



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:22 PM UTC

PDB ID : 2OM2 / pdb\_00002om2  
Title : Crystal Structure Of Human G[alpha]i1 Bound To The Goloco Motif Of Rgs14  
Authors : Siderovski, D.P.; Kimple, R.J.  
Deposited on : 2007-01-20  
Resolution : 2.20 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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

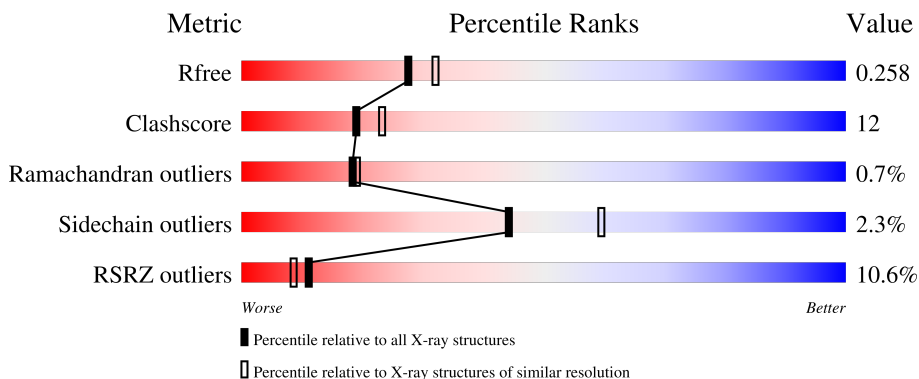
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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  $\geq 3$ , 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	325	
1	C	325	
2	B	36	
2	D	36	

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 6039 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 Guanine nucleotide-binding protein G(i), alpha-1 subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	320	2566	1630	433	488	15	0	0	0
1	C	318	2553	1621	431	486	15	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	30	GLY	-	cloning artifact	UNP P63096
C	1030	GLY	-	cloning artifact	UNP P63096

- Molecule 2 is a protein called Regulator of G-protein signalling 14 GoLoco motif peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	36	288	179	52	57	0	0	0
2	D	36	288	179	52	57	0	0	0

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		

- Molecule 4 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>11</sub>P<sub>2</sub>).



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

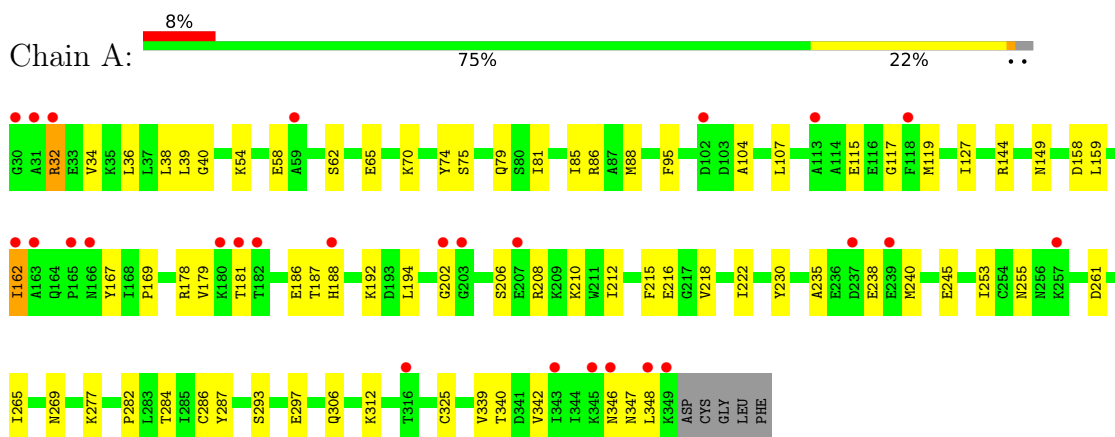
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	128	Total	O	0	0
			128	128		
5	B	8	Total	O	0	0
			8	8		
5	C	145	Total	O	0	0
			145	145		
5	D	5	Total	O	0	0
			5	5		

