



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:06 PM UTC

PDB ID : 1ST4 / pdb_00001st4
Title : Structure of DcpS bound to m7GpppA
Authors : Gu, M.; Fabrega, C.; Liu, S.W.; Liu, H.; Kiledjian, M.; Lima, C.D.
Deposited on : 2004-03-24
Resolution : 2.02 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

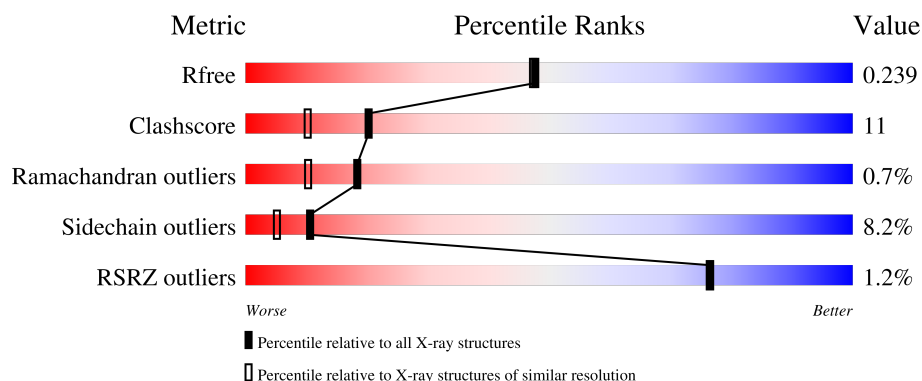
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.02 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	13299 (2.04-2.00)
Clashscore	190562	1022 (2.02-2.02)
Ramachandran outliers	187476	1014 (2.02-2.02)
Sidechain outliers	187428	1014 (2.02-2.02)
RSRZ outliers	180081	13314 (2.04-2.00)

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	% 63% 22% • 11%
1	B	337	% 57% 23% 6% • 12%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 5403 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.

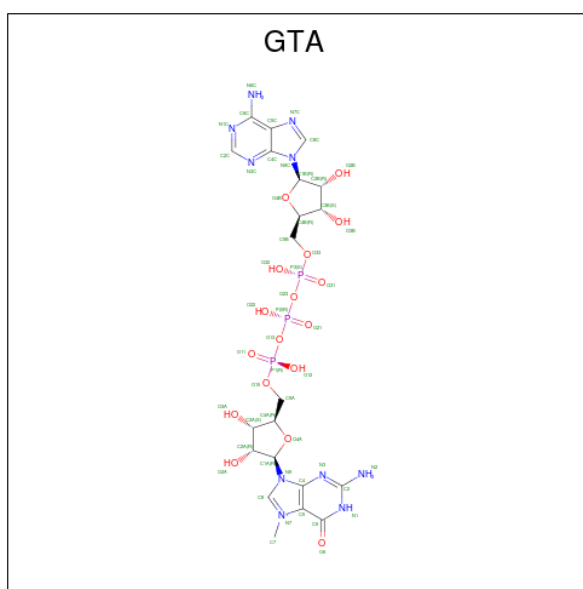
- Molecule 1 is a protein called mRNA decapping enzyme.

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 P1-7-METHYLGUANOSINE-P3-ADENOSINE-5',5'-TRIPHOSPHATE (CCD ID: GTA) (formula: C₂₁H₃₀N₁₀O₁₇P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			51	21	10	17	3		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			51	21	10	17	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		

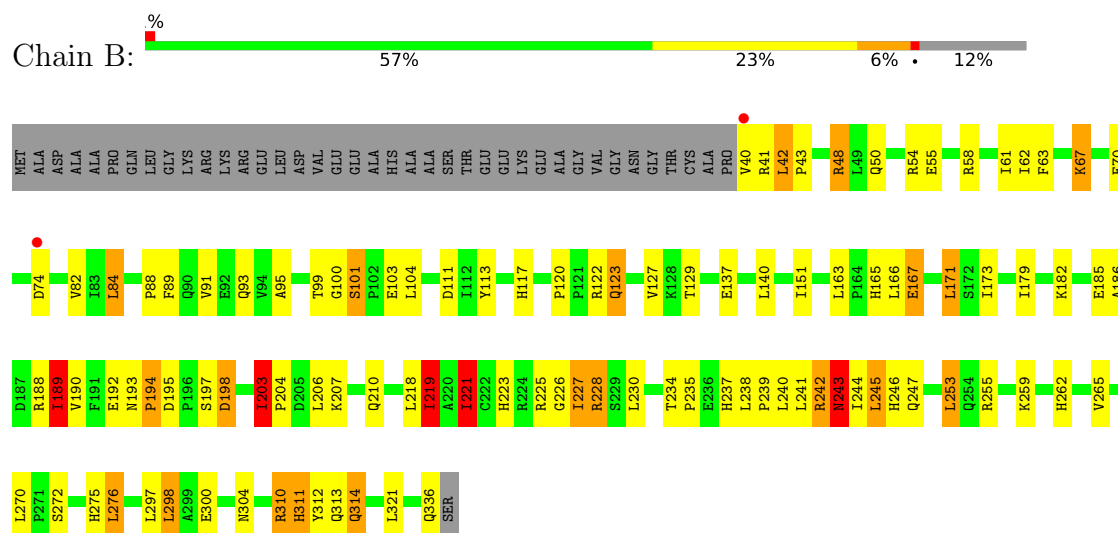
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	169	Total	O	0	0
			169	169		
4	A	232	Total	O	0	0
			232	232		

