



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:21 AM UTC

PDB ID : 1H2T / pdb_00001h2t
Title : Structure of the human nuclear cap-binding-complex (CBC) in complex with a cap analogue m7GpppG
Authors : Mazza, C.; Segref, A.; Mattaj, I.W.; Cusack, S.
Deposited on : 2002-08-16
Resolution : 2.10 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

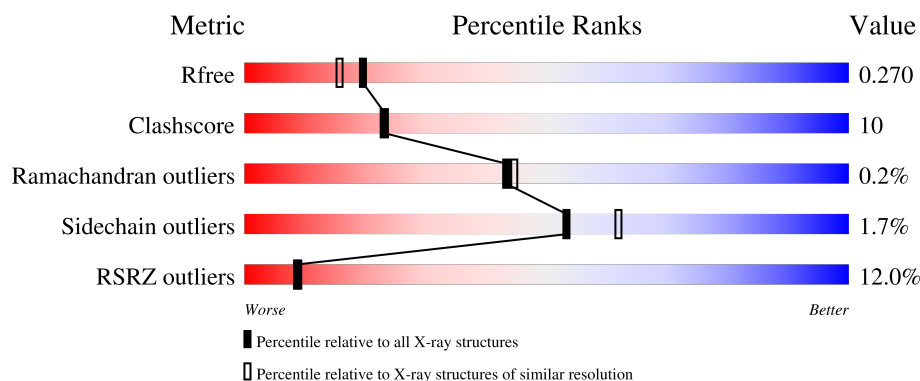
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	C	723	12% 75% 21% • •
2	Z	156	11% 65% 28% • 6%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 7356 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 80 KDA NUCLEAR CAP BINDING PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	C	704	5746	3711	969	1028	38	0	0	0

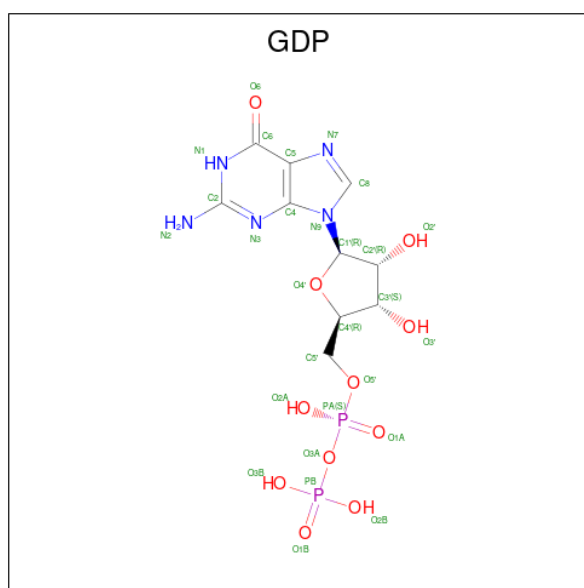
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	479	SER	ALA	engineered mutation	UNP Q09161

- Molecule 2 is a protein called 20 KDA NUCLEAR CAP BINDING PROTEIN.

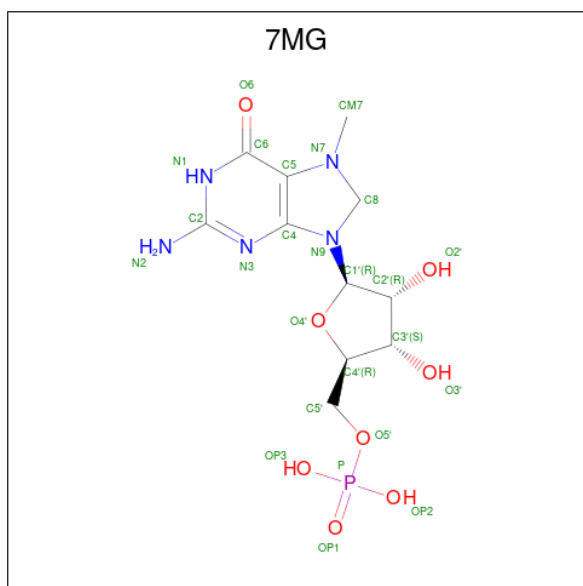
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	Z	146	1193	743	213	231	6	0	0	0

- Molecule 3 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	Z	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 4 is 7N-METHYL-8-HYDROGUANOSINE-5'-MONOPHOSPHATE (CCD ID: 7MG) (formula: $C_{11}H_{18}N_5O_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	Z	1	Total	C	N	O	P	0	0
			24	11	5	7	1		

