



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:23 AM UTC

PDB ID : 6G15 / pdb_00006g15
Title : Crystal structure of pppGpp bound RbgA from S. aureus
Authors : Pausch, P.; Bange, G.
Deposited on : 2018-03-20
Resolution : 1.65 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

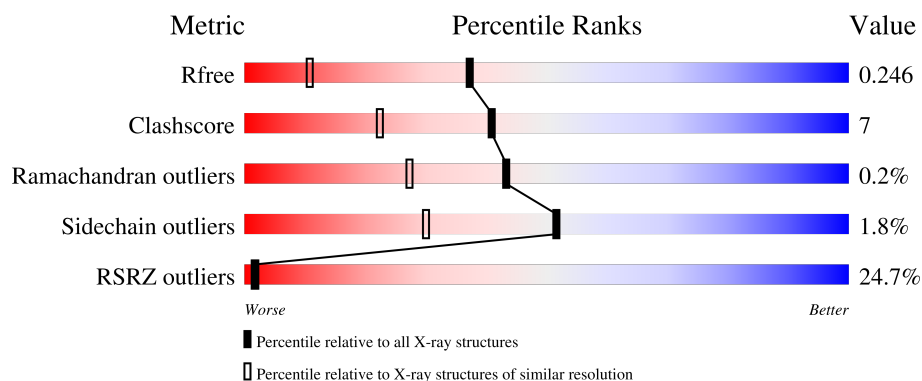
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.65 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	2563 (1.66-1.66)
Clashscore	190562	2662 (1.66-1.66)
Ramachandran outliers	187476	2621 (1.66-1.66)
Sidechain outliers	187428	2621 (1.66-1.66)
RSRZ outliers	180081	2564 (1.66-1.66)

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	A	301	23% 86% 9% • 5%
1	B	301	24% 83% 13% • •

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5112 atoms, of which 22 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.

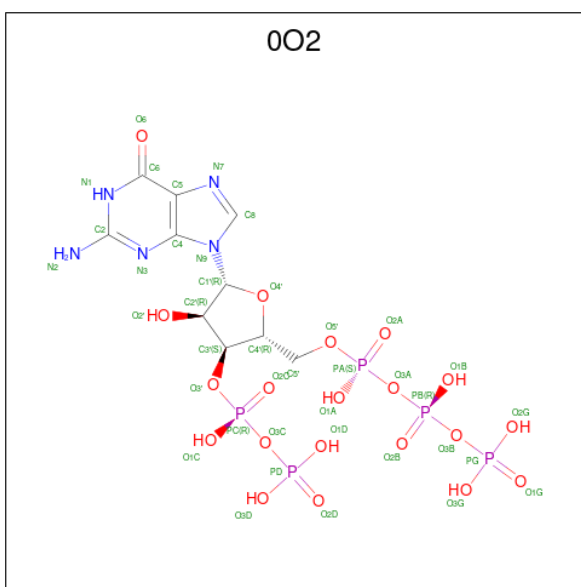
- Molecule 1 is a protein called Ribosome biogenesis GTPase A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	287	Total	C	N	O	S	0	0	0
			2297	1474	397	419	7			
1	B	289	Total	C	N	O	S	0	0	0
			2314	1484	401	422	7			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	MET	-	initiating methionine	UNP A0A0H2XK72
A	-5	GLY	-	expression tag	UNP A0A0H2XK72
A	-4	HIS	-	expression tag	UNP A0A0H2XK72
A	-3	HIS	-	expression tag	UNP A0A0H2XK72
A	-2	HIS	-	expression tag	UNP A0A0H2XK72
A	-1	HIS	-	expression tag	UNP A0A0H2XK72
A	0	HIS	-	expression tag	UNP A0A0H2XK72
A	1	HIS	-	expression tag	UNP A0A0H2XK72
B	-6	MET	-	initiating methionine	UNP A0A0H2XK72
B	-5	GLY	-	expression tag	UNP A0A0H2XK72
B	-4	HIS	-	expression tag	UNP A0A0H2XK72
B	-3	HIS	-	expression tag	UNP A0A0H2XK72
B	-2	HIS	-	expression tag	UNP A0A0H2XK72
B	-1	HIS	-	expression tag	UNP A0A0H2XK72
B	0	HIS	-	expression tag	UNP A0A0H2XK72
B	1	HIS	-	expression tag	UNP A0A0H2XK72

- Molecule 2 is guanosine 5'-(tetrahydrogen triphosphate) 3'-(trihydrogen diphosphate) (CCD ID: 002) (formula: C₁₀H₁₈N₅O₂₀P₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total 51	C 10	H 11	N 5	O 20	P 5	0	0
2	B	1	Total 51	C 10	H 11	N 5	O 20	P 5	0	0