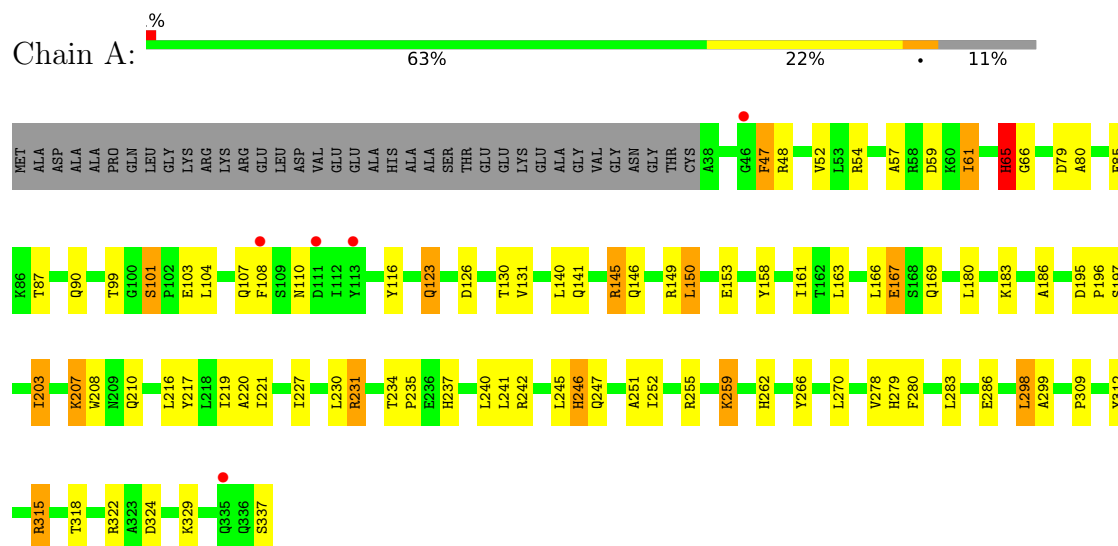
3 Residue-property plots

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	60.04Å 95.45Å 177.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.02 20.00 – 2.02	Depositor EDS
% Data completeness (in resolution range)	97.0 (20.00-2.02) 95.3 (20.00-2.02)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.22 (at 2.02Å)	Xtriage
Refinement program	CNS, REFMAC 5.1.24	Depositor
R, R_{free}	0.201 , 0.249 0.197 , 0.239	Depositor DCC
R_{free} test set	3281 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	34.0	Xtriage
Anisotropy	0.088	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 37.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5403	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.12% 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: YT3, GTA

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	1.80	39/2515 (1.6%)	1.49	13/3413 (0.4%)
1	B	1.62	20/2495 (0.8%)	1.46	20/3386 (0.6%)
All	All	1.71	59/5010 (1.2%)	1.47	33/6799 (0.5%)

All (59) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	203	ILE	CA-CB	9.16	1.65	1.55
1	B	310	ARG	CA-C	8.41	1.64	1.52
1	A	207	LYS	CE-NZ	7.88	1.73	1.49
1	A	65	HIS	C-O	7.75	1.33	1.24
1	A	186	ALA	CA-CB	7.75	1.65	1.53
1	B	265	VAL	CA-CB	7.57	1.63	1.54
1	A	131	VAL	C-O	7.35	1.31	1.24
1	B	129	THR	CA-CB	-7.22	1.43	1.53
1	B	244	ILE	CA-CB	6.71	1.61	1.54
1	A	221	ILE	CA-C	6.53	1.60	1.52
1	A	220	ALA	CA-CB	6.48	1.62	1.53
1	A	299	ALA	CA-CB	6.27	1.63	1.53
1	A	278	VAL	CA-C	6.24	1.59	1.52
1	B	101	SER	CA-C	6.18	1.60	1.52
1	B	61	ILE	C-O	6.14	1.30	1.24
1	A	90	GLN	C-O	6.09	1.31	1.23
1	A	130	THR	C-O	6.05	1.31	1.24
1	B	243	ASN	CA-C	-6.02	1.45	1.52
1	A	48	ARG	C-O	-6.01	1.17	1.24
1	A	241	LEU	C-O	5.97	1.31	1.24
1	A	242	ARG	CA-C	-5.95	1.44	1.52
1	B	120	PRO	CA-C	5.88	1.57	1.52
1	A	61	ILE	CG1-CD1	5.85	1.74	1.51
1	B	221	ILE	CA-CB	-5.74	1.47	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	113	TYR	CA-C	-5.71	1.45	1.52
1	A	279	HIS	N-CA	5.71	1.53	1.46
1	B	219	ILE	CA-CB	5.71	1.62	1.54
1	B	240	LEU	CA-C	5.66	1.60	1.52
1	B	197	SER	CA-C	5.63	1.60	1.53
1	A	216	LEU	N-CA	5.60	1.53	1.46
1	A	283	LEU	CA-C	5.50	1.59	1.52
1	A	246	HIS	C-O	-5.46	1.17	1.24
1	A	87	THR	C-O	5.40	1.29	1.23
1	B	321	LEU	C-O	5.33	1.30	1.23
1	A	52	VAL	CA-CB	5.33	1.59	1.53
1	A	80	ALA	C-O	5.32	1.30	1.23
1	A	123	GLN	CA-C	5.31	1.60	1.52
1	A	280	PHE	CD1-CE1	5.30	1.54	1.38
1	A	217	TYR	CG-CD2	5.29	1.50	1.39
1	A	255	ARG	NE-CZ	5.28	1.38	1.33
1	B	227	ILE	N-CA	5.27	1.52	1.46
1	A	180	LEU	C-O	-5.25	1.17	1.24
1	A	283	LEU	N-CA	-5.22	1.40	1.46
1	A	108	PHE	N-CA	5.21	1.52	1.46
1	A	197	SER	CA-C	5.20	1.59	1.52
1	A	251	ALA	CA-C	5.20	1.59	1.52
1	A	227	ILE	CA-CB	-5.19	1.48	1.53
1	B	241	LEU	C-O	5.18	1.30	1.24
1	A	183	LYS	C-O	-5.16	1.17	1.24
1	A	141	GLN	CG-CD	5.14	1.65	1.52
1	A	266	TYR	CA-C	-5.13	1.46	1.52
1	B	111	ASP	CA-C	5.13	1.57	1.53
1	A	262	HIS	CA-C	5.13	1.60	1.52
1	A	169	GLN	CA-C	5.09	1.59	1.52
1	B	298	LEU	N-CA	5.08	1.52	1.46
1	A	207	LYS	N-CA	5.08	1.52	1.46
1	A	85	GLU	C-O	5.02	1.29	1.24
1	A	252	ILE	N-CA	5.02	1.52	1.46
1	B	127	VAL	CA-CB	5.01	1.60	1.54