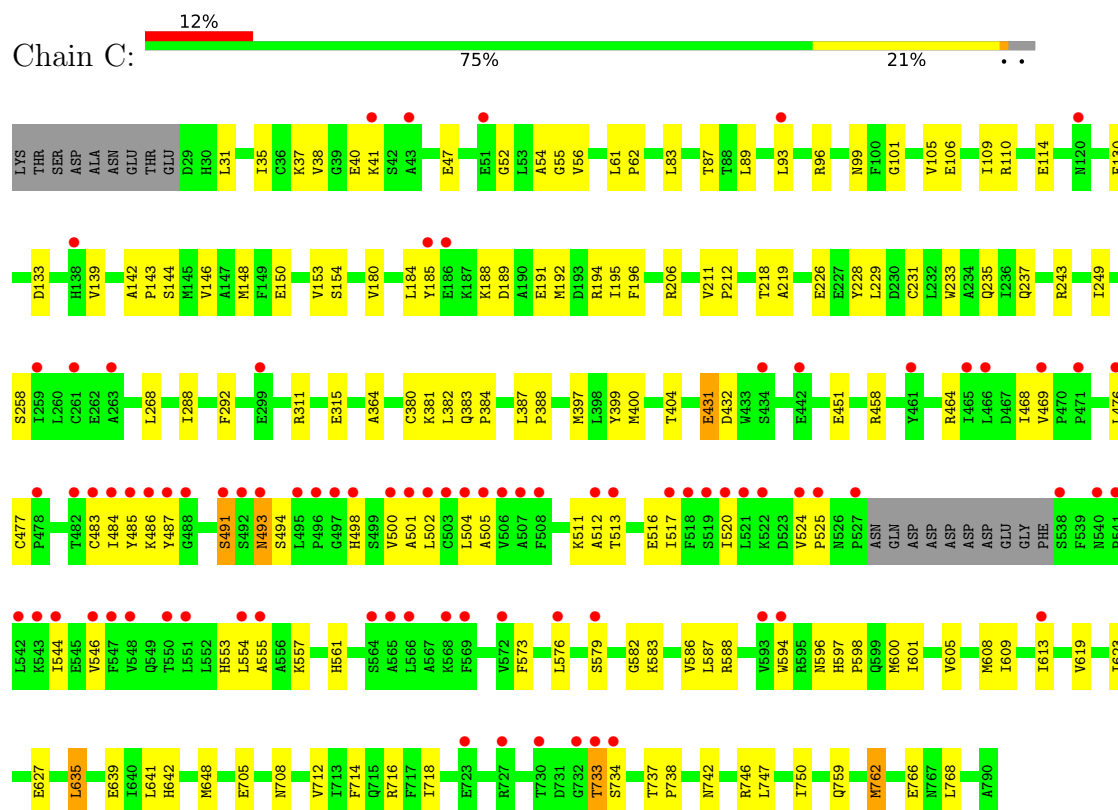
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	302	Total	O	0	0
			302	302		
5	Z	63	Total	O	0	0
			63	63		

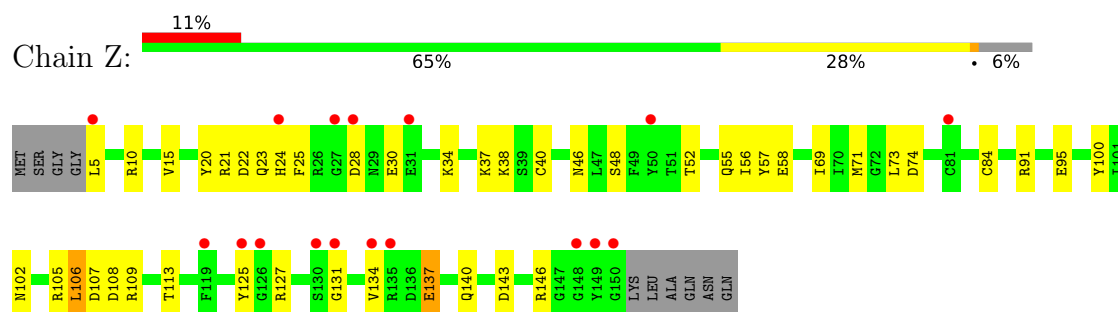
3 Residue-property plots [i](#)

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: 80 KDA NUCLEAR CAP BINDING PROTEIN



• Molecule 2: 20 KDA NUCLEAR CAP BINDING PROTEIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	112.78Å 112.78Å 158.31Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.76 – 2.10 19.76 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.6 (19.76-2.10) 99.5 (19.76-2.10)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.80 (at 2.01Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.232 , 0.269 0.232 , 0.270	Depositor DCC
R_{free} test set	3839 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	37.0	Xtriage
Anisotropy	0.207	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 50.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.018 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7356	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.47% 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: 7MG, GDP

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	C	0.42	0/5900	0.84	10/8015 (0.1%)
2	Z	0.38	0/1213	0.84	3/1619 (0.2%)
All	All	0.41	0/7113	0.84	13/9634 (0.1%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Z	105	ARG	N-CA-C	6.66	120.91	110.32
1	C	228	TYR	N-CA-C	6.63	119.36	111.33
2	Z	40	CYS	N-CA-C	-6.23	104.16	112.94
1	C	635	LEU	N-CA-C	6.15	118.77	111.33
1	C	139	VAL	N-CA-C	-6.06	106.99	111.90
1	C	768	LEU	N-CA-C	6.04	120.78	113.41
1	C	747	LEU	N-CA-C	-5.78	104.90	111.14
1	C	249	ILE	N-CA-C	5.70	116.76	109.30
1	C	762	MET	N-CA-C	5.52	117.73	111.11
1	C	288	ILE	N-CA-C	5.44	116.02	108.84
1	C	364	ALA	N-CA-C	5.32	116.85	108.55
2	Z	100	TYR	N-CA-C	5.32	121.51	114.12
1	C	226	GLU	N-CA-C	5.16	118.52	110.32

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	C	5746	0	5723	113	0
2	Z	1193	0	1147	30	0
3	Z	28	0	12	2	0
4	Z	24	0	16	1	0
5	C	302	0	0	6	0
5	Z	63	0	0	3	0
All	All	7356	0	6898	143	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 10.