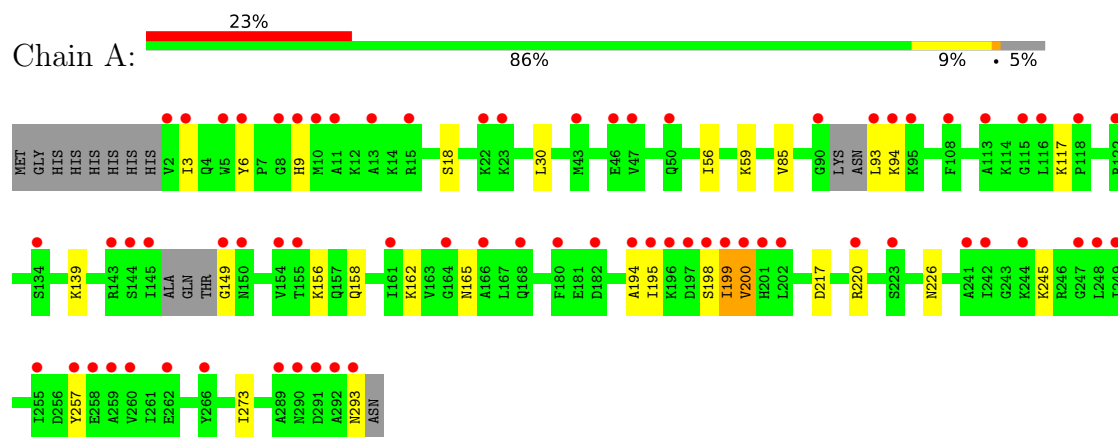
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	197	Total O 197 197	0	0
3	B	202	Total O 202 202	0	0

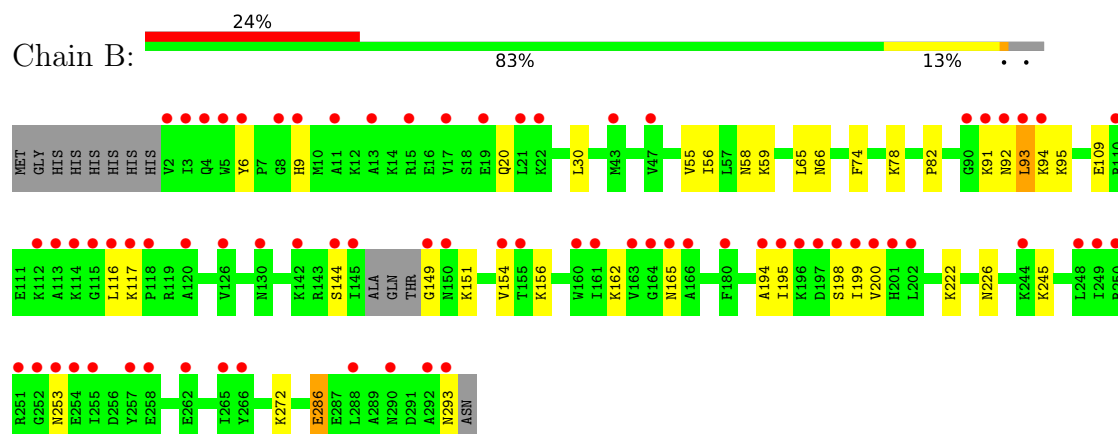
3 Residue-property plots [i](#)

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: Ribosome biogenesis GTPase A



• Molecule 1: Ribosome biogenesis GTPase A



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	72.08Å 78.47Å 125.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.89 – 1.65 48.89 – 1.65	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.89-1.65) 92.4 (48.89-1.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.16 (at 1.65Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.218 , 0.244 0.224 , 0.246	Depositor DCC
R_{free} test set	4447 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	28.7	Xtriage
Anisotropy	0.383	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 31.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5112	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 43.99 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.6280e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: 0O2

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.51	0/2337	0.74	1/3146 (0.0%)
1	B	0.54	1/2355 (0.0%)	0.73	2/3171 (0.1%)
All	All	0.53	1/4692 (0.0%)	0.74	3/6317 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	66	ASN	C-O	-5.42	1.17	1.24

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	6	TYR	N-CA-C	-6.24	102.60	108.22
1	B	6	TYR	N-CA-C	-5.68	103.11	108.22
1	B	65	LEU	N-CA-C	5.21	116.96	111.28

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	A	2297	0	2365	29	0
1	B	2314	0	2385	38	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	40	11	17	0	0
2	B	40	11	17	1	0
3	A	197	0	0	9	1
3	B	202	0	0	10	1
All	All	5090	22	4784	62	1

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 7.

