



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 25, 2019 – 08:17 PM EDT

PDB ID : 1H2T  
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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.0 (224370), CSD as540be (2019)  
Xtriage (Phenix) : 1.13  
EDS : rb-20031633  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20031633

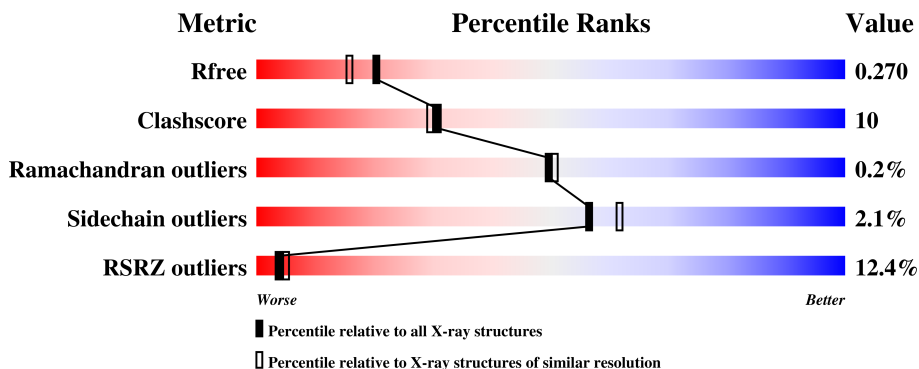
# 1 Overall quality at a glance

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))
$R_{free}$	111664	4608 (2.10-2.10)
Clashscore	122126	5109 (2.10-2.10)
Ramachandran outliers	120053	5059 (2.10-2.10)
Sidechain outliers	120020	5060 (2.10-2.10)
RSRZ outliers	108989	4497 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div>11%</div> <div>77%</div> <div>19%</div> <div>••</div> </div>
2	Z	156	<div> <div>14%</div> <div>67%</div> <div>25%</div> <div>• 6%</div> </div>

## 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

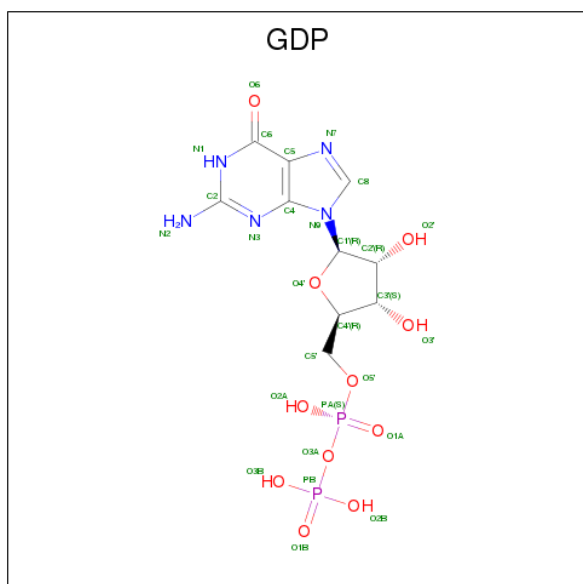
There is a discrepancy between the modelled and reference sequences:

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.

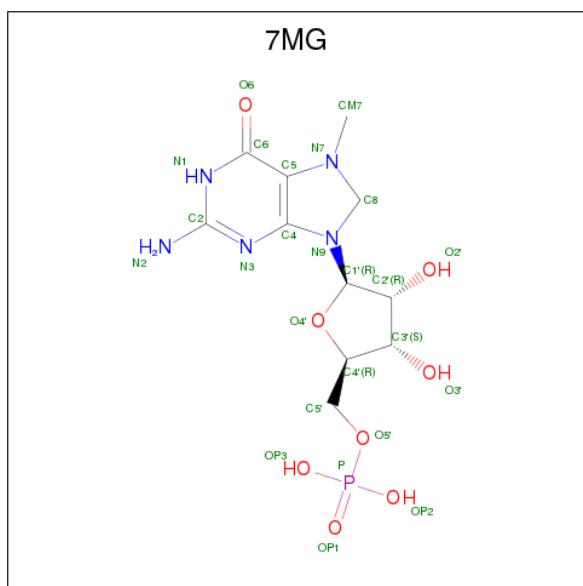
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	Z	146	1193	743	213	231	6	0	0	0

- Molecule 3 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: 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 (three-letter code: 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		