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	203	ILE	CB-CA-C	-10.38	98.68	109.89
1	B	194	PRO	N-CA-C	7.22	123.30	113.98
1	B	190	VAL	N-CA-C	-7.20	105.62	111.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	47	PHE	N-CA-C	-7.15	96.13	107.93
1	B	243	ASN	CA-C-O	-7.00	113.37	121.07
1	B	313	GLN	N-CA-C	-6.91	105.38	113.88
1	B	226	GLY	CA-C-N	-6.78	113.89	122.43
1	B	226	GLY	C-N-CA	-6.78	113.89	122.43
1	B	244	ILE	N-CA-C	6.54	117.23	110.36
1	B	246	HIS	N-CA-C	6.27	117.92	111.14
1	A	259	LYS	N-CA-C	6.07	119.06	110.50
1	B	243	ASN	N-CA-C	-5.84	103.90	111.02
1	A	219	ILE	CB-CG1-CD1	-5.80	101.61	113.80
1	A	47	PHE	CA-C-N	-5.80	114.82	123.00
1	A	47	PHE	C-N-CA	-5.80	114.82	123.00
1	B	198	ASP	N-CA-C	5.62	119.69	112.26
1	B	189	ILE	CA-C-N	-5.52	115.83	122.35
1	B	189	ILE	C-N-CA	-5.52	115.83	122.35
1	B	198	ASP	CA-C-N	-5.43	117.04	122.69
1	B	198	ASP	C-N-CA	-5.43	117.04	122.69
1	A	247	GLN	N-CA-C	-5.28	105.58	112.23
1	A	166	LEU	N-CA-C	5.19	116.62	111.07
1	B	48	ARG	NE-CZ-NH2	-5.18	114.53	119.20
1	B	89	PHE	N-CA-C	-5.17	102.88	110.52
1	B	173	ILE	N-CA-C	5.16	116.50	111.91
1	A	107	GLN	N-CA-C	5.15	119.55	113.12
1	B	210	GLN	N-CA-C	5.13	119.38	113.38
1	B	312	TYR	N-CA-C	5.11	119.27	113.19
1	B	242	ARG	N-CA-C	-5.06	105.04	111.11
1	A	220	ALA	CA-C-N	-5.03	116.96	123.19
1	A	220	ALA	C-N-CA	-5.03	116.96	123.19
1	A	242	ARG	CA-C-N	-5.01	113.18	120.29
1	A	242	ARG	C-N-CA	-5.01	113.18	120.29

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	45	0
1	B	2439	0	2428	77	0
2	A	51	0	26	3	0
2	B	51	0	26	1	0
3	A	3	0	0	0	0
4	A	232	0	0	11	0
4	B	169	0	0	15	1
All	All	5403	0	4925	112	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 11.