All (62) 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:B:92:ASN:HB3	1:B:95:LYS:HE2	1.37	1.04
1:B:116:LEU:O	3:B:401:HOH:O	1.94	0.85
1:B:92:ASN:HB3	1:B:95:LYS:CE	2.07	0.83
1:B:20:GLN:NE2	3:B:403:HOH:O	2.14	0.81
1:A:158:GLN:OE1	3:A:401:HOH:O	1.98	0.80
1:A:220:ARG:NE	1:A:273:ILE:O	2.16	0.77
1:B:198:SER:HB3	1:B:199:ILE:HD12	1.66	0.74
1:A:9:HIS:CE1	1:B:199:ILE:HG12	2.22	0.73
1:A:220:ARG:NH2	3:A:406:HOH:O	2.23	0.72
1:B:222:LYS:NZ	3:B:406:HOH:O	2.23	0.72
1:A:195:ILE:HG13	1:A:195:ILE:O	1.90	0.71
1:A:293:ASN:O	3:A:402:HOH:O	2.09	0.69
1:B:195:ILE:O	1:B:195:ILE:HG13	1.93	0.67
1:B:149:GLY:N	1:B:156:LYS:HB2	2.10	0.65
1:A:226:ASN:OD1	1:A:245:LYS:NZ	2.30	0.65
1:A:257:TYR:CE2	1:B:151:LYS:HE2	2.33	0.64
1:B:199:ILE:HG22	1:B:199:ILE:O	1.97	0.63
2:B:301:O2:O1G	3:B:404:HOH:O	2.16	0.63
1:A:149:GLY:N	1:A:156:LYS:HB2	2.15	0.62
1:A:139:LYS:NZ	3:A:403:HOH:O	2.14	0.61
1:B:198:SER:CB	1:B:199:ILE:HD12	2.31	0.60
1:B:194:ALA:HB2	3:B:451:HOH:O	2.03	0.58
1:B:199:ILE:HD12	1:B:199:ILE:N	2.19	0.58
1:A:199:ILE:HD11	1:B:9:HIS:HE1	1.69	0.56
1:A:93:LEU:HD21	3:A:524:HOH:O	2.05	0.55
1:A:18:SER:OG	3:A:405:HOH:O	2.18	0.54
1:B:198:SER:HB3	1:B:199:ILE:CD1	2.38	0.53
1:A:199:ILE:HD11	1:B:9:HIS:CE1	2.44	0.51
1:A:85:VAL:CG1	1:A:93:LEU:HD22	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:30:LEU:HD12	1:B:56:ILE:HB	1.92	0.51
1:A:3:ILE:HG23	1:B:199:ILE:HD11	1.94	0.50
1:A:200:VAL:HG13	3:A:484:HOH:O	2.11	0.50
1:A:9:HIS:CE1	1:B:199:ILE:CG1	2.95	0.49
1:A:199:ILE:N	1:A:199:ILE:HD12	2.28	0.48
1:B:272:LYS:NZ	3:B:412:HOH:O	2.44	0.48
1:A:30:LEU:HD12	1:A:56:ILE:HB	1.95	0.48
1:B:144:SER:OG	3:B:405:HOH:O	2.20	0.48
1:A:217:ASP:OD2	1:A:220:ARG:HD3	2.13	0.47
1:B:109:GLU:HG3	3:B:440:HOH:O	2.14	0.47
1:A:162:LYS:HZ1	1:A:165:ASN:C	2.22	0.47
1:B:30:LEU:HD11	1:B:58:ASN:HB2	1.96	0.47
1:A:93:LEU:HA	1:A:93:LEU:HD23	1.66	0.47
1:B:162:LYS:HZ1	1:B:165:ASN:C	2.22	0.47
1:B:226:ASN:OD1	1:B:245:LYS:NZ	2.48	0.46
1:A:85:VAL:HB	1:A:93:LEU:CD2	2.45	0.46
1:B:151:LYS:HB2	1:B:154:VAL:HG21	1.98	0.45
1:B:286:GLU:HB2	3:B:501:HOH:O	2.17	0.45
1:B:59:LYS:NZ	3:B:402:HOH:O	2.11	0.43
1:B:199:ILE:O	1:B:199:ILE:CG2	2.65	0.43
1:B:93:LEU:HD23	1:B:93:LEU:N	2.33	0.43
1:B:91:LYS:O	1:B:92:ASN:HB2	2.19	0.43
1:B:55:VAL:O	1:B:82:PRO:HA	2.19	0.42
1:B:151:LYS:HB2	1:B:154:VAL:CG2	2.49	0.42
1:B:162:LYS:HA	1:B:162:LYS:HD2	1.88	0.42
1:B:94:LYS:HD2	1:B:94:LYS:HA	1.80	0.42
1:A:162:LYS:HA	1:A:162:LYS:HD2	1.80	0.41
1:B:74:PHE:CZ	1:B:78:LYS:HE2	2.55	0.41
1:A:194:ALA:HB2	3:A:496:HOH:O	2.20	0.41
1:A:198:SER:OG	1:A:199:ILE:N	2.50	0.41
1:A:198:SER:HB3	1:A:199:ILE:HD12	2.03	0.41
1:B:92:ASN:HB3	1:B:95:LYS:NZ	2.34	0.40
1:A:59:LYS:NZ	3:A:417:HOH:O	2.55	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:523:HOH:O	3:B:562:HOH:O[2_455]	2.06	0.14

