



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:47 AM UTC

PDB ID : 1ST0 / pdb_00001st0
Title : Structure of DcpS bound to m7GpppG
Authors : Gu, M.; Fabrega, C.; Liu, S.W.; Liu, H.; Kiledjian, M.; Lima, C.D.
Deposited on : 2004-03-24
Resolution : 1.90 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

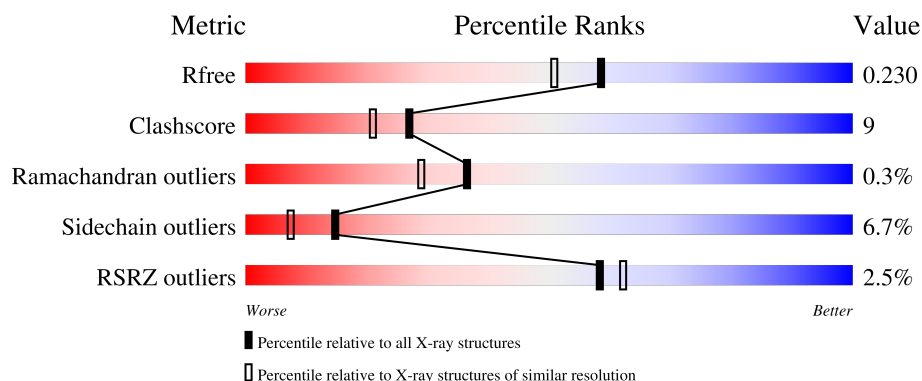
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

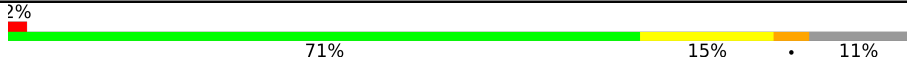
The reported resolution of this entry is 1.90 Å.

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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	337	
1	B	337	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 5647 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.

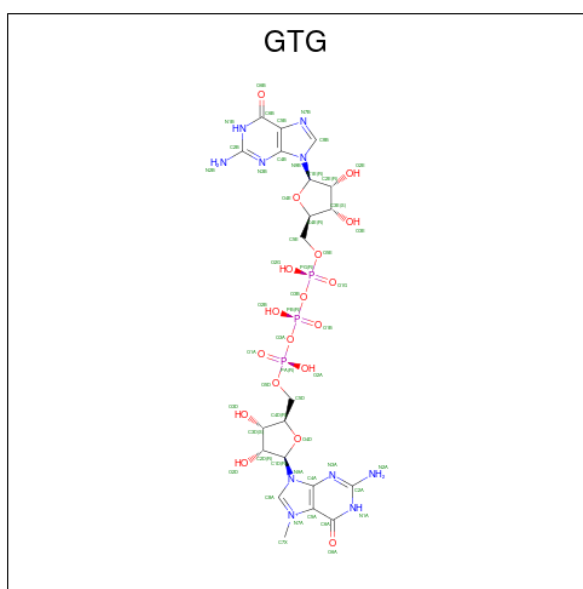
- Molecule 1 is a protein called mRNA decapping enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	297	Total	C	N	O	S	0	0	0
			2439	1554	435	447	3			
1	A	300	Total	C	N	O	S	0	0	0
			2458	1565	438	452	3			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	277	ASN	HIS	engineered mutation	UNP Q96C86
B	277	ASN	HIS	engineered mutation	UNP Q96C86

- Molecule 2 is 7-METHYL-GUANOSINE-5'-TRIPHOSPHATE-5'-GUANOSINE (CCD ID: GTG) (formula: C₂₁H₃₀N₁₀O₁₈P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			52	21	10	18	3		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			52	21	10	18	3		

- Molecule 3 is YTTRIUM (III) ION (CCD ID: YT3) (formula: Y).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total	Y	0	0
			3	3		

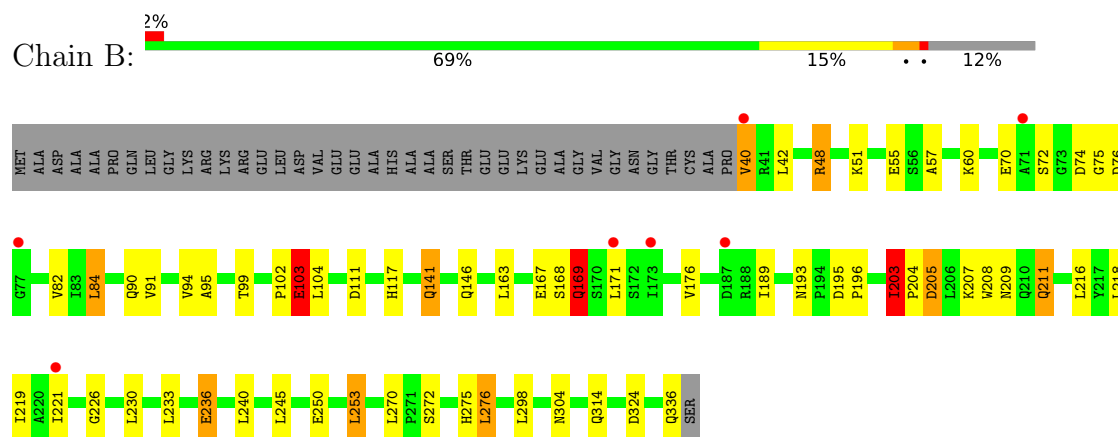
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	294	Total	O	0	0
			294	294		
4	A	349	Total	O	0	0
			349	349		