All (143) 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:C:153:VAL:HG21	1:C:195:ILE:HG23	1.61	0.81
1:C:150:GLU:HG2	1:C:195:ILE:HD11	1.60	0.81
1:C:716:ARG:HA	1:C:716:ARG:HH11	1.49	0.75
1:C:513:THR:HG22	1:C:516:GLU:HG3	1.68	0.75
2:Z:107:ASP:HB3	5:Z:2023:HOH:O	1.88	0.74
1:C:146:VAL:O	1:C:150:GLU:HG3	1.94	0.68
2:Z:143:ASP:HB3	2:Z:146:ARG:HB2	1.73	0.68
2:Z:22:ASP:HB3	2:Z:25:PHE:HB2	1.78	0.66
2:Z:57:TYR:CD2	2:Z:69:ILE:HD12	2.32	0.64
1:C:399:TYR:CD2	1:C:400:MET:HE2	2.34	0.63
1:C:153:VAL:HG21	1:C:195:ILE:CG2	2.29	0.62
1:C:516:GLU:O	1:C:520:ILE:HG13	2.00	0.62
1:C:191:GLU:HA	1:C:194:ARG:NH1	2.14	0.61
1:C:144:SER:HB3	1:C:268:LEU:HB2	1.82	0.61
1:C:712:VAL:O	1:C:716:ARG:HG2	2.01	0.61
1:C:54:ALA:HA	1:C:93:LEU:HD11	1.81	0.61
1:C:61:LEU:N	1:C:62:PRO:HD2	2.16	0.60
1:C:500:VAL:HG11	1:C:524:VAL:HG22	1.83	0.60
1:C:609:ILE:HD11	1:C:619:VAL:HG21	1.83	0.60
1:C:154:SER:HB3	5:C:2053:HOH:O	2.01	0.59
1:C:83:LEU:HD11	1:C:130:PHE:HA	1.82	0.59
1:C:623:ILE:HD13	1:C:641:LEU:HB2	1.85	0.58
1:C:211:VAL:HB	1:C:212:PRO:HD3	1.86	0.58
1:C:635:LEU:O	1:C:639:GLU:HG3	2.04	0.57
1:C:218:THR:OG1	1:C:404:THR:HB	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:382:LEU:C	1:C:384:PRO:HD3	2.29	0.56
3:Z:1151:GDP:O1B	4:Z:1152:7MG:H81	2.07	0.54
1:C:87:THR:HG21	1:C:133:ASP:HB3	1.90	0.54
1:C:505:ALA:HA	1:C:554:LEU:HD11	1.90	0.54
1:C:557:LYS:HD3	1:C:561:HIS:NE2	2.22	0.54
1:C:493:ASN:N	1:C:493:ASN:HD22	2.06	0.53
1:C:387:LEU:HB3	1:C:388:PRO:HD3	1.89	0.53
1:C:399:TYR:HD2	1:C:400:MET:HE2	1.74	0.53
1:C:35:ILE:O	1:C:38:VAL:HG12	2.08	0.52
1:C:431:GLU:H	1:C:431:GLU:CD	2.17	0.52
1:C:55:GLY:HA2	1:C:96:ARG:NH1	2.24	0.52
1:C:498:HIS:NE2	1:C:502:LEU:HD11	2.24	0.52
2:Z:73:LEU:O	2:Z:125:TYR:HA	2.10	0.52
2:Z:46:ASN:HA	2:Z:146:ARG:HH21	1.75	0.51
1:C:258:SER:HB2	5:C:2106:HOH:O	2.10	0.51
1:C:52:GLY:O	1:C:56:VAL:HG23	2.11	0.51
2:Z:21:ARG:HG3	2:Z:21:ARG:HH11	1.76	0.51
2:Z:91:ARG:O	2:Z:95:GLU:HG3	2.11	0.50
1:C:493:ASN:HD22	1:C:494:SER:N	2.10	0.50
2:Z:56:ILE:HD13	2:Z:84:CYS:SG	2.52	0.50
1:C:588:ARG:HA	5:C:2242:HOH:O	2.12	0.50
1:C:582:GLY:O	1:C:586:VAL:HG23	2.13	0.49
1:C:142:ALA:HB3	1:C:143:PRO:HD3	1.95	0.49
2:Z:52:THR:OG1	2:Z:55:GLN:HG3	2.12	0.49
1:C:517:ILE:HA	1:C:520:ILE:HD12	1.95	0.48
1:C:37:LYS:O	1:C:40:GLU:HG3	2.14	0.48
1:C:605:VAL:HA	1:C:608:MET:HE2	1.95	0.48
1:C:608:MET:HB3	1:C:613:ILE:HB	1.95	0.48
1:C:458:ARG:HD2	2:Z:58:GLU:CD	2.39	0.48
1:C:555:ALA:C	1:C:557:LYS:H	2.22	0.48
2:Z:34:LYS:O	2:Z:38:LYS:HD3	2.14	0.48
1:C:642:HIS:CE1	1:C:750:ILE:HD13	2.49	0.48
1:C:648:MET:CE	1:C:705:GLU:HG2	2.44	0.47
2:Z:28:ASP:OD2	2:Z:30:GLU:HB3	2.15	0.47
1:C:188:LYS:HD2	1:C:191:GLU:OE2	2.14	0.47
1:C:525:PRO:HD3	5:C:2228:HOH:O	2.14	0.47
2:Z:24:HIS:HB3	5:Z:2015:HOH:O	2.14	0.47
1:C:484:ILE:HD11	1:C:596:ASN:ND2	2.29	0.47
1:C:733:THR:HG22	1:C:734:SER:H	1.80	0.47
1:C:109:ILE:HD11	1:C:268:LEU:HD22	1.97	0.46
2:Z:20:TYR:O	2:Z:21:ARG:HG3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:648:MET:HE1	1:C:705:GLU:HG2	1.97	0.46
1:C:476:LEU:HD12	1:C:476:LEU:N	2.30	0.46
2:Z:106:LEU:O	2:Z:107:ASP:HB2	2.16	0.46
1:C:469:VAL:HG21	1:C:477:CYS:SG	2.56	0.46
1:C:605:VAL:HA	1:C:608:MET:CE	2.46	0.46
1:C:383:GLN:N	1:C:384:PRO:HD3	2.30	0.46
1:C:642:HIS:HE1	1:C:750:ILE:HD13	1.80	0.46