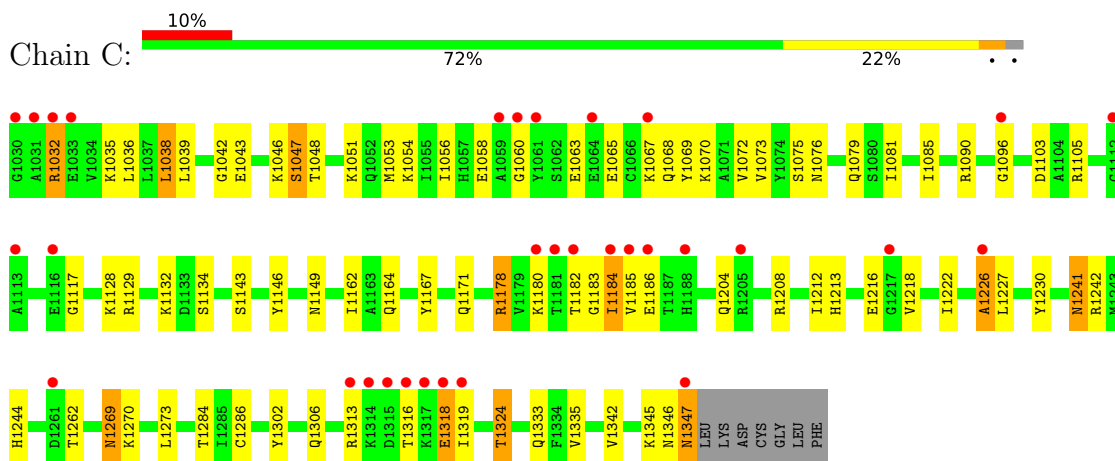
### 3 Residue-property plots

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.

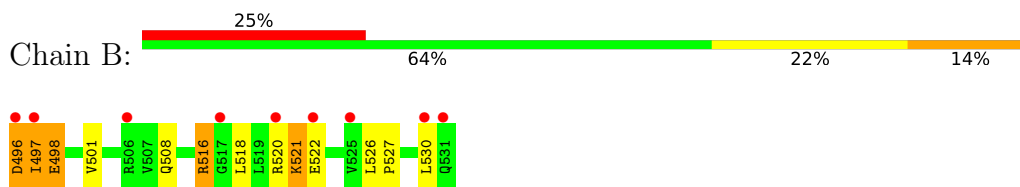
- Molecule 1: Guanine nucleotide-binding protein G(i), alpha-1 subunit



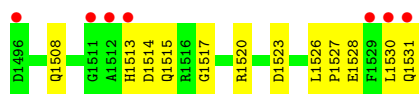
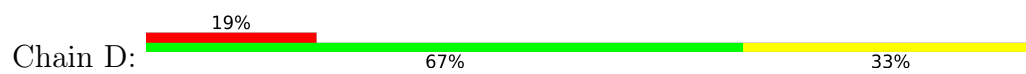
- Molecule 1: Guanine nucleotide-binding protein G(i), alpha-1 subunit



- Molecule 2: Regulator of G-protein signalling 14 GoLoco motif peptide



- Molecule 2: Regulator of G-protein signalling 14 GoLoco motif peptide



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	69.59Å 82.31Å 187.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.20 20.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (20.00-2.20) 99.7 (20.00-2.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.57 (at 2.20Å)	Xtrriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.227 , 0.260 0.228 , 0.258	Depositor DCC
$R_{free}$ test set	5636 reflections (10.15%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	32.8	Xtrriage
Anisotropy	0.187	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 44.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	6039	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.85% 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: MG, 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	A	0.40	0/2612	0.84	4/3519 (0.1%)
1	C	0.40	0/2599	0.84	7/3501 (0.2%)
2	B	0.35	0/290	0.97	3/388 (0.8%)
2	D	0.35	0/290	0.82	1/388 (0.3%)
All	All	0.39	0/5791	0.84	15/7796 (0.2%)

