaccharides 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.

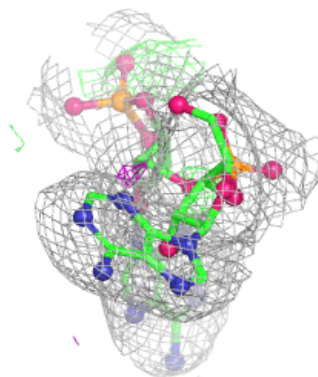
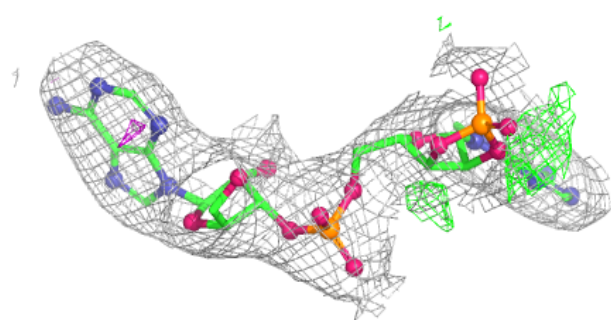
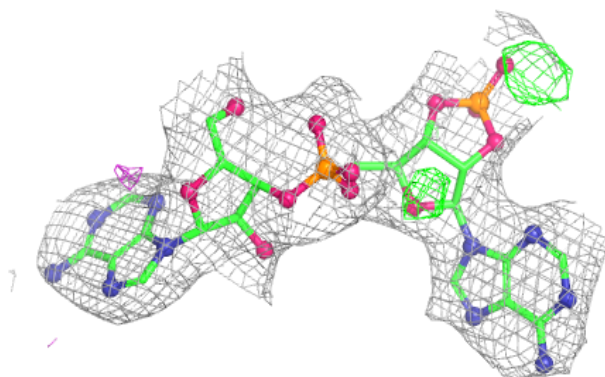
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q < 0.9
2	LQJ	AAA	301	44/44	0.93	0.07	39,74,95,107	0
2	LQJ	BBB	301	44/44	0.94	0.07	62,89,108,128	0

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.

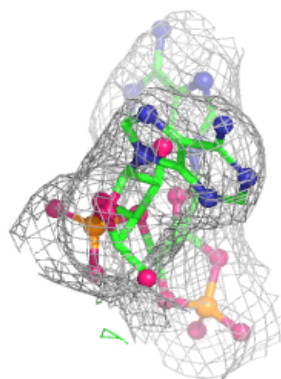
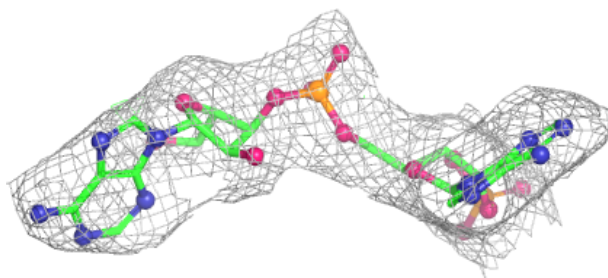
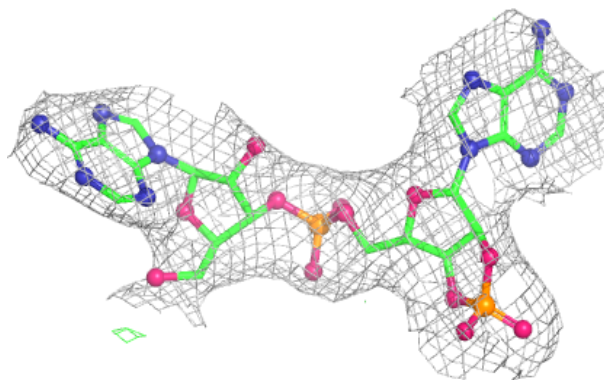
Electron density around LQJ AAA 301:

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



Electron density around LQJ 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.