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	281/301 (93%)	274 (98%)	6 (2%)	1 (0%)	30	15
1	B	285/301 (95%)	276 (97%)	9 (3%)	0	100	100
All	All	566/602 (94%)	550 (97%)	15 (3%)	1 (0%)	43	27

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	199	ILE

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	246/258 (95%)	243 (99%)	3 (1%)	63	45
1	B	248/258 (96%)	242 (98%)	6 (2%)	43	20
All	All	494/516 (96%)	485 (98%)	9 (2%)	51	30

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	94	LYS
1	A	117	LYS
1	A	200	VAL
1	B	93	LEU
1	B	117	LYS

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Mol	Chain	Res	Type
1	B	200	VAL
1	B	253	ASN
1	B	286	GLU
1	B	293	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	HIS
1	A	20	GLN
1	A	130	ASN
1	A	275	ASN
1	B	9	HIS
1	B	20	GLN
1	B	130	ASN
1	B	275	ASN

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](#)

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	0O2	A	301	-	40,42,42	3.00	12 (30%)	61,68,68	2.45	18 (29%)
2	0O2	B	301	-	40,42,42	3.04	12 (30%)	61,68,68	2.40	21 (34%)

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	0O2	A	301	-	-	5/33/49/49	0/3/3/3
2	0O2	B	301	-	-	7/33/49/49	0/3/3/3

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	0O2	C5-N7	8.61	1.56	1.39
2	A	301	0O2	C5-N7	8.41	1.56	1.39
2	B	301	0O2	O6-C6	8.36	1.39	1.23
2	A	301	0O2	O6-C6	7.76	1.38	1.23
2	B	301	0O2	C8-N9	-6.76	1.22	1.37
2	A	301	0O2	C8-N9	-6.69	1.22	1.37
2	A	301	0O2	C2-N3	6.27	1.48	1.33
2	B	301	0O2	C2-N3	5.86	1.47	1.33
2	B	301	0O2	C4-N9	-5.22	1.24	1.38
2	A	301	0O2	C4-N9	-5.07	1.25	1.38
2	B	301	0O2	O4'-C1'	4.88	1.53	1.42
2	A	301	0O2	O4'-C1'	4.85	1.53	1.42
2	A	301	0O2	C2'-C3'	-3.78	1.44	1.53
2	A	301	0O2	O4'-C4'	3.74	1.53	1.45
2	B	301	0O2	O4'-C4'	3.62	1.53	1.45
2	B	301	0O2	C2'-C3'	-3.42	1.45	1.53
2	A	301	0O2	C2-N2	3.35	1.42	1.34
2	A	301	0O2	C4-N3	3.30	1.41	1.34
2	B	301	0O2	C2-N2	3.06	1.41	1.34
2	B	301	0O2	C4-N3	2.85	1.40	1.34
2	B	301	0O2	C1'-N9	-2.77	1.39	1.47
2	A	301	0O2	C1'-N9	-2.60	1.40	1.47
2	A	301	0O2	C3'-C4'	-2.11	1.47	1.52
2	B	301	0O2	C3'-C4'	-2.09	1.47	1.52

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	0O2	C8-N9-C4	8.42	121.81	106.03
2	B	301	0O2	C8-N9-C4	8.35	121.67	106.03
2	A	301	0O2	C5-C4-N3	-7.04	117.18	128.39
2	A	301	0O2	N9-C4-N3	6.89	139.73	125.95
2	B	301	0O2	C5-C4-N3	-6.69	117.74	128.39
2	B	301	0O2	N9-C4-N3	6.11	138.16	125.95
2	A	301	0O2	C2-N3-C4	5.15	121.16	112.30
2	B	301	0O2	C2-N3-C4	5.09	121.06	112.30
2	B	301	0O2	C4-C5-N7	-4.02	104.30	110.67
2	A	301	0O2	O2G-PG-O3B	3.97	117.96	104.64
2	B	301	0O2	C2-N1-C6	-3.66	118.47	125.11
2	A	301	0O2	C2-N1-C6	-3.56	118.66	125.11
2	A	301	0O2	C4-C5-N7	-3.41	105.27	110.67
2	B	301	0O2	O3G-PG-O3B	3.33	115.80	104.64
2	A	301	0O2	C1'-N9-C8	-3.15	117.78	126.73
2	B	301	0O2	O1D-PD-O3C	3.11	115.06	104.64
2	A	301	0O2	C5-C6-N1	3.05	121.01	113.25
2	A	301	0O2	O3G-PG-O3B	2.97	114.61	104.64
2	B	301	0O2	O3D-PD-O3C	2.94	114.49	104.64
2	A	301	0O2	O1D-PD-O3C	2.87	114.28	104.64
2	B	301	0O2	C5-C6-N1	2.87	120.56	113.25
2	B	301	0O2	O2G-PG-O3B	2.74	113.84	104.64
2	B	301	0O2	C1'-N9-C8	-2.60	119.34	126.73
2	A	301	0O2	C2'-C3'-C4'	2.59	107.77	103.24
2	B	301	0O2	C1'-N9-C4	-2.58	118.86	126.49
2	B	301	0O2	O1C-PC-O2C	-2.54	100.64	112.44
2	A	301	0O2	C3'-C2'-C1'	2.48	105.35	99.89
2	B	301	0O2	C3'-C2'-C1'	2.44	105.25	99.89
2	A	301	0O2	C8-N7-C5	-2.44	99.92	104.26
2	A	301	0O2	O3D-PD-O3C	2.38	112.63	104.64
2	B	301	0O2	O1A-PA-O3A	2.35	113.61	107.27
2	B	301	0O2	C6-C5-N7	2.32	134.52	130.29
2	A	301	0O2	O1C-PC-O2C	-2.29	101.77	112.44
2	B	301	0O2	C8-N7-C5	-2.21	100.32	104.26
2	B	301	0O2	C2'-C3'-C4'	2.16	107.01	103.24
2	B	301	0O2	C4'-O4'-C1'	-2.11	104.81	109.47
2	A	301	0O2	C1'-N9-C4	-2.09	120.30	126.49
2	B	301	0O2	N9-C8-N7	-2.06	109.58	113.40
2	A	301	0O2	O6-C6-C5	-2.02	121.20	126.53