1:C:762:MET:O	1:C:766:GLU:HG3	2.15	0.46
1:C:501:ALA:HA	1:C:504:LEU:HD12	1.97	0.46
2:Z:134:VAL:O	2:Z:137:GLU:HB2	2.16	0.46
1:C:544:ILE:HD11	1:C:576:LEU:O	2.16	0.45
1:C:451:GLU:CD	1:C:635:LEU:HD13	2.42	0.45
1:C:485:TYR:HB2	1:C:553:HIS:HD2	1.81	0.45
2:Z:102:ASN:HB2	2:Z:113:THR:OG1	2.16	0.45
1:C:716:ARG:HA	1:C:716:ARG:NH1	2.26	0.45
1:C:485:TYR:HB2	1:C:553:HIS:CD2	2.52	0.45
1:C:484:ILE:HD11	1:C:596:ASN:HD21	1.82	0.45
1:C:493:ASN:N	1:C:493:ASN:ND2	2.64	0.45
2:Z:48:SER:HB2	2:Z:109:ARG:HD2	1.99	0.44
1:C:544:ILE:HG12	1:C:576:LEU:HB3	1.99	0.44
1:C:41:LYS:HG3	1:C:41:LYS:O	2.16	0.44
2:Z:46:ASN:HA	2:Z:146:ARG:NH2	2.32	0.44
1:C:498:HIS:O	1:C:502:LEU:HG	2.18	0.44
1:C:742:ASN:O	1:C:746:ARG:HG2	2.17	0.44
2:Z:37:LYS:C	2:Z:38:LYS:HD2	2.43	0.44
1:C:737:THR:HB	1:C:738:PRO:HD2	2.00	0.44
2:Z:21:ARG:HG3	2:Z:21:ARG:NH1	2.32	0.44
1:C:192:MET:O	1:C:196:PHE:HD2	2.01	0.43
1:C:601:ILE:O	1:C:605:VAL:HG23	2.17	0.43
2:Z:5:LEU:HB3	2:Z:10:ARG:NH1	2.33	0.43
2:Z:108:ASP:HB2	5:Z:2053:HOH:O	2.18	0.43
1:C:233:TRP:O	1:C:237:GLN:HG2	2.17	0.43
1:C:597:HIS:CD2	1:C:600:MET:HB2	2.53	0.43
2:Z:15:VAL:HG12	2:Z:15:VAL:O	2.18	0.43
2:Z:57:TYR:CE2	2:Z:69:ILE:HD12	2.53	0.43
1:C:188:LYS:HB3	1:C:191:GLU:HB2	2.00	0.43
1:C:513:THR:CG2	1:C:516:GLU:HG3	2.43	0.43
1:C:483:CYS:HB2	1:C:594:TRP:CH2	2.53	0.43
1:C:83:LEU:CD1	1:C:130:PHE:HA	2.48	0.43
1:C:206:ARG:CZ	1:C:229:LEU:HD12	2.49	0.43
1:C:708:ASN:O	1:C:712:VAL:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:587:LEU:HD23	1:C:608:MET:HE1	2.01	0.42
1:C:180:VAL:O	1:C:180:VAL:HG22	2.18	0.42
1:C:61:LEU:N	1:C:62:PRO:CD	2.82	0.42
1:C:380:CYS:SG	1:C:387:LEU:HD12	2.59	0.42
2:Z:127:ARG:HD2	3:Z:1151:GDP:O2B	2.18	0.42
2:Z:143:ASP:OD2	2:Z:146:ARG:HG3	2.19	0.42
1:C:486:LYS:O	1:C:491:SER:HB3	2.19	0.42
1:C:517:ILE:HD12	1:C:517:ILE:N	2.35	0.42
1:C:148:MET:CE	1:C:268:LEU:HD13	2.50	0.42
1:C:579:SER:O	1:C:583:LYS:HG3	2.20	0.42
1:C:185:TYR:O	1:C:189:ASP:HB3	2.20	0.42
1:C:219:ALA:HB2	1:C:404:THR:HG21	2.01	0.42
1:C:383:GLN:HB2	1:C:387:LEU:HB2	2.01	0.42
1:C:512:ALA:HB3	1:C:517:ILE:HD11	2.02	0.42
1:C:464:ARG:O	1:C:468:ILE:HG23	2.20	0.42
1:C:487:TYR:HE1	1:C:546:VAL:HG12	1.85	0.42
1:C:101:GLY:O	1:C:105:VAL:HG23	2.20	0.41
1:C:191:GLU:HG3	1:C:194:ARG:HH12	1.85	0.41
1:C:714:PHE:O	1:C:718:ILE:HG13	2.20	0.41
1:C:513:THR:O	1:C:517:ILE:HD13	2.20	0.41
2:Z:56:ILE:HD12	2:Z:71:MET:SD	2.60	0.41
1:C:191:GLU:HA	1:C:194:ARG:HH11	1.81	0.41
1:C:47:GLU:H	1:C:47:GLU:CD	2.29	0.41
1:C:89:LEU:O	1:C:93:LEU:HD13	2.20	0.41
1:C:106:GLU:HG2	1:C:110:ARG:NH1	2.36	0.41
1:C:573:PHE:HB3	1:C:613:ILE:HD12	2.03	0.41
1:C:596:ASN:C	1:C:598:PRO:HD3	2.45	0.41
1:C:180:VAL:HG22	1:C:184:LEU:HG	2.03	0.41
1:C:231:CYS:O	1:C:235:GLN:HG3	2.20	0.41
1:C:500:VAL:HG11	1:C:524:VAL:CG2	2.51	0.41
1:C:292:PHE:CD1	1:C:397:MET:HE1	2.56	0.40
1:C:381:LYS:NZ	5:C:2183:HOH:O	2.53	0.40
1:C:485:TYR:CZ	1:C:487:TYR:HB2	2.56	0.40
1:C:99:ASN:ND2	5:C:2031:HOH:O	2.54	0.40
2:Z:74:ASP:OD2	2:Z:131:GLY:HA3	2.21	0.40
1:C:311:ARG:O	1:C:315:GLU:HG3	2.21	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	C	700/723 (97%)	672 (96%)	26 (4%)	2 (0%)	36	36
2	Z	144/156 (92%)	137 (95%)	7 (5%)	0	100	100
All	All	844/879 (96%)	809 (96%)	33 (4%)	2 (0%)	43	44