All (112) 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:A:61:ILE:CD1	1:A:61:ILE:CG1	1.74	1.57
1:A:207:LYS:CE	1:A:207:LYS:NZ	1.73	1.49
1:B:310:ARG:HB2	1:B:314:GLN:HE22	1.07	1.20
1:B:310:ARG:HB2	1:B:314:GLN:NE2	1.69	1.05
1:B:310:ARG:CB	1:B:314:GLN:NE2	2.22	1.02
1:B:91:VAL:HG23	4:B:532:HOH:O	1.63	0.96
1:A:245:LEU:HB2	1:A:298:LEU:HD13	1.53	0.88
1:B:310:ARG:CB	1:B:314:GLN:HE22	1.81	0.88
4:B:476:HOH:O	1:A:315:ARG:HD2	1.71	0.87
1:A:234:THR:H	1:A:237:HIS:HD2	1.22	0.87
1:B:41:ARG:NH2	1:A:101:SER:HB3	1.94	0.83
1:B:228:ARG:HH11	1:B:228:ARG:HG3	1.45	0.80
1:B:203:ILE:HD13	1:B:203:ILE:H	1.47	0.79
1:B:310:ARG:HB3	1:B:314:GLN:NE2	1.98	0.78
1:B:123:GLN:HG2	4:B:564:HOH:O	1.84	0.76
1:B:310:ARG:HB3	1:B:314:GLN:HE21	1.51	0.76
1:B:123:GLN:CG	4:B:564:HOH:O	2.35	0.72
1:B:304:ASN:OD1	1:A:315:ARG:NH2	2.23	0.71
1:A:110:ASN:HB3	4:A:595:HOH:O	1.90	0.71
1:A:65:HIS:HD2	4:A:686:HOH:O	1.74	0.68
1:B:219:ILE:HD13	1:B:219:ILE:H	1.59	0.68
1:B:122:ARG:NH2	1:A:103:GLU:OE1	2.27	0.66
1:B:171:LEU:H	1:B:171:LEU:HD12	1.61	0.66
1:B:99:THR:HG22	1:A:47:PHE:O	1.96	0.65
1:A:153:GLU:OE2	1:A:231:ARG:NH1	2.28	0.63
1:B:219:ILE:H	1:B:219:ILE:CD1	2.12	0.62
1:A:61:ILE:CD1	1:A:61:ILE:CB	2.73	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:LEU:HD11	1:A:312:TYR:CE2	2.34	0.62
1:B:204:PRO:HA	1:B:218:LEU:HD23	1.81	0.61
1:B:137:GLU:HA	1:B:140:LEU:HD12	1.82	0.61
1:B:193:ASN:OD1	1:B:193:ASN:C	2.44	0.60
1:B:203:ILE:N	1:B:203:ILE:CD1	2.65	0.60
1:B:228:ARG:HG3	1:B:228:ARG:NH1	2.08	0.60
1:B:203:ILE:HD13	1:B:203:ILE:N	2.15	0.59
1:A:158:TYR:CG	1:A:231:ARG:HD3	2.37	0.59
1:A:259:LYS:HE2	4:A:576:HOH:O	2.01	0.59
1:B:219:ILE:CD1	1:B:219:ILE:N	2.66	0.58
1:A:145:ARG:NH1	4:A:667:HOH:O	2.36	0.58
1:A:322:ARG:HD3	4:A:668:HOH:O	2.03	0.58
1:B:95:ALA:O	1:B:99:THR:HG23	2.05	0.57
1:B:42:LEU:HD13	1:A:104:LEU:HD11	1.87	0.57
1:B:93:GLN:NE2	1:B:123:GLN:HB2	2.20	0.56
1:B:255:ARG:NH1	4:B:608:HOH:O	2.39	0.55
1:A:234:THR:H	1:A:237:HIS:CD2	2.14	0.53
1:B:171:LEU:HD13	1:B:272:SER:O	2.09	0.53
1:B:242:ARG:O	1:B:243:ASN:C	2.52	0.52
1:B:234:THR:HB	1:B:235:PRO:CD	2.39	0.52
1:B:203:ILE:HD13	1:B:219:ILE:O	2.10	0.52
1:A:123:GLN:HB2	4:A:564:HOH:O	2.11	0.50
1:B:247:GLN:HB2	4:B:610:HOH:O	2.12	0.49
1:B:43:PRO:HD3	1:A:116:TYR:OH	2.13	0.49
1:A:65:HIS:HE1	1:A:79:ASP:OD1	1.94	0.49
1:A:246:HIS:HE1	4:A:559:HOH:O	1.96	0.49
1:B:54:ARG:HD2	1:B:63:PHE:CE1	2.49	0.47
1:A:324:ASP:C	1:A:324:ASP:OD2	2.57	0.47
1:B:223:HIS:N	4:B:558:HOH:O	2.48	0.47
1:B:255:ARG:HB2	4:B:486:HOH:O	2.15	0.47
1:B:310:ARG:O	1:B:311:HIS:C	2.58	0.47
1:B:237:HIS:O	1:B:238:LEU:C	2.58	0.46
1:B:275:HIS:O	1:B:276:LEU:C	2.58	0.46
1:B:239:PRO:O	1:B:243:ASN:HB2	2.16	0.46
1:A:47:PHE:CE1	1:A:66:GLY:HA3	2.51	0.46
1:B:207:LYS:HE3	2:B:452:GTA:O2A	2.16	0.46
2:A:451:GTA:N3C	2:A:451:GTA:H2B	2.30	0.46
1:A:158:TYR:CD2	1:A:231:ARG:HD3	2.51	0.46
1:B:41:ARG:HH22	1:A:101:SER:HB3	1.75	0.45
1:A:61:ILE:HG21	1:A:61:ILE:HD13	1.97	0.45
1:B:82:VAL:HG12	1:B:84:LEU:HD22	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:186:ALA:HA	1:B:189:ILE:HD12	1.99	0.45
1:B:194:PRO:O	1:B:195:ASP:C	2.57	0.45
1:B:165:HIS:HE1	4:B:474:HOH:O	2.00	0.45
1:B:58:ARG:NH2	1:A:59:ASP:OD2	2.49	0.45
1:B:67:LYS:NZ	4:B:597:HOH:O	2.41	0.45
1:B:262:HIS:CE1	1:A:149:ARG:CZ	3.00	0.45
1:B:192:GLU:HG2	1:B:194:PRO:HD3	1.99	0.44
1:B:41:ARG:NH2	1:A:101:SER:CB	2.73	0.44
1:B:243:ASN:O	4:B:610:HOH:O	2.21	0.44
1:A:150:LEU:CD1	1:A:318:THR:HG22	2.48	0.44
1:B:259:LYS:O	1:B:262:HIS:HB2	2.17	0.44
1:A:54:ARG:NE	4:A:730:HOH:O	2.15	0.43
1:B:88:PRO:HB3	1:A:57:ALA:HA	2.00	0.43
1:B:103:GLU:C	1:B:104:LEU:HG	2.42	0.43
4:B:535:HOH:O	1:A:286:GLU:HG2	2.19	0.43
1:B:163:LEU:O	1:B:167:GLU:HG2	2.19	0.43
1:A:167:GLU:HB2	4:A:622:HOH:O	2.18	0.43
1:B:253:LEU:C	1:B:253:LEU:HD23	2.44	0.43
1:B:310:ARG:HD2	1:B:314:GLN:NE2	2.34	0.43
1:B:63:PHE:CD1	1:B:63:PHE:N	2.86	0.42
1:B:117:HIS:ND1	1:A:126:ASP:OD2	2.40	0.42
1:A:237:HIS:O	1:A:240:LEU:HB3	2.20	0.42
1:B:221:ILE:H	1:B:221:ILE:HG13	1.55	0.42
1:B:48:ARG:HD3	1:B:70:GLU:OE1	2.19	0.42
1:B:227:ILE:HD13	1:B:237:HIS:CD2	2.55	0.41
1:B:123:GLN:HG3	4:B:564:HOH:O	2.08	0.41
1:A:235:PRO:HG2	1:A:309:PRO:HB3	2.03	0.41
1:B:140:LEU:H	1:B:140:LEU:HG	1.73	0.41
1:A:246:HIS:HD2	4:A:728:HOH:O	2.04	0.41
1:B:54:ARG:HG2	1:B:55:GLU:N	2.36	0.41
1:B:253:LEU:C	1:B:253:LEU:CD2	2.93	0.41
1:A:195:ASP:HA	1:A:196:PRO:HD3	1.81	0.41
2:A:451:GTA:C2C	4:A:599:HOH:O	2.69	0.41
1:B:247:GLN:CB	4:B:610:HOH:O	2.68	0.41
1:B:297:LEU:HB2	1:B:300:GLU:HG3	2.03	0.41
1:A:140:LEU:HD23	1:A:140:LEU:HA	1.88	0.41
1:B:100:GLY:O	1:B:101:SER:C	2.63	0.41
1:B:245:LEU:HD23	1:B:245:LEU:HA	1.85	0.41
1:B:314:GLN:CG	4:B:579:HOH:O	2.69	0.41
1:B:179:ILE:HD11	1:B:185:GLU:OE1	2.21	0.40
1:A:208:TRP:CE2	1:A:210:GLN:HA	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:41:ARG:HH22	1:A:101:SER:CB	2.34	0.40
1:B:242:ARG:O	1:B:243:ASN:O	2.38	0.40
2:A:451:GTA:N3C	2:A:451:GTA:C2B	2.84	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)
4:B:554:HOH:O	4:B:572:HOH:O[4_566]	2.14	0.06