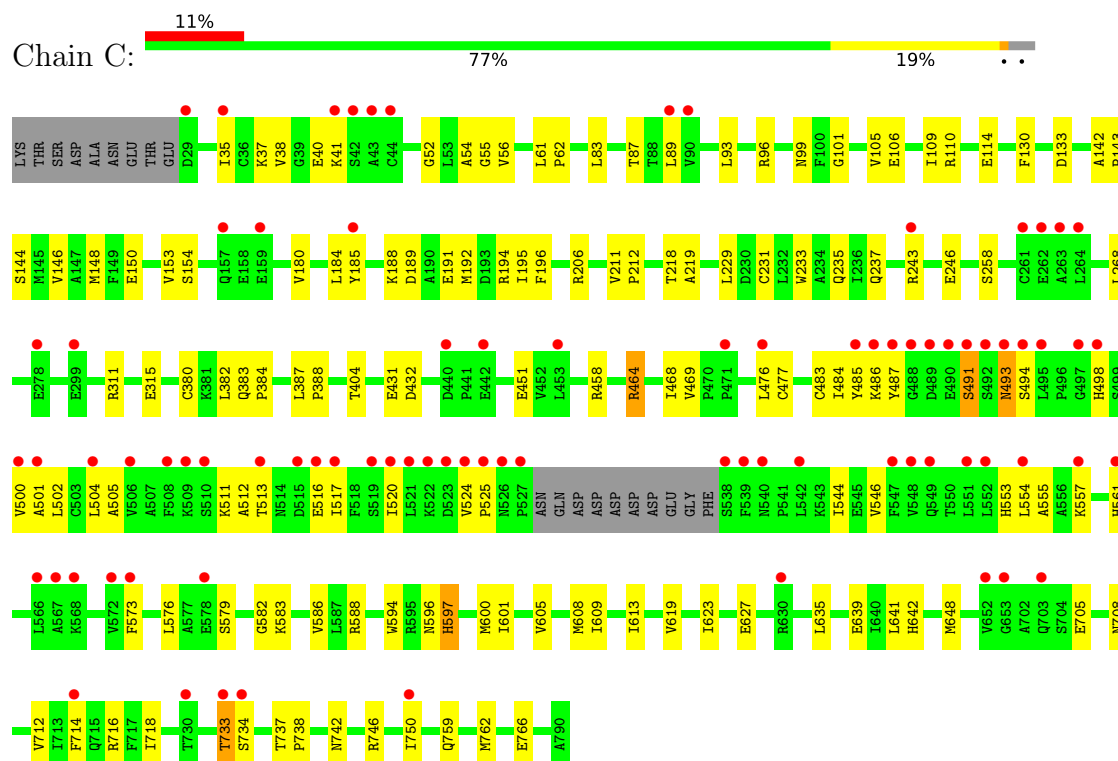
- Molecule 5 is water.

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

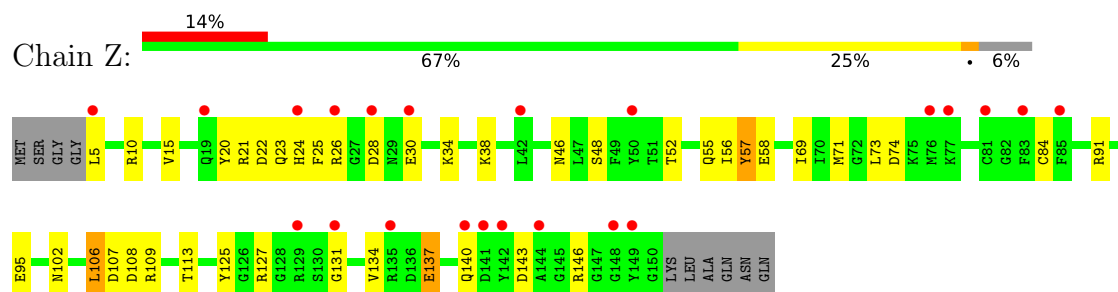
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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, $\alpha$ , $\beta$ , $\gamma$	112.78Å 112.78Å 158.31Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.76 – 2.10 19.76 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.6 (19.76-2.10) 97.1 (19.76-2.00)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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 <sup>2</sup> )	37.0	Xtriage
Anisotropy	0.207	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 52.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.018 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7356	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: GDP, 7MG

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	0.36	0/5900	0.52	0/8015
2	Z	0.35	0/1213	0.57	0/1619
All	All	0.36	0/7113	0.53	0/9634

There are no bond length outliers.

There are no bond angle outliers.