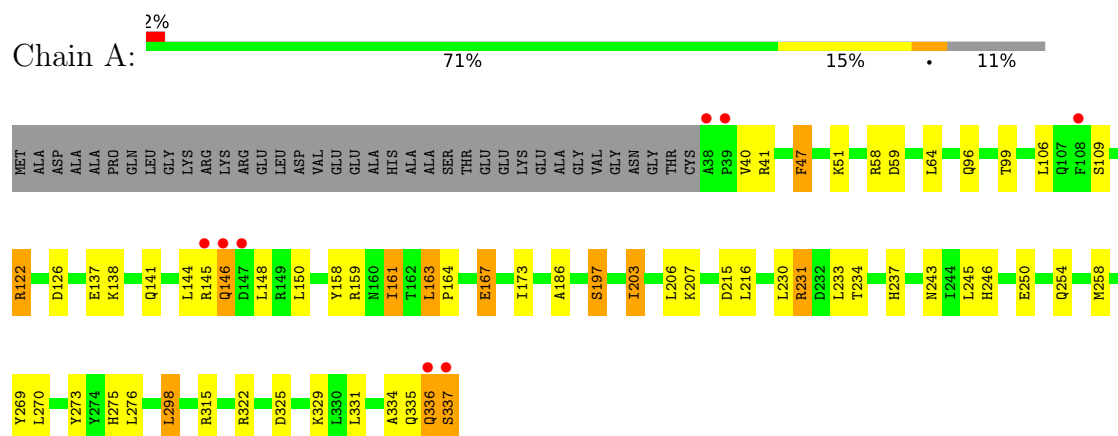
3 Residue-property plots [i](#)

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: mRNA decapping enzyme



- Molecule 1: mRNA decapping enzyme



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	59.45Å 94.78Å 178.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.90 20.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.1 (20.00-1.90) 99.1 (20.00-1.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.86 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.187 , 0.231 0.187 , 0.230	Depositor DCC
R_{free} test set	3991 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	29.1	Xtriage
Anisotropy	0.060	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 41.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5647	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.70% 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: GTG, YT3

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	1.35	7/2515 (0.3%)	1.19	5/3413 (0.1%)
1	B	1.25	2/2495 (0.1%)	1.17	4/3386 (0.1%)
All	All	1.30	9/5010 (0.2%)	1.18	9/6799 (0.1%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	203	ILE	C-O	-7.38	1.18	1.24
1	A	258	MET	SD-CE	6.23	1.95	1.79
1	B	240	LEU	CA-C	6.04	1.60	1.52
1	A	203	ILE	CA-C	5.68	1.58	1.52
1	A	47	PHE	CA-C	-5.58	1.46	1.52
1	A	243	ASN	CA-C	5.57	1.59	1.52
1	A	186	ALA	CA-CB	5.46	1.62	1.53
1	B	203	ILE	CA-CB	5.35	1.61	1.54
1	A	250	GLU	CA-CB	5.13	1.61	1.53

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	104	LEU	N-CA-C	6.03	119.31	109.24
1	A	47	PHE	N-CA-C	-6.00	97.81	108.13
1	A	203	ILE	CB-CA-C	-5.90	103.52	109.89
1	B	103	GLU	N-CA-C	5.85	118.97	107.98
1	B	75	GLY	N-CA-C	-5.77	107.10	114.37
1	A	231	ARG	NE-CZ-NH2	-5.45	114.29	119.20
1	A	231	ARG	CB-CG-CD	5.17	123.19	111.30
1	B	111	ASP	CB-CA-C	-5.14	110.67	116.63
1	A	243	ASN	N-CA-C	-5.00	105.90	111.36

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	A	2458	0	2445	48	0
1	B	2439	0	2428	50	0
2	A	52	0	26	1	0
2	B	52	0	26	3	0
3	A	3	0	0	0	1
4	A	349	0	0	12	0
4	B	294	0	0	12	0
All	All	5647	0	4925	91	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 9.