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	298/337 (88%)	280 (94%)	16 (5%)	2 (1%)	18	10
1	B	295/337 (88%)	277 (94%)	16 (5%)	2 (1%)	18	10
All	All	593/674 (88%)	557 (94%)	32 (5%)	4 (1%)	18	10

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	311	HIS
1	A	145	ARG
1	B	230	LEU
1	A	146	GLN

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	269/295 (91%)	255 (95%)	14 (5%)	21	13
1	B	267/295 (90%)	237 (89%)	30 (11%)	6	1
All	All	536/590 (91%)	492 (92%)	44 (8%)	10	5

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	40	VAL
1	B	42	LEU
1	B	50	GLN
1	B	62	ILE
1	B	67	LYS
1	B	74	ASP
1	B	84	LEU
1	B	123	GLN
1	B	151	ILE
1	B	166	LEU
1	B	167	GLU
1	B	171	LEU
1	B	182	LYS
1	B	188	ARG
1	B	189	ILE
1	B	198	ASP
1	B	203	ILE
1	B	206	LEU
1	B	219	ILE
1	B	221	ILE
1	B	225	ARG
1	B	228	ARG
1	B	243	ASN
1	B	245	LEU
1	B	253	LEU
1	B	270	LEU
1	B	276	LEU
1	B	298	LEU
1	B	314	GLN
1	B	336	GLN
1	A	65	HIS
1	A	99	THR
1	A	101	SER

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Mol	Chain	Res	Type
1	A	150	LEU
1	A	161	ILE
1	A	163	LEU
1	A	167	GLU
1	A	203	ILE
1	A	231	ARG
1	A	270	LEU
1	A	298	LEU
1	A	315	ARG
1	A	329	LYS
1	A	337	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	107	GLN
1	B	243	ASN
1	B	246	HIS
1	B	262	HIS
1	B	314	GLN
1	A	50	GLN
1	A	65	HIS
1	A	125	ASN
1	A	169	GLN
1	A	237	HIS
1	A	246	HIS
1	A	249	GLN
1	A	254	GLN
1	A	314	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	GTA	A	451	-	56,56,56	2.33	12 (21%)	83,88,88	2.04	28 (33%)
2	GTA	B	452	-	56,56,56	2.23	12 (21%)	83,88,88	2.30	29 (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	GTA	A	451	-	-	7/32/64/64	0/6/6/6
2	GTA	B	452	-	-	5/32/64/64	0/6/6/6

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	451	GTA	C8C-N7C	9.99	1.50	1.31
2	B	452	GTA	C8C-N7C	8.41	1.47	1.31
2	B	452	GTA	C8C-N9C	6.75	1.49	1.37
2	A	451	GTA	C8C-N9C	6.31	1.48	1.37
2	B	452	GTA	C4-N3	5.30	1.46	1.34
2	A	451	GTA	C5B-C4B	-5.10	1.36	1.51
2	B	452	GTA	C5B-C4B	-4.60	1.37	1.51
2	B	452	GTA	C5-N7	-4.37	1.34	1.39
2	A	451	GTA	P3-O23	3.94	1.63	1.59
2	A	451	GTA	P1-O13	3.84	1.63	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	451	GTA	C5-N7	-3.79	1.34	1.39
2	A	451	GTA	C6-N1	-3.77	1.31	1.38
2	B	452	GTA	P2-O13	3.67	1.63	1.59
2	A	451	GTA	C6C-N6C	-3.35	1.25	1.34
2	B	452	GTA	P1-O13	3.30	1.63	1.59
2	A	451	GTA	C8-N7	3.15	1.38	1.33
2	B	452	GTA	P3-O23	-3.01	1.56	1.59
2	A	451	GTA	C2C-N1C	2.82	1.38	1.33
2	B	452	GTA	C6C-N6C	-2.68	1.27	1.34
2	B	452	GTA	C2C-N1C	2.40	1.38	1.33
2	A	451	GTA	C8-N9	2.30	1.41	1.35
2	A	451	GTA	C4-N3	2.21	1.39	1.34
2	B	452	GTA	C8-N7	2.19	1.36	1.33
2	B	452	GTA	C2C-N3C	2.02	1.37	1.33