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	108	0
2	Z	1193	0	1147	29	0
3	Z	28	0	12	2	0
4	Z	24	0	16	1	0
5	C	302	0	0	5	0
5	Z	63	0	0	3	0
All	All	7356	0	6898	137	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 (137) 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: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
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:HD22	1:C:493:ASN:N	2.06	0.53
1:C:387:LEU:HB3	1:C:388:PRO:HD3	1.89	0.53
1:C:35:ILE:O	1:C:38:VAL:HG12	2.08	0.52
1:C:498:HIS:NE2	1:C:502:LEU:HD11	2.24	0.52
1:C:55:GLY:HA2	1:C:96:ARG:NH1	2.24	0.52
1:C:382:LEU:C	1:C:384:PRO:HD3	2.29	0.52
1:C:605:VAL:HA	1:C:608:MET:HE2	1.91	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:148:MET:HE3	1:C:268:LEU:HD13	1.91	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:608:MET:HB3	1:C:613:ILE:HB	1.95	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:431:GLU:CD	1:C:431:GLU:H	2.17	0.47
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
2:Z:24:HIS:HB3	5:Z:2015:HOH:O	2.14	0.47
1:C:525:PRO:HD3	5:C:2228: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
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: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
1:C:605:VAL:HA	1:C:608:MET:CE	2.46	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:648:MET:HE3	1:C:705:GLU:HG2	1.98	0.45
1:C:493:ASN:N	1:C:493:ASN:ND2	2.64	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:41:LYS:O	1:C:41:LYS:HG3	2.16	0.45
1:C:484:ILE:HD11	1:C:596:ASN:HD21	1.82	0.45
2:Z:48:SER:HB2	2:Z:109:ARG:HD2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:544:ILE:HG12	1:C:576:LEU:HB3	1.99	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
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:108:ASP:HB2	5:Z:2053:HOH:O	2.18	0.43
2:Z:5:LEU:HB3	2:Z:10:ARG:NH1	2.33	0.43
1:C:233:TRP:O	1:C:237:GLN:HG2	2.17	0.43
1:C:458:ARG:HD2	2:Z:58:GLU:CD	2.39	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:555:ALA:C	1:C:557:LYS:H	2.22	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
1:C:180:VAL:HG22	1:C:180:VAL:O	2.18	0.42
1:C:380:CYS:SG	1:C:387:LEU:HD12	2.59	0.42
1:C:61:LEU:N	1:C:62:PRO:CD	2.82	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:N	1:C:517:ILE:HD12	2.35	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:38:VAL:HG13	1:C:38:VAL:O	2.20	0.42
1:C:383:GLN:HB2	1:C:387:LEU:HB2	2.01	0.42
1:C:219:ALA:HB2	1:C:404:THR:HG21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:89:LEU:O	1:C:93:LEU:HD13	2.20	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:451:GLU:CD	1:C:635:LEU:HD13	2.42	0.41
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:148:MET:CE	1:C:268:LEU:HD13	2.50	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 [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	C	700/723 (97%)	672 (96%)	26 (4%)	2 (0%)	43	43
2	Z	144/156 (92%)	137 (95%)	7 (5%)	0	100	100
All	All	844/879 (96%)	809 (96%)	33 (4%)	2 (0%)	49	51

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%)	635 (98%)	10 (2%)	65	72
2	Z	123/130 (95%)	117 (95%)	6 (5%)	27	25
All	All	768/792 (97%)	752 (98%)	16 (2%)	56	62

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	114	GLU
1	C	243	ARG
1	C	246	GLU
1	C	432	ASP
1	C	464	ARG
1	C	493	ASN
1	C	597	HIS
1	C	627	GLU
1	C	733	THR
1	C	759	GLN
2	Z	23	GLN
2	Z	26	ARG
2	Z	57	TYR
2	Z	106	LEU
2	Z	137	GLU
2	Z	140	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	49	ASN
1	C	99	ASN
1	C	122	ASN
1	C	198	ASN
1	C	245	GLN
1	C	343	ASN

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Mol	Chain	Res	Type
1	C	493	ASN
1	C	596	ASN
1	C	649	ASN
1	C	703	GLN
1	C	706	GLN
1	C	708	ASN
1	C	753	GLN
1	C	756	GLN
2	Z	140	GLN

### 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 carbohydrates 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	24,30,30	1.09	2 (8%)	27,47,47	2.34	6 (22%)
4	7MG	Z	1152	3	20,26,27	1.25	2 (10%)	24,39,42	1.70	3 (12%)

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	-	0/12/32/32	0/3/3/3
4	7MG	Z	1152	3	-	0/7/37/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	Z	1152	7MG	C8-N9	-3.35	1.37	1.45
3	Z	1151	GDP	C8-N7	-2.13	1.30	1.34
3	Z	1151	GDP	C6-N1	3.68	1.39	1.33
4	Z	1152	7MG	C6-N1	3.75	1.39	1.33