All (91) 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:102:PRO:HA	4:B:942:HOH:O	1.26	1.33
1:A:254:GLN:HG3	4:A:962:HOH:O	1.48	1.11
1:B:205:ASP:HB2	1:B:219:ILE:CD1	1.84	1.06
1:B:205:ASP:HB2	1:B:219:ILE:HD12	1.11	1.05
1:B:91:VAL:HG23	4:A:829:HOH:O	1.62	0.97
1:B:90:GLN:HG3	4:B:906:HOH:O	1.69	0.93
1:B:205:ASP:OD2	1:B:207:LYS:HG2	1.69	0.92
1:A:40:VAL:HG12	1:A:41:ARG:H	1.36	0.91
1:A:322:ARG:HD3	4:A:836:HOH:O	1.77	0.84
1:A:40:VAL:HG12	1:A:41:ARG:N	1.95	0.81
1:A:245:LEU:HB2	1:A:298:LEU:HD13	1.62	0.80
1:A:234:THR:H	1:A:237:HIS:HD2	1.29	0.78
1:B:205:ASP:CB	1:B:219:ILE:HD12	2.05	0.74
1:B:168:SER:O	1:B:169:GLN:HB2	1.88	0.73
1:A:40:VAL:CG1	1:A:41:ARG:H	2.04	0.71
1:B:163:LEU:O	1:B:167:GLU:HG2	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:74:ASP:HB3	1:B:76:ASP:H	1.55	0.70
1:A:246:HIS:HE1	4:A:845:HOH:O	1.78	0.65
1:B:51:LYS:HE2	4:B:867:HOH:O	1.97	0.65
1:A:158:TYR:CG	1:A:231:ARG:HD3	2.32	0.64
1:A:234:THR:H	1:A:237:HIS:CD2	2.14	0.63
1:B:169:GLN:HA	1:B:169:GLN:OE1	1.99	0.62
1:B:176:VAL:HG13	1:B:221:ILE:HG21	1.81	0.61
1:B:48:ARG:HD3	1:B:70:GLU:OE1	2.01	0.61
1:A:197:SER:HB3	4:A:926:HOH:O	2.00	0.61
1:A:254:GLN:HG3	4:A:1047:HOH:O	2.00	0.60
1:B:103:GLU:CD	1:A:122:ARG:NH1	2.60	0.59
1:A:137:GLU:OE1	1:A:141:GLN:NE2	2.36	0.59
1:A:322:ARG:HG2	1:A:325:ASP:HB2	1.85	0.58
1:B:236:GLU:O	1:B:236:GLU:HG3	2.02	0.57
1:B:314:GLN:HG2	4:B:822:HOH:O	2.03	0.56
1:A:331:LEU:O	1:A:335:GLN:HG3	2.05	0.56
1:A:163:LEU:HB3	1:A:164:PRO:HD3	1.88	0.56
1:B:103:GLU:OE2	1:A:122:ARG:NH1	2.39	0.55
1:B:272:SER:HB2	2:B:652:GTG:O3A	2.08	0.53
1:B:336:GLN:HB2	4:B:865:HOH:O	2.09	0.53
1:A:207:LYS:NZ	2:A:651:GTG:O2G	2.30	0.52
1:B:230:LEU:HD12	1:B:233:LEU:HD12	1.91	0.52
1:B:74:ASP:HB2	4:B:887:HOH:O	2.10	0.51
1:A:96:GLN:HG2	4:A:959:HOH:O	2.11	0.51
1:A:51:LYS:HE2	1:A:144:LEU:CD1	2.43	0.49
1:B:314:GLN:NE2	4:B:815:HOH:O	2.44	0.48
1:B:117:HIS:ND1	1:A:126:ASP:OD2	2.46	0.48
1:A:41:ARG:HG2	4:A:1001:HOH:O	2.13	0.48
1:B:204:PRO:HA	1:B:218:LEU:HD23	1.96	0.48
1:B:94:VAL:CG1	1:A:64:LEU:HD11	2.43	0.48
1:A:322:ARG:CD	4:A:836:HOH:O	2.49	0.48
1:B:99:THR:HG22	1:A:47:PHE:O	2.15	0.47
1:B:141:GLN:HG3	4:B:896:HOH:O	2.14	0.47
1:B:40:VAL:HG11	4:B:899:HOH:O	2.15	0.47
1:B:193:ASN:OD1	1:B:193:ASN:C	2.56	0.47
4:B:709:HOH:O	1:A:315:ARG:HD2	2.15	0.47
1:A:40:VAL:CG1	1:A:41:ARG:N	2.63	0.47
1:B:209:ASN:CG	1:B:211:GLN:HG3	2.40	0.46
1:A:51:LYS:HE2	1:A:144:LEU:HD13	1.98	0.46
1:B:226:GLY:O	4:B:778:HOH:O	2.21	0.46
1:A:233:LEU:HA	1:A:237:HIS:CD2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:95:ALA:O	1:B:99:THR:HG23	2.15	0.46
1:B:103:GLU:O	1:B:103:GLU:CG	2.64	0.45
1:A:158:TYR:CD1	1:A:231:ARG:HD3	2.52	0.45
1:A:231:ARG:HD2	1:A:269:TYR:OH	2.16	0.45
1:A:237:HIS:HE1	4:A:837:HOH:O	1.99	0.45
1:B:82:VAL:HG12	1:B:84:LEU:HD22	1.97	0.44
1:B:146:GLN:HG3	1:B:324:ASP:CG	2.42	0.44
2:B:652:GTG:O1G	2:B:652:GTG:H2'	2.17	0.44
1:A:138:LYS:HE3	4:A:1029:HOH:O	2.17	0.44
1:B:94:VAL:HG11	1:A:64:LEU:HD11	1.99	0.44
1:B:57:ALA:O	1:B:60:LYS:HE3	2.17	0.44
1:B:253:LEU:C	1:B:253:LEU:HD22	2.42	0.44
1:B:103:GLU:HB3	4:B:753:HOH:O	2.16	0.44
1:B:189:ILE:HA	1:B:203:ILE:HG22	1.99	0.44
1:A:336:GLN:HG2	1:A:337:SER:N	2.33	0.44
1:A:106:LEU:HD11	1:A:109:SER:HB2	2.00	0.43
1:A:215:ASP:O	1:A:216:LEU:C	2.61	0.43
1:B:221:ILE:HG23	1:B:275:HIS:CD2	2.55	0.42
1:A:161:ILE:HD11	1:A:334:ALA:HB2	2.01	0.42
1:A:167:GLU:HB2	4:A:971:HOH:O	2.19	0.42
1:B:209:ASN:OD1	1:B:211:GLN:HG3	2.20	0.41
1:B:304:ASN:OD1	1:A:315:ARG:NH2	2.32	0.41
1:A:146:GLN:HB3	1:A:148:LEU:HG	2.02	0.41
1:A:230:LEU:HA	1:A:230:LEU:HD12	1.81	0.41
1:B:195:ASP:HA	1:B:196:PRO:HD3	1.96	0.41
1:B:168:SER:O	1:B:169:GLN:CB	2.65	0.41
1:A:59:ASP:N	1:A:59:ASP:OD2	2.54	0.41
1:A:206:LEU:C	1:A:206:LEU:HD23	2.46	0.41
1:B:219:ILE:HD11	2:B:652:GTG:O3D	2.20	0.41
1:B:208:TRP:CE2	1:B:216:LEU:HA	2.56	0.41
1:B:103:GLU:CD	1:A:122:ARG:HH12	2.28	0.41
1:B:275:HIS:O	1:B:276:LEU:C	2.64	0.40
1:A:173:ILE:HG22	1:A:273:TYR:HB3	2.04	0.40
1:A:275:HIS:O	1:A:276:LEU:C	2.64	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:701:YT3:Y	3:A:702:YT3:Y[3_655]	2.07	0.13