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	0O2	C3'-O3'-PC-O1C
2	A	301	0O2	C3'-O3'-PC-O3C
2	A	301	0O2	PD-O3C-PC-O3'
2	B	301	0O2	C3'-O3'-PC-O2C
2	B	301	0O2	C3'-O3'-PC-O3C
2	B	301	0O2	PD-O3C-PC-O3'
2	B	301	0O2	C3'-O3'-PC-O1C
2	A	301	0O2	C3'-O3'-PC-O2C
2	B	301	0O2	PD-O3C-PC-O1C
2	B	301	0O2	PD-O3C-PC-O2C
2	A	301	0O2	PA-O3A-PB-O1B
2	B	301	0O2	PA-O3A-PB-O1B

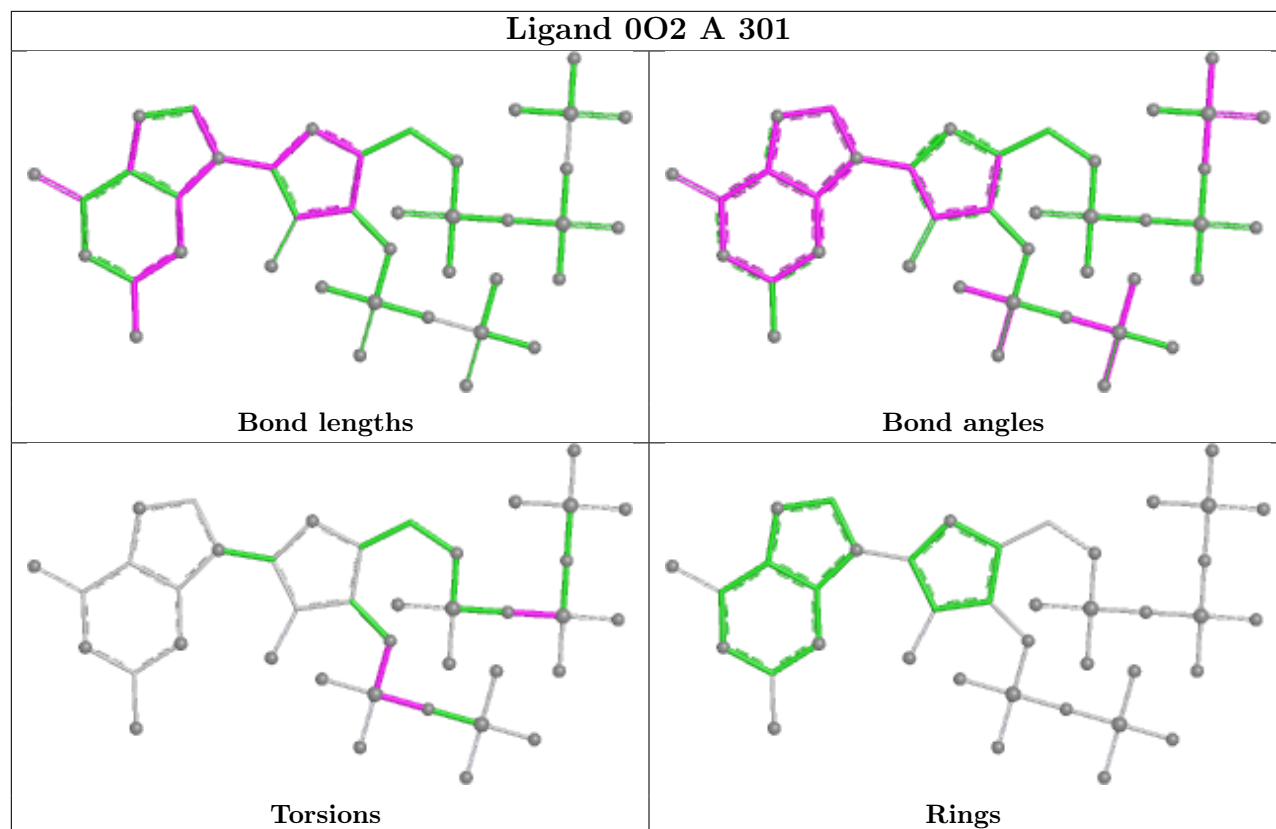
There are no ring outliers.