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1182	THR	CB-CA-C	-7.24	108.22	116.54
2	B	498	GLU	N-CA-C	-6.92	103.52	112.23
1	C	1226	ALA	N-CA-C	6.73	119.62	111.82
1	A	253	ILE	N-CA-C	6.58	116.68	110.30
1	C	1324	THR	N-CA-C	6.49	118.80	109.14
1	A	162	ILE	N-CA-C	6.12	116.87	110.62
1	A	297	GLU	N-CA-C	5.81	117.29	111.07
1	C	1269	ASN	N-CA-C	5.41	118.44	110.59
2	B	516	ARG	N-CA-C	5.28	120.20	113.18
1	C	1048	THR	N-CA-C	-5.20	105.70	111.36
2	D	1528	GLU	N-CA-C	5.13	117.53	111.33
1	C	1164	GLN	CA-C-N	5.13	125.42	119.47
1	C	1164	GLN	C-N-CA	5.13	125.42	119.47
2	B	518	LEU	N-CA-C	-5.03	103.77	110.55
1	A	269	ASN	N-CA-C	5.02	117.87	110.59

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	2566	0	2540	53	0
1	C	2553	0	2527	64	0
2	B	288	0	290	22	0
2	D	288	0	290	8	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
4	A	28	0	12	1	0
4	C	28	0	12	2	0
5	A	128	0	0	4	0
5	B	8	0	0	0	0
5	C	145	0	0	5	0
5	D	5	0	0	0	0
All	All	6039	0	5671	135	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 12.