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	452	GTA	N9C-C8C-N7C	-8.42	101.99	113.94
2	A	451	GTA	N9C-C8C-N7C	-7.86	102.78	113.94
2	B	452	GTA	C5C-C4C-N3C	-5.87	118.63	126.72
2	A	451	GTA	N3C-C2C-N1C	-5.02	120.99	128.58
2	A	451	GTA	C5-C6-N1	4.70	121.55	111.84
2	B	452	GTA	N3C-C2C-N1C	-4.67	121.51	128.58
2	B	452	GTA	C5C-N7C-C8C	4.38	110.34	103.45
2	A	451	GTA	O4B-C1B-N9C	4.27	116.29	108.09
2	B	452	GTA	C5-C6-N1	4.04	120.19	111.84
2	A	451	GTA	C4C-N9C-C8C	3.81	109.74	105.74
2	B	452	GTA	C2C-N3C-C4C	3.70	120.86	111.83
2	B	452	GTA	C1B-N9C-C8C	-3.63	119.04	127.09
2	A	451	GTA	O6-C6-C5	-3.61	119.96	128.01
2	B	452	GTA	C5-C4-N3	-3.53	121.47	128.15
2	B	452	GTA	O33-C5B-C4B	3.52	120.97	108.99
2	B	452	GTA	O23-P2-O21	3.49	121.21	110.70
2	B	452	GTA	C6C-C5C-C4C	3.48	121.93	117.18
2	B	452	GTA	O4B-C4B-C5B	3.46	120.42	109.33
2	B	452	GTA	O6-C6-C5	-3.31	120.63	128.01
2	A	451	GTA	O12-P1-O13	-3.20	98.63	107.27
2	B	452	GTA	C5C-C4C-N9C	3.04	109.13	105.81
2	A	451	GTA	O3A-C3A-C4A	-3.01	102.44	111.08
2	A	451	GTA	C5-C4-N9	2.99	112.25	105.88
2	B	452	GTA	N3C-C4C-N9C	2.95	132.19	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	451	GTA	C5C-C4C-N9C	2.92	109.00	105.81
2	B	452	GTA	O22-P2-O21	2.83	125.62	112.44
2	B	452	GTA	C6-C5-N7	2.82	135.70	132.17
2	B	452	GTA	C4C-N9C-C8C	2.81	108.69	105.74
2	B	452	GTA	C5-C4-N9	2.70	111.65	105.88
2	A	451	GTA	C5C-N7C-C8C	2.70	107.69	103.45
2	B	452	GTA	O3A-C3A-C2A	2.60	120.16	111.82
2	A	451	GTA	C2-N1-C6	-2.52	120.55	125.11
2	B	452	GTA	O13-P2-O21	-2.50	103.19	110.70
2	A	451	GTA	O32-P3-O23	-2.49	100.55	107.27
2	B	452	GTA	C2-N3-C4	2.46	116.53	112.30
2	A	451	GTA	C3B-C2B-C1B	2.44	106.08	101.46
2	A	451	GTA	O22-P2-O21	2.41	123.66	112.44
2	A	451	GTA	O15-C5A-C4A	-2.39	100.86	108.99
2	A	451	GTA	O4B-C4B-C5B	2.36	116.89	109.33
2	B	452	GTA	C2A-C1A-N9	2.34	119.78	113.25
2	B	452	GTA	O4A-C1A-C2A	-2.31	101.68	106.62
2	B	452	GTA	C4C-N9C-C1B	2.30	132.01	126.63
2	A	451	GTA	O2A-C2A-C1A	-2.28	102.24	110.10
2	A	451	GTA	C2C-N1C-C6C	2.24	122.40	118.73
2	A	451	GTA	C8-N9-C4	-2.19	101.68	107.09
2	B	452	GTA	C7-N7-C8	2.17	128.08	124.79
2	A	451	GTA	C6-C5-N7	2.16	134.88	132.17
2	B	452	GTA	O12-P1-O13	-2.15	101.45	107.27
2	A	451	GTA	C2C-N3C-C4C	2.15	117.09	111.83
2	A	451	GTA	O33-C5B-C4B	2.13	116.26	108.99
2	B	452	GTA	O2A-C2A-C3A	2.13	118.63	111.82
2	A	451	GTA	C5-C4-N3	-2.08	124.21	128.15
2	A	451	GTA	O4A-C1A-N9	-2.06	103.69	108.36
2	A	451	GTA	C5C-C4C-N3C	-2.06	123.88	126.72
2	A	451	GTA	C8-N7-C5	-2.06	105.21	107.78
2	A	451	GTA	C2A-C3A-C4A	2.04	106.54	102.61
2	B	452	GTA	O3B-C3B-C4B	-2.03	105.26	111.08

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	452	GTA	C5B-O33-P3-O23
2	B	452	GTA	C5B-O33-P3-O32
2	A	451	GTA	P2-O13-P1-O15
2	A	451	GTA	C5B-O33-P3-O31