1 monomer is involved in 1 short contact:

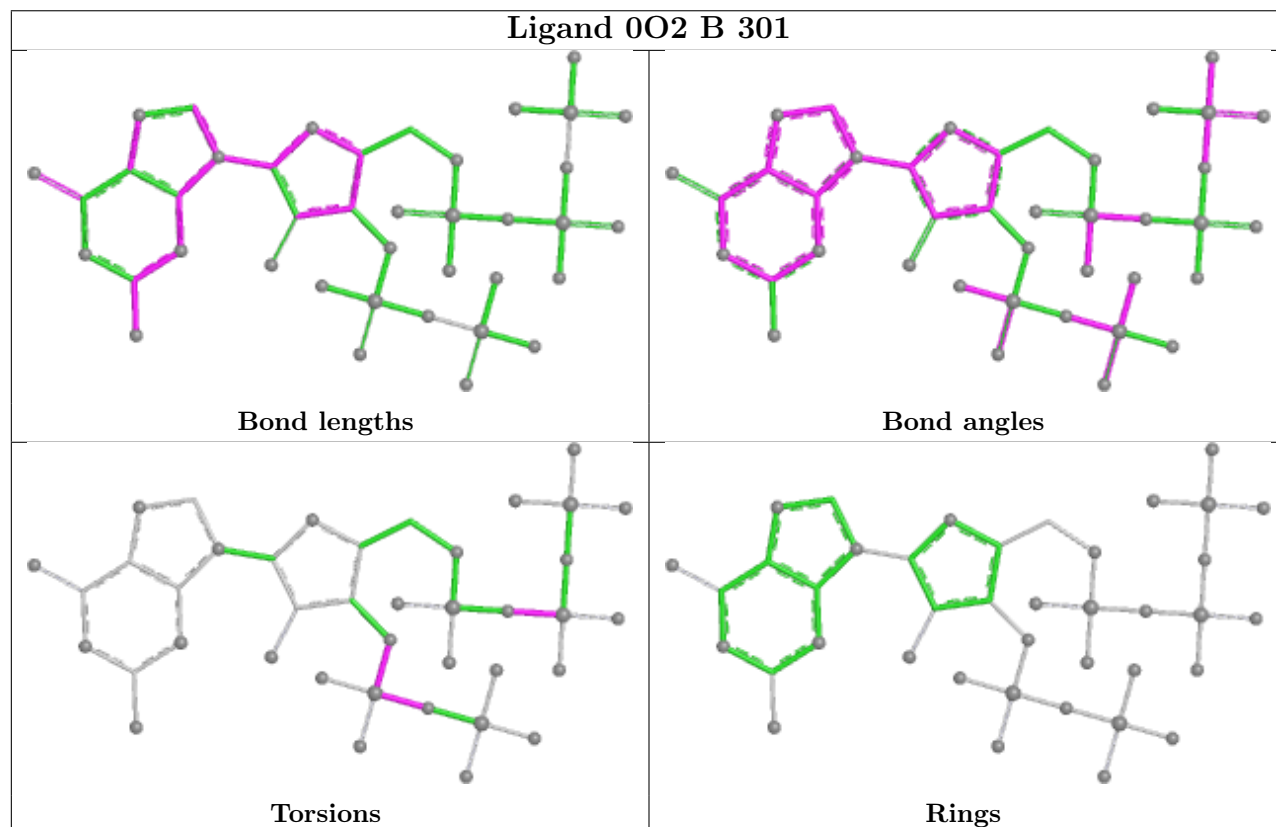
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	301	0O2	1	0

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 0O2 A 301



Ligand 0O2 B 301



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	A	287/301 (95%)	1.21	69 (24%) 2 2	23, 39, 77, 97	0
1	B	289/301 (96%)	1.24	73 (25%) 1 1	23, 38, 81, 110	0
All	All	576/602 (95%)	1.22	142 (24%) 2 2	23, 39, 78, 110	0