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	298/337 (88%)	285 (96%)	12 (4%)	1 (0%)	36	29
1	B	295/337 (88%)	284 (96%)	10 (3%)	1 (0%)	36	29
All	All	593/674 (88%)	569 (96%)	22 (4%)	2 (0%)	36	29

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	169	GLN
1	A	145	ARG

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	269/295 (91%)	253 (94%)	16 (6%)	18	10
1	B	267/295 (90%)	247 (92%)	20 (8%)	12	6
All	All	536/590 (91%)	500 (93%)	36 (7%)	15	7

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	40	VAL
1	B	42	LEU
1	B	48	ARG
1	B	55	GLU

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Mol	Chain	Res	Type
1	B	72	SER
1	B	84	LEU
1	B	103	GLU
1	B	141	GLN
1	B	169	GLN
1	B	171	LEU
1	B	203	ILE
1	B	205	ASP
1	B	211	GLN
1	B	236	GLU
1	B	245	LEU
1	B	250	GLU
1	B	253	LEU
1	B	270	LEU
1	B	276	LEU
1	B	298	LEU
1	A	58	ARG
1	A	99	THR
1	A	122	ARG
1	A	146	GLN
1	A	150	LEU
1	A	159	ARG
1	A	161	ILE
1	A	163	LEU
1	A	167	GLU
1	A	197	SER
1	A	203	ILE
1	A	270	LEU
1	A	298	LEU
1	A	329	LYS
1	A	336	GLN
1	A	337	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	105	GLN
1	B	123	GLN
1	B	125	ASN
1	B	165	HIS
1	A	50	GLN
1	A	165	HIS