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	491	SER
1	C	511	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	C	645/662 (97%)	636 (99%)	9 (1%)	59	67
2	Z	123/130 (95%)	119 (97%)	4 (3%)	33	37
All	All	768/792 (97%)	755 (98%)	13 (2%)	53	62

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

Mol	Chain	Res	Type
1	C	31	LEU
1	C	114	GLU
1	C	243	ARG
1	C	431	GLU

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Mol	Chain	Res	Type
1	C	432	ASP
1	C	493	ASN
1	C	627	GLU
1	C	733	THR
1	C	759	GLN
2	Z	23	GLN
2	Z	106	LEU
2	Z	137	GLU
2	Z	140	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	49	ASN
1	C	99	ASN
1	C	111	GLN
1	C	122	ASN
1	C	198	ASN
1	C	245	GLN
1	C	267	ASN
1	C	493	ASN
1	C	540	ASN
1	C	549	GLN
1	C	596	ASN
1	C	597	HIS
1	C	649	ASN
1	C	703	GLN
1	C	708	ASN
1	C	753	GLN
1	C	756	GLN
2	Z	23	GLN
2	Z	140	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](#)

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	$\# Z > 2$
3	GDP	Z	1151	4	29,30,30	0.62	0	45,47,47	0.53	1 (2%)
4	7MG	Z	1152	3	23,26,27	2.72	2 (8%)	27,39,42	1.75	3 (11%)

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
3	GDP	Z	1151	4	-	0/16/32/32	0/3/3/3
4	7MG	Z	1152	3	-	0/7/37/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	Z	1152	7MG	C8-N9	-12.49	1.37	1.45
4	Z	1152	7MG	C5-N7	3.16	1.39	1.35

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	Z	1152	7MG	N9-C8-N7	6.68	112.83	103.37
4	Z	1152	7MG	C4-C5-N7	5.33	111.67	105.38
3	Z	1151	GDP	O2B-PB-O1B	2.25	119.59	110.83
4	Z	1152	7MG	C6-C5-C4	-2.03	118.83	122.40

There are no chirality outliers.