All (142) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	200	VAL	8.2
1	B	2	VAL	7.9
1	A	2	VAL	6.8
1	B	199	ILE	6.8
1	A	199	ILE	6.5
1	A	200	VAL	5.8
1	B	145	ILE	5.7
1	A	145	ILE	5.6
1	A	3	ILE	5.1
1	A	93	LEU	4.7
1	B	3	ILE	4.7
1	A	6	TYR	4.6
1	B	115	GLY	4.6
1	B	6	TYR	4.5
1	B	252	GLY	4.5
1	A	249	ILE	4.5
1	B	198	SER	4.5
1	B	249	ILE	4.3
1	B	197	ASP	4.3
1	B	5	TRP	4.3
1	A	180	PHE	4.2
1	A	248	LEU	4.1
1	A	116	LEU	3.9
1	A	293	ASN	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	197	ASP	3.8
1	A	90	GLY	3.7
1	B	113	ALA	3.6
1	B	293	ASN	3.6
1	A	5	TRP	3.6
1	B	91	LYS	3.5
1	B	180	PHE	3.5
1	B	15	ARG	3.5
1	B	248	LEU	3.5
1	B	93	LEU	3.5
1	B	195	ILE	3.4
1	B	92	ASN	3.4
1	A	292	ALA	3.4
1	A	122	ARG	3.3
1	A	149	GLY	3.3
1	B	149	GLY	3.3
1	A	258	GLU	3.3
1	B	43	MET	3.2
1	A	255	ILE	3.2
1	B	17	VAL	3.2
1	A	257	TYR	3.1
1	B	114	LYS	3.1
1	B	11	ALA	3.1
1	A	155	THR	3.1
1	B	155	THR	3.1
1	A	144	SER	3.1
1	A	223	SER	3.1
1	A	195	ILE	3.1
1	B	196	LYS	3.1
1	B	117	LYS	3.0
1	B	257	TYR	3.0
1	B	166	ALA	3.0
1	A	113	ALA	3.0
1	B	154	VAL	2.9
1	B	160	TRP	2.9
1	B	116	LEU	2.9
1	A	241	ALA	2.9
1	B	194	ALA	2.9
1	A	202	LEU	2.9
1	A	262	GLU	2.9
1	B	90	GLY	2.8
1	A	198	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	161	ILE	2.8
1	A	154	VAL	2.8
1	A	94	LYS	2.8
1	B	22	LYS	2.8
1	B	251	ARG	2.7
1	B	255	ILE	2.7
1	A	259	ALA	2.7
1	B	201	HIS	2.7
1	B	13	ALA	2.7
1	B	292	ALA	2.6
1	B	253	ASN	2.6
1	B	21	LEU	2.6
1	A	115	GLY	2.5
1	B	165	ASN	2.5
1	B	126	VAL	2.5
1	B	9	HIS	2.5
1	A	10	MET	2.5
1	A	43	MET	2.5
1	B	150	ASN	2.5
1	A	266	TYR	2.4
1	A	260	VAL	2.4
1	B	161	ILE	2.4
1	A	50	GLN	2.4
1	A	164	GLY	2.4
1	A	13	ALA	2.4
1	A	15	ARG	2.4
1	A	201	HIS	2.4
1	A	166	ALA	2.4
1	B	110	ARG	2.4
1	A	9	HIS	2.4
1	A	220	ARG	2.3
1	A	196	LYS	2.3
1	A	168	GLN	2.3
1	B	118	PRO	2.3
1	A	11	ALA	2.3
1	A	289	ALA	2.3
1	B	202	LEU	2.3
1	B	288	LEU	2.3
1	B	262	GLU	2.3
1	A	8	GLY	2.3
1	A	23	LYS	2.3
1	A	244	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	95	LYS	2.2
1	B	94	LYS	2.2
1	A	108	PHE	2.2
1	A	247	GLY	2.2
1	B	4	GLN	2.2
1	B	254	GLU	2.2
1	B	250	ARG	2.2
1	B	244	LYS	2.2
1	A	182	ASP	2.2
1	A	291	ASP	2.2
1	A	134	SER	2.2
1	B	164	GLY	2.2
1	B	290	ASN	2.2
1	B	266	TYR	2.2
1	A	118	PRO	2.2
1	A	242	ILE	2.2
1	A	47	VAL	2.1
1	B	163	VAL	2.1
1	A	194	ALA	2.1
1	B	112	LYS	2.1
1	A	22	LYS	2.1
1	B	142	LYS	2.1
1	A	46	GLU	2.1
1	B	265	ILE	2.1
1	B	8	GLY	2.0
1	A	290	ASN	2.0
1	B	19	GLU	2.0
1	A	143	ARG	2.0
1	B	258	GLU	2.0
1	A	150	ASN	2.0
1	B	130	ASN	2.0
1	B	120	ALA	2.0
1	B	144	SER	2.0
1	B	47	VAL	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 [i](#)