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Mol	Chain	Res	Type
1	A	169	GLN
1	A	174	GLN
1	A	237	HIS
1	A	246	HIS
1	A	249	GLN
1	A	314	GLN
1	A	336	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 5 ligands modelled in this entry, 3 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	$\# Z > 2$
2	GTG	B	652	-	57,57,57	1.94	10 (17%)	85,90,90	1.96	23 (27%)
2	GTG	A	651	-	57,57,57	2.04	14 (24%)	85,90,90	2.01	26 (30%)

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	GTG	B	652	-	-	7/32/64/64	0/6/6/6
2	GTG	A	651	-	-	8/32/64/64	0/6/6/6

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	651	GTG	PB-O3B	-6.38	1.52	1.59
2	B	652	GTG	C4A-N3A	5.50	1.46	1.34
2	B	652	GTG	C5E-C4E	-5.46	1.35	1.51
2	B	652	GTG	PA-O3A	5.45	1.65	1.59
2	B	652	GTG	C8B-N7B	5.17	1.47	1.32
2	A	651	GTG	C5A-N7A	-5.10	1.33	1.39
2	A	651	GTG	C5E-C4E	-5.05	1.36	1.51
2	B	652	GTG	PB-O3A	4.38	1.64	1.59
2	A	651	GTG	PA-O3A	-4.36	1.54	1.59
2	B	652	GTG	C8B-N9B	4.21	1.47	1.37
2	A	651	GTG	C4A-N3A	4.18	1.43	1.34
2	B	652	GTG	C8A-N7A	3.61	1.39	1.33
2	A	651	GTG	PG-O3B	3.57	1.63	1.59
2	A	651	GTG	C5B-N7B	-3.16	1.32	1.39
2	A	651	GTG	C8B-N7B	3.13	1.41	1.32
2	A	651	GTG	C4B-N9B	-2.96	1.30	1.38
2	A	651	GTG	C8A-N7A	2.72	1.37	1.33
2	A	651	GTG	C5B-C6B	-2.71	1.34	1.44
2	B	652	GTG	C5A-N7A	-2.29	1.36	1.39
2	B	652	GTG	PB-O3B	2.23	1.61	1.59
2	A	651	GTG	O4E-C1E	2.21	1.47	1.42
2	B	652	GTG	C7X-N7A	2.15	1.50	1.46
2	A	651	GTG	C2A-N3A	2.14	1.38	1.33
2	A	651	GTG	C8B-N9B	2.10	1.42	1.37