All (135) 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:86:ARG:HH11	1:A:86:ARG:HG3	1.46	0.81
1:C:1313:ARG:HB3	1:C:1316:THR:HB	1.63	0.79
1:A:40:GLY:H	2:B:508:GLN:NE2	1.79	0.79
1:A:86:ARG:HD3	2:B:527:PRO:HB3	1.65	0.77
1:C:1046:LYS:O	1:C:1047:SER:HB2	1.85	0.75
1:C:1212:ILE:O	1:C:1216:GLU:HG2	1.92	0.69
2:B:496:ASP:C	2:B:498:GLU:H	2.01	0.69
1:A:282:PRO:HB2	1:A:284:THR:HG22	1.76	0.67
1:A:40:GLY:H	2:B:508:GLN:HE21	1.40	0.67
2:B:520:ARG:HG3	2:B:521:LYS:HD3	1.76	0.67
1:C:1054:LYS:HE2	1:C:1060:GLY:O	1.94	0.67
2:D:1526:LEU:HD12	2:D:1527:PRO:HD2	1.77	0.67
1:C:1038:LEU:HD12	1:C:1222:ILE:HB	1.78	0.66
2:B:526:LEU:HD12	2:B:527:PRO:HD2	1.78	0.65
1:C:1042:GLY:O	1:C:1242:ARG:NH2	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:ARG:O	2:B:516:ARG:O	2.15	0.65
2:B:497:ILE:O	2:B:501:VAL:HG23	1.98	0.63
1:A:277:LYS:HE3	5:A:4052:HOH:O	1.99	0.63
2:B:527:PRO:HG2	2:B:530:LEU:HD12	1.81	0.63
1:C:1070:LYS:HE3	1:C:1117:GLY:O	2.00	0.62
2:B:520:ARG:NE	2:B:521:LYS:HD2	2.15	0.62
1:A:208:ARG:NH1	2:B:498:GLU:HB2	2.14	0.62
1:C:1128:LYS:HE2	1:C:1132:LYS:HE2	1.83	0.61
1:A:86:ARG:HG3	1:A:86:ARG:NH1	2.13	0.60
1:C:1218:VAL:HG23	1:C:1262:THR:HG23	1.84	0.60
1:C:1226:ALA:O	1:C:1270:LYS:HB2	2.02	0.60
2:B:521:LYS:HE3	2:B:522:GLU:HG3	1.84	0.59
1:C:1081:ILE:O	1:C:1085:ILE:HG12	2.02	0.59
1:C:1178:ARG:HD3	2:D:1515:GLN:O	2.03	0.59
1:A:265:ILE:N	1:A:265:ILE:HD12	2.19	0.58
1:C:1241:ASN:ND2	1:C:1244:HIS:H	2.01	0.58
1:C:1204:GLN:HG2	5:C:4208:HOH:O	2.04	0.57
1:A:39:LEU:HA	2:B:508:GLN:HE22	1.69	0.57
1:A:235:ALA:HB3	1:A:238:GLU:HG2	1.86	0.56
1:C:1241:ASN:HD22	1:C:1241:ASN:C	2.14	0.56
1:C:1318:GLU:O	1:C:1319:ILE:HD13	2.06	0.56
1:C:1035:LYS:HE2	1:C:1218:VAL:HG12	1.87	0.55
1:C:1347:ASN:HD22	1:C:1347:ASN:C	2.14	0.55
1:C:1056:ILE:HG23	1:C:1333:GLN:HE21	1.72	0.55
1:C:1046:LYS:O	4:C:356:GDP:O1B	2.25	0.54
2:D:1531:GLN:OXT	2:D:1531:GLN:HG3	2.06	0.54
1:A:179:VAL:O	2:B:516:ARG:HG2	2.08	0.54
1:A:192:LYS:HD2	1:A:340:THR:HG21	1.90	0.54
1:A:75:SER:O	1:A:79:GLN:HG3	2.09	0.53
1:C:1046:LYS:O	1:C:1047:SER:CB	2.52	0.53
1:A:208:ARG:HD2	2:B:498:GLU:OE1	2.08	0.53
1:A:342:VAL:O	1:A:346:ASN:HB2	2.08	0.52
1:A:74:TYR:HE1	1:A:162:ILE:HG22	1.75	0.52
1:C:1149:ASN:HB2	1:C:1178:ARG:CZ	2.40	0.51
1:C:1069:TYR:O	1:C:1072:VAL:HG12	2.11	0.50
1:C:1171:GLN:HA	1:C:1171:GLN:HE21	1.76	0.50
1:C:1051:LYS:HG3	5:C:4151:HOH:O	2.11	0.50
1:C:1128:LYS:HE2	1:C:1132:LYS:CE	2.41	0.50
1:A:104:ALA:O	1:A:107:LEU:HB3	2.11	0.50
1:A:208:ARG:O	1:A:212:ILE:HG12	2.12	0.50
1:A:70:LYS:HE3	1:A:117:GLY:O	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:527:PRO:CG	2:B:530:LEU:HD12	2.42	0.49
1:C:1226:ALA:O	1:C:1227:LEU:HB2	2.11	0.49
2:B:496:ASP:O	2:B:497:ILE:HB	2.11	0.49
1:C:1075:SER:O	1:C:1079:GLN:HG3	2.12	0.49
1:A:346:ASN:C	1:A:348:LEU:H	2.21	0.49
1:C:1162:ILE:HA	1:C:1167:TYR:CD1	2.48	0.49
1:C:1208:ARG:O	1:C:1212:ILE:HG12	2.12	0.49
1:A:167:TYR:CE2	1:A:169:PRO:HG3	2.47	0.48
1:C:1318:GLU:O	1:C:1318:GLU:OE1	2.31	0.48
2:B:521:LYS:CE	2:B:522:GLU:HG3	2.43	0.48
1:A:38:LEU:HD23	1:A:222:ILE:HB	1.95	0.48
1:A:186:GLU:OE2	1:A:188:HIS:CE1	2.66	0.48
2:D:1513:HIS:O	2:D:1514:ASP:HB2	2.14	0.48
1:C:1105:ARG:HD3	2:D:1530:LEU:O	2.13	0.48