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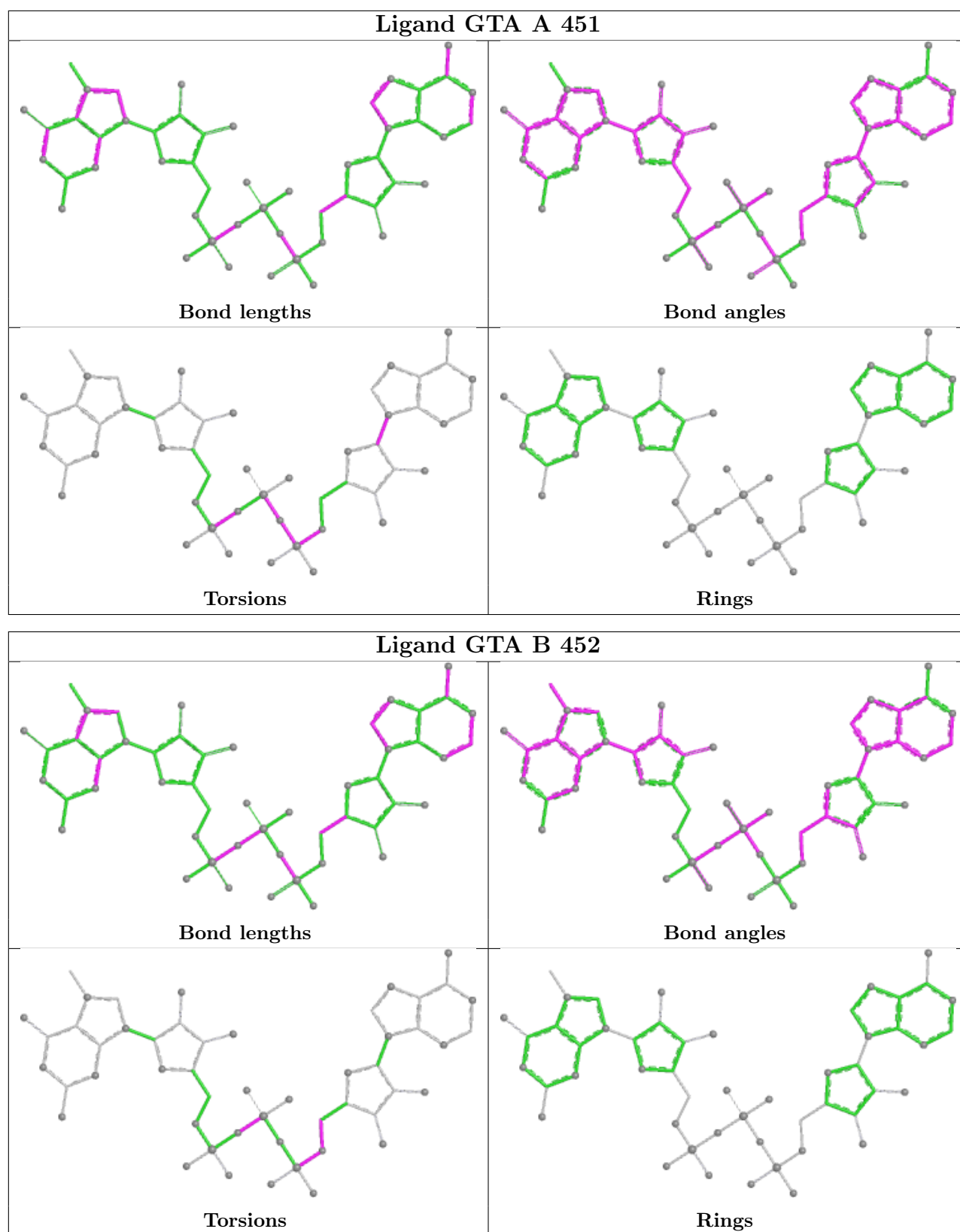
Mol	Chain	Res	Type	Atoms
2	A	451	GTA	P2-O23-P3-O33
2	B	452	GTA	C4B-C5B-O33-P3
2	B	452	GTA	C5B-O33-P3-O31
2	A	451	GTA	C2B-C1B-N9C-C8C
2	A	451	GTA	C2B-C1B-N9C-C4C
2	A	451	GTA	O4B-C1B-N9C-C8C
2	A	451	GTA	P3-O23-P2-O21
2	B	452	GTA	P1-O13-P2-O21

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	451	GTA	3	0
2	B	452	GTA	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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%)	-0.24	5 (1%) 69 69	20, 36, 65, 105	0
1	B	297/337 (88%)	0.19	2 (0%) 84 84	25, 47, 67, 82	0
All	All	597/674 (88%)	-0.03	7 (1%) 76 76	20, 42, 65, 105	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	108	PHE	4.3
1	B	40	VAL	4.1
1	A	113	TYR	3.1
1	A	335	GLN	2.6
1	A	46	GLY	2.3
1	B	74	ASP	2.1
1	A	111	ASP	2.1

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](#)