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	651	GTG	N9B-C8B-N7B	-8.29	98.03	113.40
2	B	652	GTG	N9B-C8B-N7B	-6.53	101.30	113.40
2	B	652	GTG	C6A-C5A-N7A	5.54	139.12	132.17
2	A	651	GTG	C8B-N9B-C4B	5.18	115.74	106.03
2	B	652	GTG	C5A-C6A-N1A	5.01	122.19	111.84
2	B	652	GTG	C5B-C4B-N3B	-4.42	121.36	128.39
2	A	651	GTG	C6A-C5A-N7A	4.42	137.71	132.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	651	GTG	O4E-C1E-N9B	-4.03	99.23	108.36
2	A	651	GTG	C8B-N7B-C5B	3.54	110.58	104.26
2	B	652	GTG	C2B-N3B-C4B	3.42	118.19	112.30
2	A	651	GTG	O3A-PA-O1A	-3.25	100.93	110.70
2	B	652	GTG	C2A-N3A-C4A	3.18	117.78	112.30
2	B	652	GTG	O2G-PG-O3B	3.18	115.86	107.27
2	A	651	GTG	C5A-C6A-N1A	3.13	118.31	111.84
2	A	651	GTG	C2B-N3B-C4B	3.12	117.67	112.30
2	B	652	GTG	O4E-C1E-N9B	3.05	115.27	108.36
2	B	652	GTG	O6A-C6A-C5A	-2.99	121.34	128.01
2	B	652	GTG	C5A-C4A-N9A	2.99	112.26	105.88
2	B	652	GTG	O4E-C4E-C3E	2.97	111.05	105.15
2	B	652	GTG	C5A-C4A-N3A	-2.96	122.56	128.15
2	B	652	GTG	C8B-N7B-C5B	2.95	109.52	104.26
2	A	651	GTG	O4E-C4E-C3E	2.87	110.84	105.15
2	B	652	GTG	C3E-C2E-C1E	2.84	106.84	101.46
2	B	652	GTG	O5E-C5E-C4E	2.79	118.49	108.99
2	A	651	GTG	O4D-C1D-N9A	-2.77	102.09	108.36
2	A	651	GTG	C5A-C4A-N9A	2.76	111.76	105.88
2	A	651	GTG	N9B-C4B-N3B	2.72	131.40	125.95
2	A	651	GTG	O4E-C4E-C5E	2.63	117.75	109.33
2	A	651	GTG	C5B-C4B-N3B	-2.60	124.26	128.39
2	B	652	GTG	O3B-PB-O1B	-2.53	103.09	110.70