1:C:1180:LYS:HG3	2:D:1517:GLY:HA3	1.94	0.48
1:A:230:TYR:O	1:A:286:CYS:HB2	2.13	0.48
1:A:255:ASN:OD1	1:A:312:LYS:HG2	2.12	0.48
1:A:127:ILE:HG22	1:A:159:LEU:HD11	1.96	0.48
1:A:81:ILE:O	1:A:85:ILE:HG12	2.15	0.47
1:C:1090:ARG:NH2	5:C:4113:HOH:O	2.48	0.47
1:A:255:ASN:CG	1:A:312:LYS:HG2	2.40	0.47
1:A:62:SER:OG	1:A:65:GLU:HG3	2.14	0.46
1:C:1241:ASN:HD22	1:C:1244:HIS:H	1.62	0.46
1:A:206:SER:CB	1:A:210:LYS:HD3	2.45	0.46
1:A:212:ILE:O	1:A:216:GLU:HG3	2.16	0.46
2:D:1530:LEU:O	2:D:1531:GLN:C	2.59	0.46
1:A:34:VAL:HG12	1:A:36:LEU:HD13	1.98	0.46
1:A:206:SER:HB3	1:A:210:LYS:HD3	1.97	0.46
1:C:1069:TYR:O	1:C:1073:VAL:HG23	2.15	0.45
1:C:1313:ARG:O	1:C:1316:THR:N	2.49	0.45
1:C:1324:THR:HG22	1:C:1335:VAL:HG21	1.99	0.45
2:B:521:LYS:HE3	2:B:522:GLU:CG	2.47	0.45
1:C:1039:LEU:C	1:C:1046:LYS:HD3	2.42	0.45
1:C:1043:GLU:O	4:C:356:GDP:H5''	2.17	0.45
1:A:119:MET:HA	5:A:4139:HOH:O	2.17	0.45
1:C:1167:TYR:HA	5:C:4271:HOH:O	2.16	0.44
1:C:1213:HIS:HA	1:C:1216:GLU:CG	2.47	0.44
1:A:54:LYS:O	1:A:58:GLU:HB2	2.17	0.44
1:C:1043:GLU:OE2	1:C:1178:ARG:NH2	2.41	0.44
1:C:1230:TYR:O	1:C:1286:CYS:HB2	2.18	0.44
1:A:86:ARG:NH1	1:A:86:ARG:CG	2.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:ASP:O	1:A:162:ILE:HG12	2.17	0.43
1:A:347:ASN:O	1:A:348:LEU:C	2.61	0.43
2:B:520:ARG:HA	2:B:520:ARG:HD2	1.75	0.43
1:C:1183:GLY:O	1:C:1184:ILE:C	2.60	0.43
1:C:1226:ALA:O	1:C:1269:ASN:O	2.36	0.43
1:C:1342:VAL:HG22	1:C:1345:LYS:NZ	2.33	0.43
1:C:1096:GLY:HA3	1:C:1134:SER:OG	2.17	0.43
1:A:88:MET:HE1	1:A:95:PHE:CD1	2.54	0.43
1:A:240:MET:HG3	1:A:245:GLU:HG3	2.01	0.43
1:A:287:TYR:CE1	1:A:306:GLN:HG3	2.53	0.43
1:C:1213:HIS:HA	1:C:1216:GLU:HG2	2.01	0.43
1:C:1171:GLN:HA	1:C:1171:GLN:NE2	2.33	0.42
1:A:265:ILE:HG12	1:A:339:VAL:HG13	2.01	0.42
1:C:1103:ASP:OD1	1:C:1129:ARG:NH1	2.52	0.42
1:C:1185:VAL:HG12	1:C:1186:GLU:N	2.34	0.42
2:B:496:ASP:C	2:B:498:GLU:N	2.67	0.42
1:C:1076:ASN:CG	1:C:1178:ARG:HG3	2.44	0.42
1:A:32:ARG:HH11	1:A:194:LEU:HD21	1.84	0.42
1:A:215:PHE:O	1:A:218:VAL:HG12	2.19	0.42
1:C:1302:TYR:O	1:C:1306:GLN:HG2	2.20	0.42
1:C:1063:GLU:O	1:C:1067:LYS:HG3	2.19	0.42
1:C:1128:LYS:HE3	5:C:4252:HOH:O	2.20	0.42
1:A:115:GLU:O	1:A:115:GLU:HG3	2.18	0.42
1:C:1270:LYS:HD3	1:C:1273:LEU:HD12	2.02	0.42
1:C:1065:GLU:O	1:C:1068:GLN:HB2	2.20	0.41
1:A:149:ASN:HB2	1:A:178:ARG:CZ	2.50	0.41
1:A:186:GLU:HG2	1:A:187:THR:N	2.35	0.41
2:D:1520:ARG:HG2	2:D:1523:ASP:OD2	2.19	0.41
1:C:1346:ASN:O	1:C:1347:ASN:C	2.63	0.41
1:C:1054:LYS:HA	1:C:1058:GLU:CG	2.51	0.41
1:A:144:ARG:HG2	5:A:4096:HOH:O	2.20	0.41
1:A:181:THR:HG21	5:A:4062:HOH:O	2.21	0.41
1:A:40:GLY:N	2:B:508:GLN:NE2	2.59	0.40
1:A:325:CYS:HA	4:A:355:GDP:O6	2.21	0.40
1:C:1053:MET:HA	1:C:1053:MET:HE2	2.03	0.40
1:C:1143:SER:HA	1:C:1146:TYR:CE1	2.57	0.40
1:C:1241:ASN:ND2	1:C:1244:HIS:ND1	2.67	0.40
1:C:1035:LYS:CE	1:C:1218:VAL:HG12	2.51	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	A	318/325 (98%)	305 (96%)	12 (4%)	1 (0%)	36	42
1	C	316/325 (97%)	299 (95%)	14 (4%)	3 (1%)	14	14
2	B	34/36 (94%)	31 (91%)	2 (6%)	1 (3%)	3	2
2	D	34/36 (94%)	31 (91%)	3 (9%)	0	100	100
All	All	702/722 (97%)	666 (95%)	31 (4%)	5 (1%)	18	19