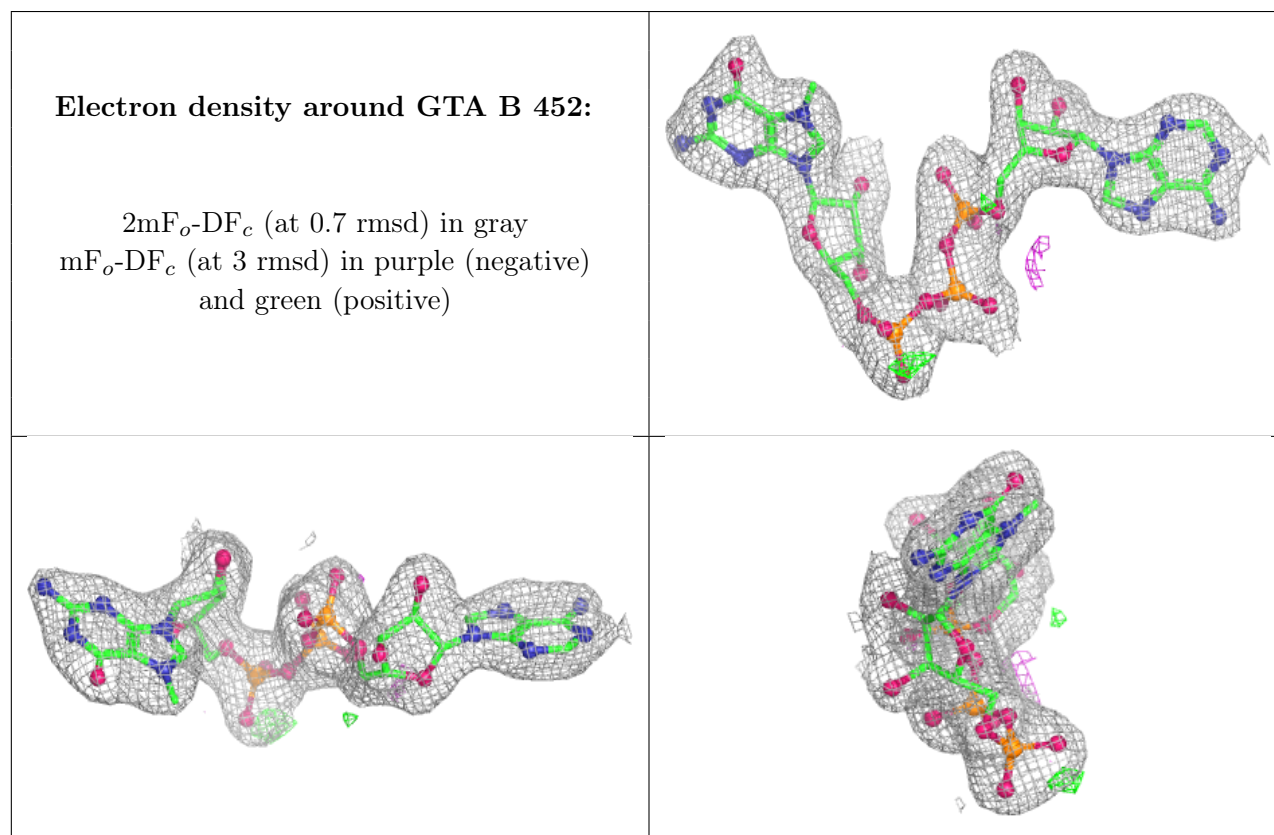
There are no oligosaccharides in this entry.

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.

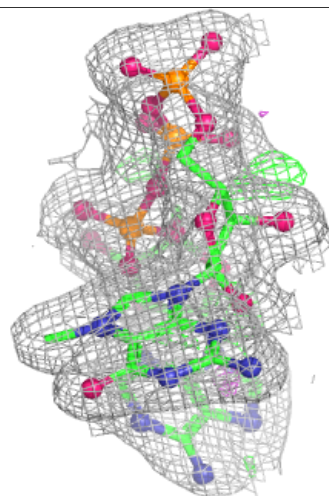
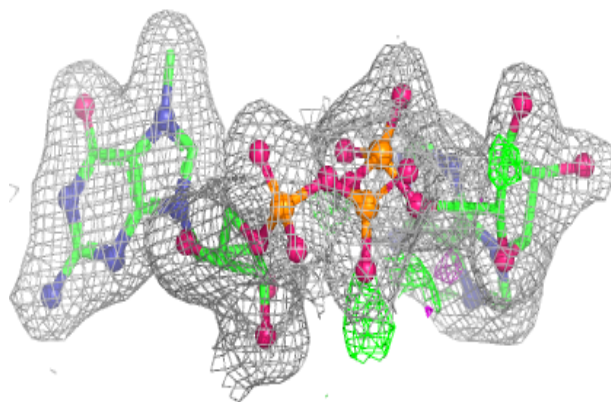
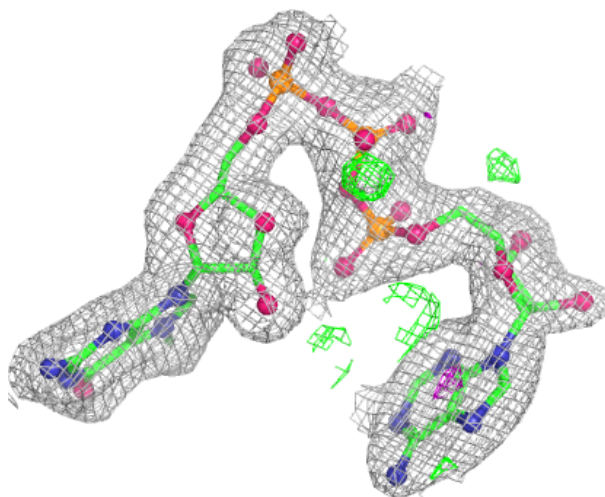
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	YT3	A	503	1/1	0.84	0.13	148,148,148,148	0
2	GTA	B	452	51/51	0.96	0.07	36,53,63,64	0
3	YT3	A	502	1/1	0.98	0.07	104,104,104,104	0
2	GTA	A	451	51/51	0.98	0.06	18,28,53,57	0
3	YT3	A	501	1/1	0.99	0.03	60,60,60,60	0

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 GTA A 451:

$2mF_o-DF_c$ (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.