2	A	651	GTG	O6B-C6B-C5B	-2.52	119.88	126.53
2	A	651	GTG	O2G-PG-O1G	2.51	124.12	112.44
2	A	651	GTG	O2B-PB-O3B	2.48	113.97	107.27
2	A	651	GTG	O3A-PB-O1B	-2.39	103.52	110.70
2	B	652	GTG	C8B-N9B-C4B	2.32	110.38	106.03
2	A	651	GTG	O3E-C3E-C4E	-2.27	104.55	111.08
2	A	651	GTG	O2G-PG-O3B	-2.27	101.13	107.27
2	B	652	GTG	C6A-C5A-C4A	-2.27	115.09	119.01
2	A	651	GTG	O6A-C6A-C5A	-2.26	122.97	128.01
2	A	651	GTG	N1B-C2B-N3B	-2.24	119.22	123.32
2	B	652	GTG	O2B-PB-O1B	2.21	122.74	112.44
2	B	652	GTG	O4E-C4E-C5E	2.20	116.39	109.33
2	A	651	GTG	C3D-C2D-C1D	-2.15	97.40	101.46
2	A	651	GTG	C5A-C4A-N3A	-2.13	124.13	128.15
2	B	652	GTG	C2B-N1B-C6B	-2.08	121.33	125.11
2	A	651	GTG	C1E-N9B-C8B	-2.06	120.89	126.73
2	B	652	GTG	C7X-N7A-C8A	2.05	127.89	124.79
2	A	651	GTG	C3E-C2E-C1E	2.03	105.31	101.46
2	B	652	GTG	O3B-PG-O1G	-2.03	104.59	110.70

There are no chirality outliers.

All (15) torsion outliers are listed below:

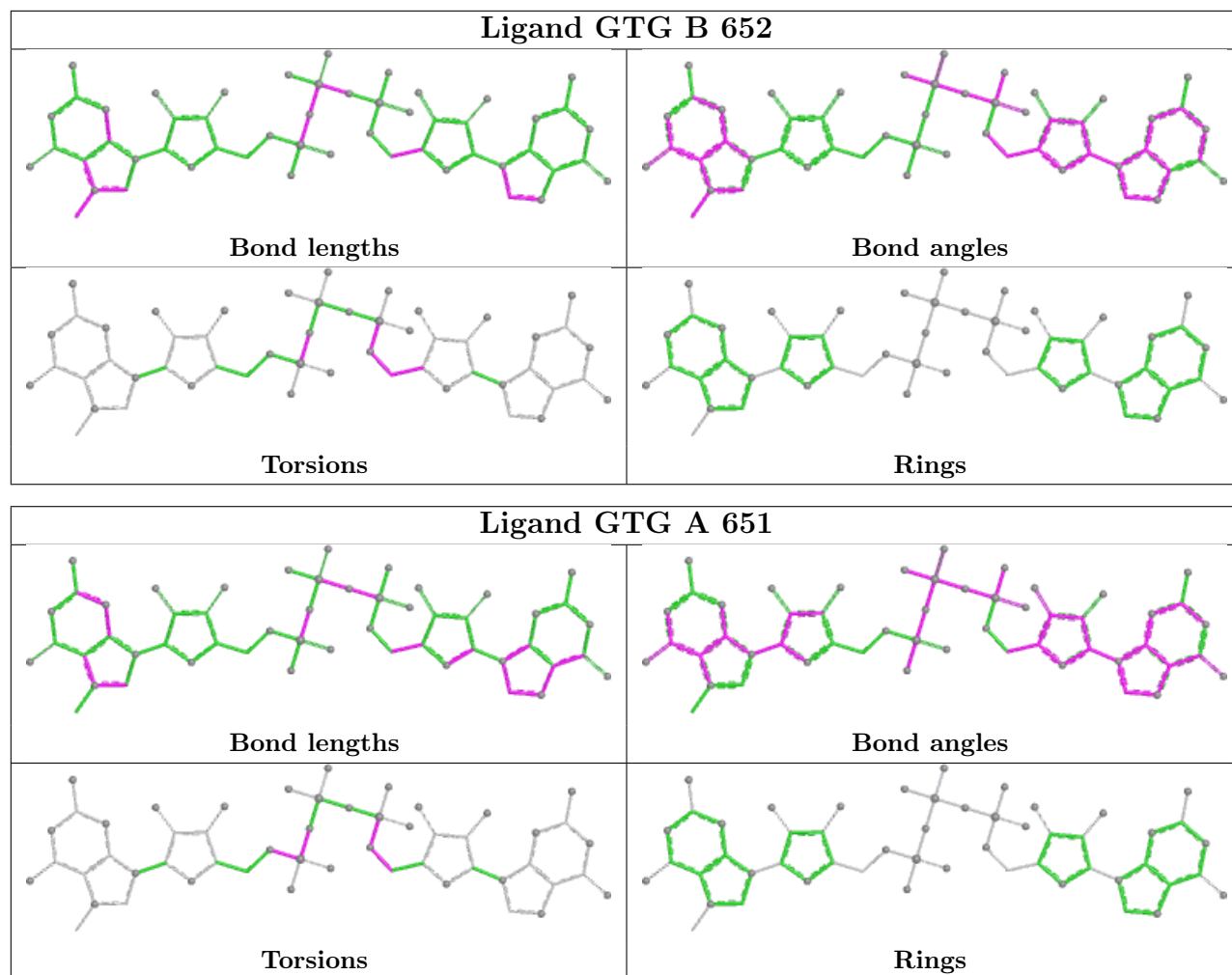
Mol	Chain	Res	Type	Atoms
2	B	652	GTG	C5E-O5E-PG-O3B
2	B	652	GTG	C5E-O5E-PG-O1G
2	B	652	GTG	C5E-O5E-PG-O2G
2	A	651	GTG	C5D-O5D-PA-O2A
2	A	651	GTG	C5D-O5D-PA-O3A
2	A	651	GTG	C5E-O5E-PG-O3B
2	A	651	GTG	C5E-O5E-PG-O1G
2	A	651	GTG	C5E-O5E-PG-O2G
2	B	652	GTG	O4E-C4E-C5E-O5E
2	B	652	GTG	C3E-C4E-C5E-O5E
2	B	652	GTG	PB-O3A-PA-O5D
2	A	651	GTG	PB-O3A-PA-O5D
2	B	652	GTG	C4E-C5E-O5E-PG
2	A	651	GTG	C4E-C5E-O5E-PG
2	A	651	GTG	PB-O3A-PA-O1A