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	202	GLY
1	C	1047	SER
1	C	1184	ILE
2	B	497	ILE
1	C	1032	ARG

### 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	276/281 (98%)	273 (99%)	3 (1%)	65	79
1	C	275/281 (98%)	267 (97%)	8 (3%)	37	51
2	B	32/32 (100%)	30 (94%)	2 (6%)	16	19
2	D	32/32 (100%)	31 (97%)	1 (3%)	35	48
All	All	615/626 (98%)	601 (98%)	14 (2%)	44	59

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	ARG
1	A	261	ASP
1	A	293	SER
2	B	496	ASP
2	B	521	LYS
1	C	1032	ARG
1	C	1036	LEU
1	C	1038	LEU
1	C	1178	ARG
1	C	1241	ASN
1	C	1284	THR
1	C	1318	GLU
1	C	1347	ASN
2	D	1508	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	GLN
1	A	106	GLN
1	A	147	GLN
1	A	172	GLN
1	A	188	HIS
1	A	294	ASN
1	A	333	GLN
1	A	347	ASN
2	B	508	GLN
2	B	531	GLN
1	C	1106	GLN
1	C	1171	GLN
1	C	1172	GLN
1	C	1188	HIS
1	C	1195	HIS
1	C	1241	ASN
1	C	1311	ASN
1	C	1322	HIS
1	C	1333	GLN
1	C	1347	ASN
2	D	1513	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 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
4	GDP	A	355	3	29,30,30	1.02	2 (6%)	45,47,47	1.06	4 (8%)
4	GDP	C	356	3	29,30,30	1.17	3 (10%)	45,47,47	1.10	4 (8%)

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
4	GDP	A	355	3	-	8/16/32/32	0/3/3/3
4	GDP	C	356	3	-	7/16/32/32	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	355	GDP	PA-O2A	-2.50	1.43	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	356	GDP	PA-O2A	-2.36	1.44	1.55
4	C	356	GDP	PB-O2B	-2.35	1.46	1.54
4	C	356	GDP	C4-N3	2.24	1.39	1.34
4	A	355	GDP	PB-O2B	-2.20	1.46	1.54

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	356	GDP	O4'-C1'-N9	-2.75	102.13	108.36
4	C	356	GDP	O4'-C4'-C5'	-2.62	100.93	109.33
4	C	356	GDP	C2'-C3'-C4'	2.62	107.68	102.61
4	A	355	GDP	O4'-C4'-C5'	-2.42	101.57	109.33
4	A	355	GDP	C2'-C3'-C4'	2.41	107.27	102.61
4	A	355	GDP	O5'-C5'-C4'	2.34	116.97	108.99
4	C	356	GDP	O5'-C5'-C4'	2.28	116.77	108.99
4	A	355	GDP	O4'-C1'-N9	-2.10	103.61	108.36

There are no chirality outliers.