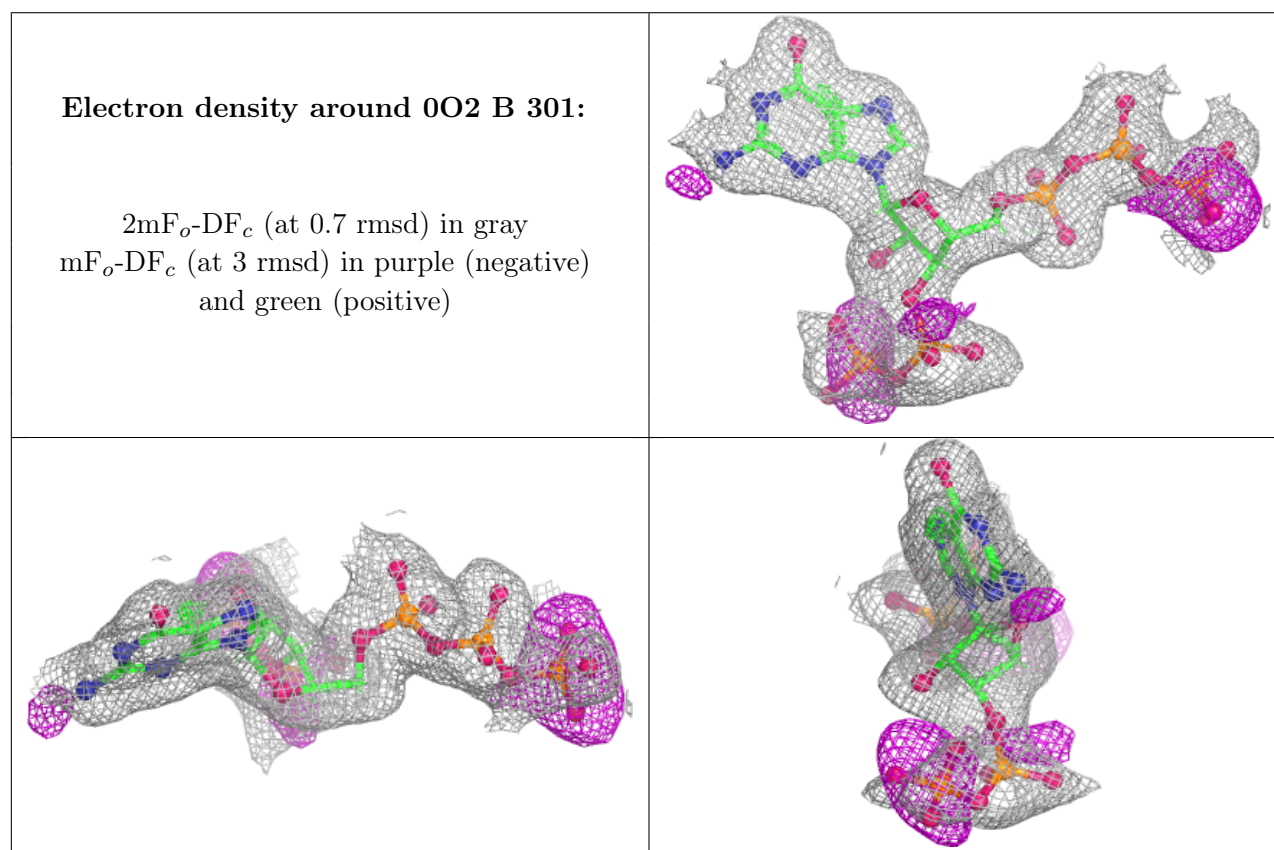
There are no oligosaccharides in this entry.

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.

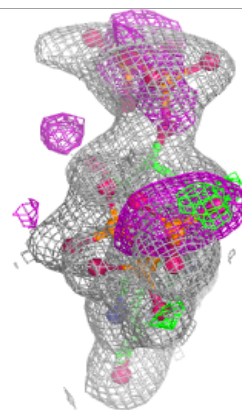
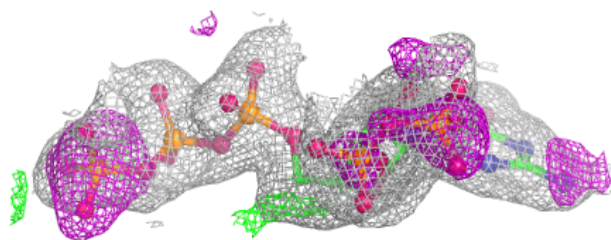
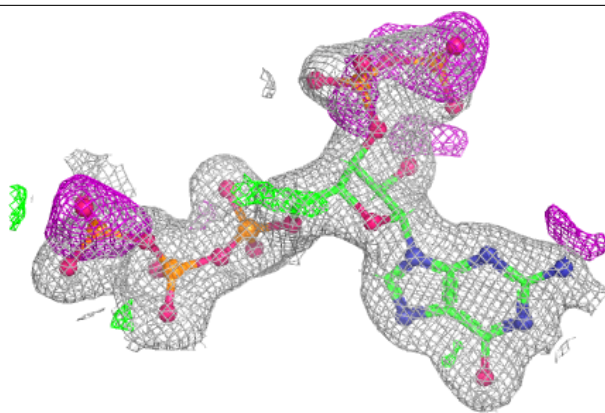
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	0O2	B	301	40/40	0.89	0.12	32,44,64,71	0
2	0O2	A	301	40/40	0.91	0.11	30,42,70,76	0

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 0O2 A 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.