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	652	GTG	3	0
2	A	651	GTG	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.



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	A	300/337 (89%)	-0.22	8 (2%) 56 60	17, 30, 55, 79	0
1	B	297/337 (88%)	0.16	7 (2%) 59 63	21, 37, 60, 76	0
All	All	597/674 (88%)	-0.03	15 (2%) 58 62	17, 34, 57, 79	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	145	ARG	3.8
1	B	171	LEU	2.9
1	A	108	PHE	2.9
1	B	77	GLY	2.8
1	A	38	ALA	2.8
1	A	337	SER	2.7
1	A	147	ASP	2.6
1	A	39	PRO	2.6
1	B	187	ASP	2.4
1	A	146	GLN	2.3
1	B	71	ALA	2.2
1	B	40	VAL	2.2
1	A	336	GLN	2.2
1	B	173	ILE	2.1
1	B	221	ILE	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](#)

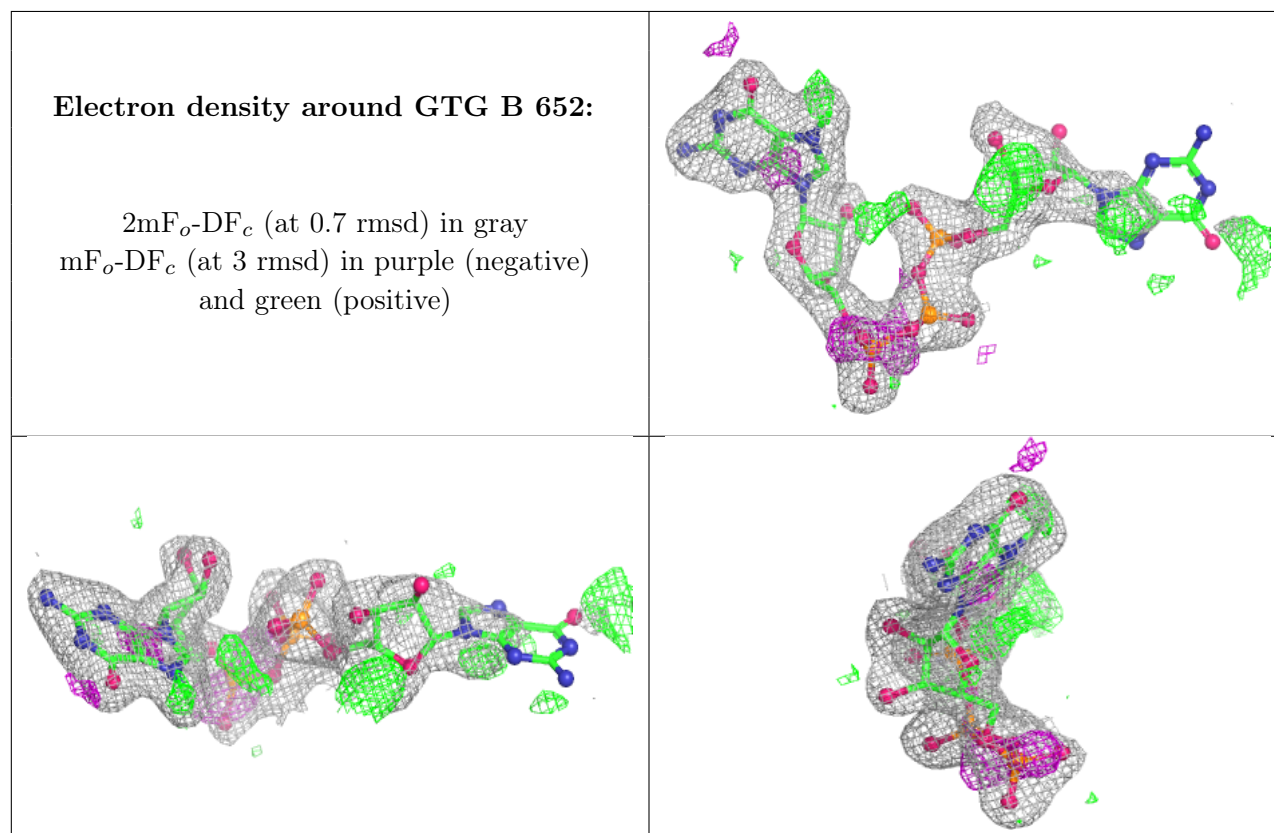
There are no oligosaccharides in this entry.

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.

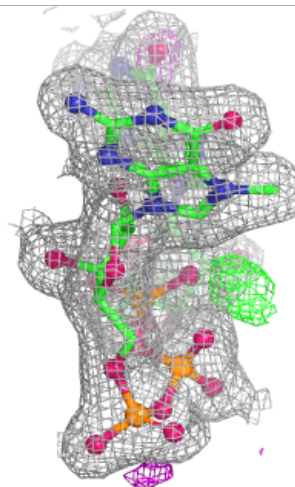
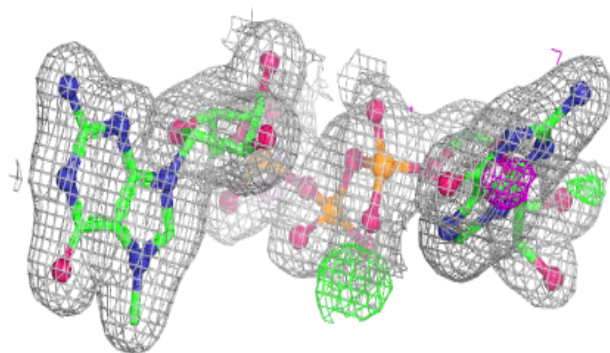
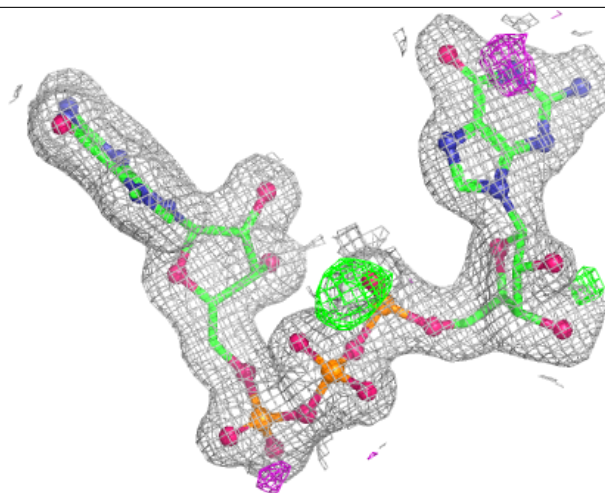
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	GTG	B	652	52/52	0.90	0.15	35,52,89,90	11
2	GTG	A	651	52/52	0.98	0.05	17,25,39,41	0
3	YT3	A	701	1/1	0.99	0.10	55,55,55,55	0
3	YT3	A	702	1/1	0.99	0.10	94,94,94,94	0
3	YT3	A	703	1/1	0.99	0.18	66,66,66,66	0

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 GTG A 651:

$2mF_o-DF_c$ (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.