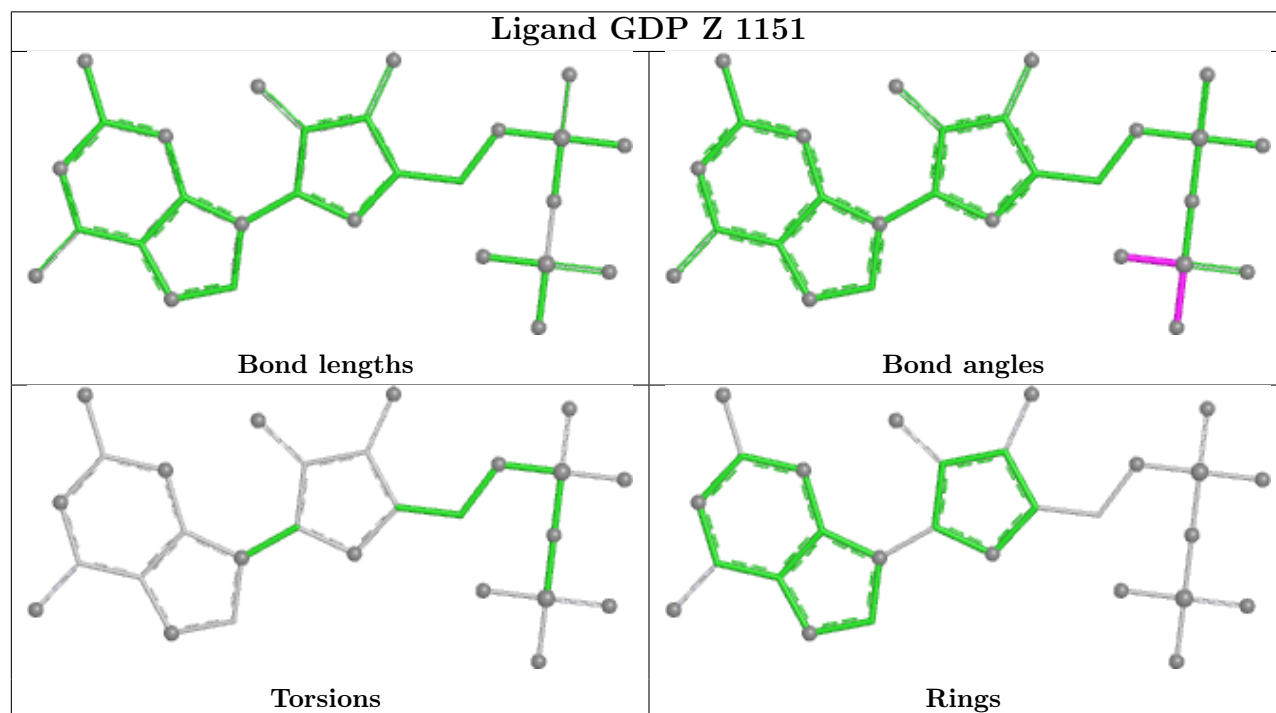
There are no torsion outliers.

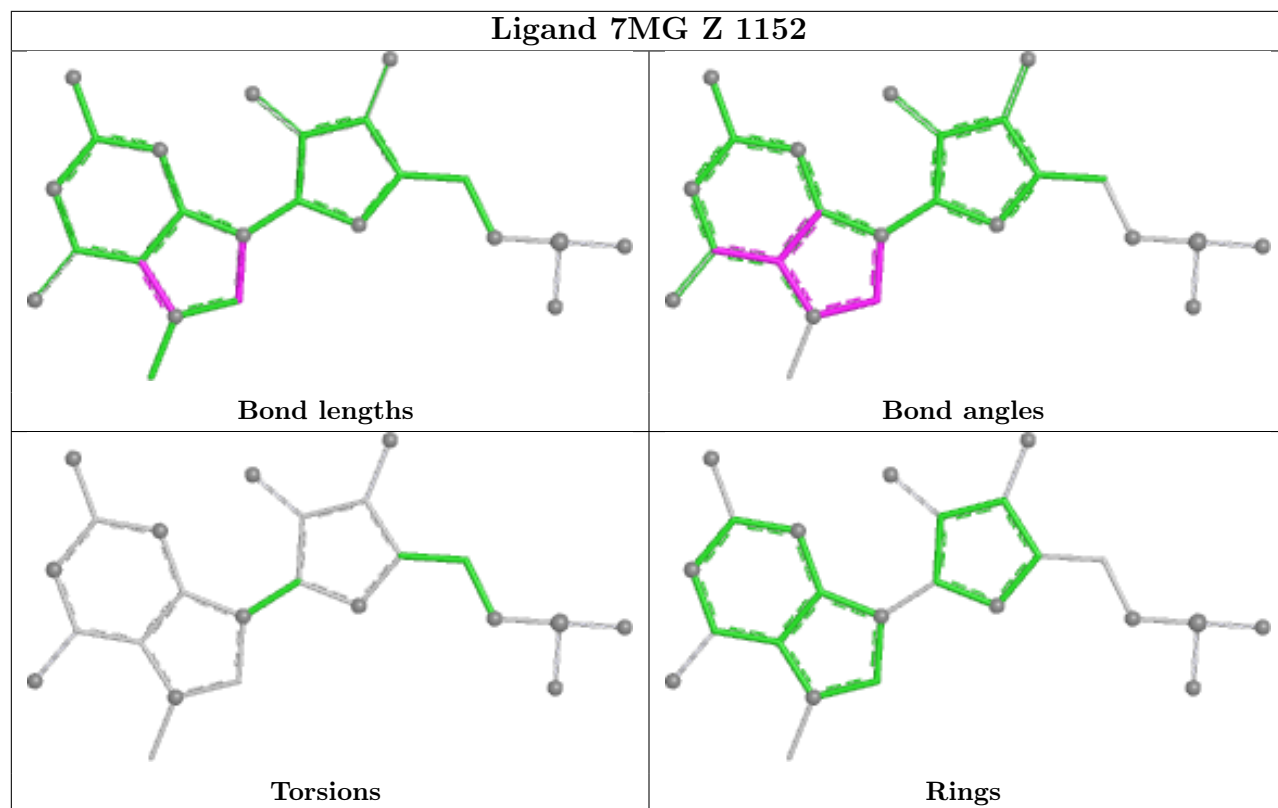
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	Z	1151	GDP	2	0
4	Z	1152	7MG	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