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Z	1151	GDP	C5-C6-N1	-8.56	111.55	123.47
3	Z	1151	GDP	C2-N3-C4	-2.95	111.99	115.36
3	Z	1151	GDP	N3-C2-N1	-2.51	123.85	127.25
4	Z	1152	7MG	C8-N7-C5	-2.22	103.03	108.96
3	Z	1151	GDP	C6-C5-C4	-2.01	118.86	120.79
3	Z	1151	GDP	O2B-PB-O1B	2.30	119.59	110.53
4	Z	1152	7MG	C6-C5-C4	3.38	118.83	115.20
4	Z	1152	7MG	C6-N1-C2	6.43	125.22	116.06
3	Z	1151	GDP	C6-N1-C2	6.44	125.23	116.06

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

## 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

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	C	704/723 (97%)	0.57	83 (11%) <b>4</b> <b>5</b>	21, 41, 83, 106	0
2	Z	146/156 (93%)	0.77	22 (15%) <b>2</b> <b>3</b>	22, 47, 69, 79	0
All	All	850/879 (96%)	0.60	105 (12%) <b>4</b> <b>5</b>	21, 42, 79, 106	0

All (105) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	488	GLY	10.4
1	C	527	PRO	8.0
1	C	43	ALA	6.9
1	C	41	LYS	6.4
1	C	489	ASP	6.2
1	C	493	ASN	5.9
2	Z	50	TYR	5.8
1	C	491	SER	5.8
1	C	538	SER	5.5
2	Z	26	ARG	5.4
1	C	492	SER	5.3
1	C	490	GLU	5.1
1	C	525	PRO	4.7
1	C	513	THR	4.2
1	C	494	SER	4.2
2	Z	24	HIS	4.2
2	Z	149	TYR	4.2
2	Z	129	ARG	4.1
1	C	471	PRO	4.1
1	C	652	VAL	3.9
1	C	495	LEU	3.9
1	C	733	THR	3.9
1	C	540	ASN	3.7
2	Z	76	MET	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	508	PHE	3.6
1	C	524	VAL	3.6
1	C	262	GLU	3.5
1	C	526	ASN	3.4
1	C	263	ALA	3.4
2	Z	5	LEU	3.3
2	Z	131	GLY	3.3
1	C	554	LEU	3.3
1	C	500	VAL	3.3
1	C	515	ASP	3.3
1	C	548	VAL	3.2
1	C	557	LYS	3.1
1	C	504	LEU	3.1
2	Z	28	ASP	3.1
1	C	539	PHE	3.0
1	C	264	LEU	3.0
1	C	44	CYS	3.0
1	C	522	LYS	3.0
1	C	42	SER	2.9
1	C	510	SER	2.9
2	Z	19	GLN	2.9
1	C	243	ARG	2.9
1	C	261	CYS	2.9
1	C	630	ARG	2.9
1	C	523	ASP	2.8
1	C	519	SER	2.8
1	C	568	LYS	2.8
1	C	547	PHE	2.8
2	Z	141	ASP	2.8
1	C	299	GLU	2.8
2	Z	144	ALA	2.8
2	Z	42	LEU	2.7
1	C	578	GLU	2.7
1	C	734	SER	2.7
2	Z	142	TYR	2.7
1	C	498	HIS	2.6
1	C	521	LEU	2.6
2	Z	30	GLU	2.6
1	C	653	GLY	2.6
1	C	552	LEU	2.6
1	C	485	TYR	2.6
1	C	509	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	497	GLY	2.5
1	C	476	LEU	2.5
1	C	487	TYR	2.5
1	C	551	LEU	2.5
2	Z	77	LYS	2.5
1	C	542	LEU	2.4
1	C	185	TYR	2.4
1	C	561	HIS	2.4
1	C	159	GLU	2.4
1	C	278	GLU	2.4
2	Z	148	GLY	2.4
1	C	506	VAL	2.4
1	C	730	THR	2.3
1	C	90	VAL	2.3
1	C	89	LEU	2.3
1	C	520	ILE	2.3
1	C	35	ILE	2.3
1	C	566	LEU	2.2
1	C	714	PHE	2.2
2	Z	135	ARG	2.2
1	C	442	GLU	2.2
1	C	750	ILE	2.2
2	Z	140	GLN	2.2
1	C	453	LEU	2.2
1	C	440	ASP	2.2
1	C	549	GLN	2.2
1	C	29	ASP	2.2
2	Z	83	PHE	2.2
1	C	573	PHE	2.2
2	Z	85	PHE	2.1
1	C	516	GLU	2.1
1	C	703	GLN	2.1
1	C	567	ALA	2.1
1	C	517	ILE	2.1
1	C	486	LYS	2.1
1	C	157	GLN	2.1
2	Z	81	CYS	2.0
1	C	501	ALA	2.0
1	C	572	VAL	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 carbohydrates 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, 95<sup>th</sup> 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	0.82	0.28	54,74,84,84	0
4	7MG	Z	1152	24/25	0.93	0.13	38,47,51,56	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.