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	C	704/723 (97%)	0.60	85 (12%) 8 9	21, 41, 83, 106	0
2	Z	146/156 (93%)	0.83	17 (11%) 9 10	22, 47, 69, 79	0
All	All	850/879 (96%)	0.64	102 (12%) 9 9	21, 42, 79, 106	0

All (102) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	Z	150	GLY	7.7
1	C	527	PRO	6.5
1	C	500	VAL	5.1
1	C	501	ALA	4.8
1	C	497	GLY	4.5
2	Z	50	TYR	4.4
1	C	544	ILE	4.1
1	C	520	ILE	4.0
1	C	504	LEU	3.9
2	Z	28	ASP	3.8
1	C	488	GLY	3.8
1	C	498	HIS	3.8
1	C	525	PRO	3.7
1	C	485	TYR	3.7
1	C	185	TYR	3.6
1	C	524	VAL	3.6
1	C	484	ILE	3.5
1	C	508	PHE	3.5
1	C	569	PHE	3.5
1	C	512	ALA	3.5
1	C	507	ALA	3.4
1	C	733	THR	3.3
1	C	505	ALA	3.3
1	C	565	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	496	PRO	3.3
1	C	487	TYR	3.3
1	C	566	LEU	3.3
1	C	734	SER	3.2
1	C	506	VAL	3.2
1	C	471	PRO	3.1
1	C	517	ILE	3.1
1	C	495	LEU	3.1
1	C	732	GLY	3.1
2	Z	148	GLY	3.1
1	C	554	LEU	3.0
1	C	41	LYS	3.0
2	Z	149	TYR	3.0
1	C	540	ASN	2.9
1	C	482	THR	2.9
1	C	469	VAL	2.9
1	C	120	ASN	2.9
1	C	493	ASN	2.9
1	C	513	THR	2.8
1	C	521	LEU	2.8
1	C	492	SER	2.8
2	Z	125	TYR	2.8
1	C	502	LEU	2.8
1	C	476	LEU	2.7
1	C	542	LEU	2.7
1	C	461	TYR	2.7
1	C	519	SER	2.7
1	C	550	THR	2.6
1	C	483	CYS	2.6
2	Z	131	GLY	2.6
1	C	138	HIS	2.6
1	C	466	LEU	2.6
1	C	572	VAL	2.6
2	Z	126	GLY	2.6
1	C	576	LEU	2.6
1	C	723	GLU	2.6
2	Z	81	CYS	2.5
1	C	43	ALA	2.5
1	C	555	ALA	2.5
1	C	491	SER	2.5
1	C	518	PHE	2.5
1	C	465	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	486	LYS	2.5
1	C	546	VAL	2.5
1	C	593	VAL	2.4
1	C	730	THR	2.4
2	Z	24	HIS	2.4
1	C	263	ALA	2.4
1	C	613	ILE	2.4
1	C	579	SER	2.3
1	C	551	LEU	2.3
1	C	434	SER	2.3
2	Z	27	GLY	2.3
1	C	299	GLU	2.2
1	C	547	PHE	2.2
1	C	478	PRO	2.2
1	C	522	LYS	2.2
1	C	51	GLU	2.2
2	Z	31	GLU	2.2
2	Z	5	LEU	2.2
1	C	594	TRP	2.2
1	C	442	GLU	2.2
1	C	727	ARG	2.1
1	C	186	GLU	2.1
2	Z	119	PHE	2.1
1	C	548	VAL	2.1
2	Z	134	VAL	2.1
1	C	503	CYS	2.1
1	C	564	SER	2.1
1	C	543	LYS	2.1
1	C	93	LEU	2.1
1	C	538	SER	2.1
1	C	261	CYS	2.1
2	Z	130	SER	2.1
1	C	259	ILE	2.0
2	Z	135	ARG	2.0
1	C	568	LYS	2.0
1	C	541	PRO	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](#)

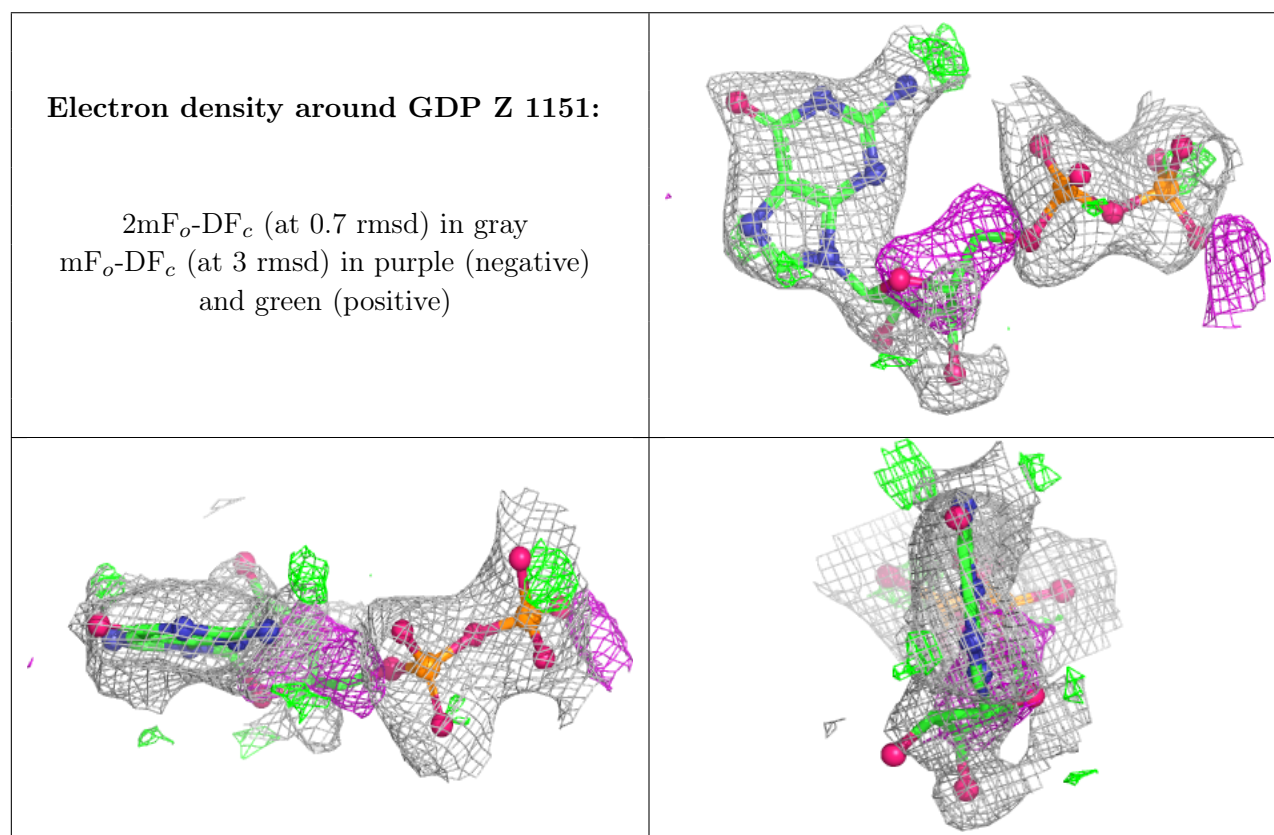
There are no oligosaccharides in this entry.

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.

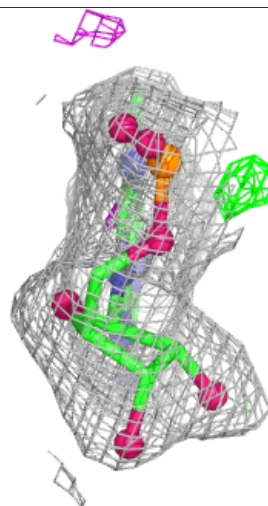
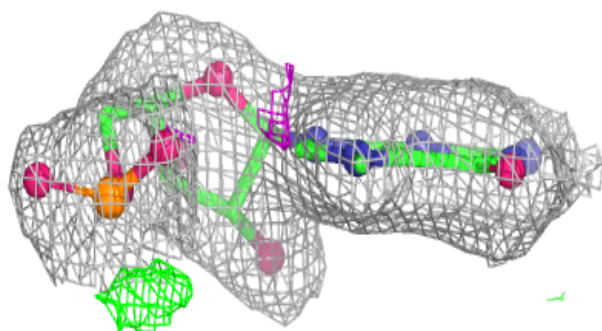
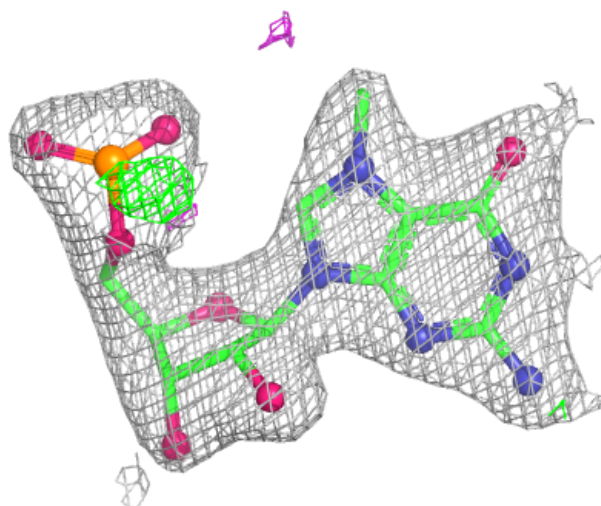
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GDP	Z	1151	28/28	0.85	0.16	54,74,84,84	0
4	7MG	Z	1152	24/25	0.92	0.10	38,47,51,56	0

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 7MG Z 1152:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.