All (15) torsion outliers are listed below:

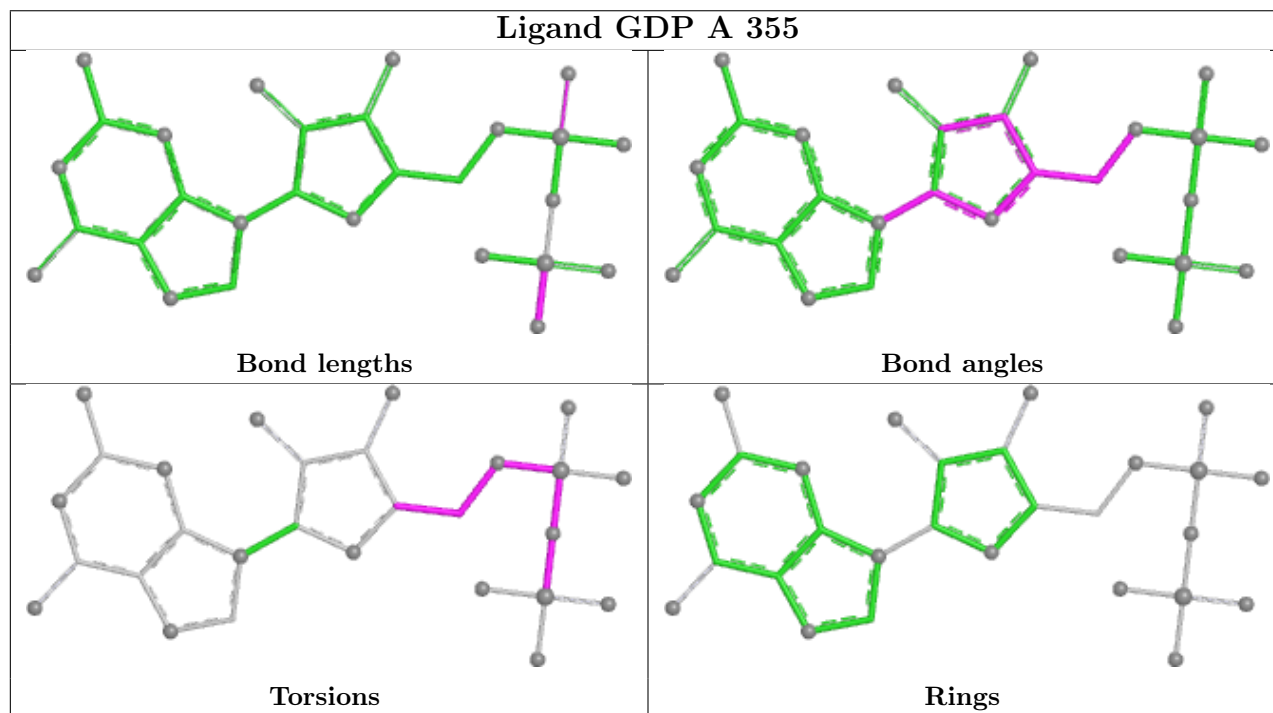
Mol	Chain	Res	Type	Atoms
4	A	355	GDP	PA-O3A-PB-O2B
4	A	355	GDP	PB-O3A-PA-O5'
4	A	355	GDP	C5'-O5'-PA-O3A
4	A	355	GDP	C5'-O5'-PA-O1A
4	A	355	GDP	C5'-O5'-PA-O2A
4	C	356	GDP	PA-O3A-PB-O2B
4	C	356	GDP	PB-O3A-PA-O5'
4	C	356	GDP	C5'-O5'-PA-O3A
4	C	356	GDP	C5'-O5'-PA-O1A
4	C	356	GDP	C5'-O5'-PA-O2A
4	A	355	GDP	C4'-C5'-O5'-PA
4	C	356	GDP	C4'-C5'-O5'-PA
4	A	355	GDP	PA-O3A-PB-O3B
4	C	356	GDP	PA-O3A-PB-O3B
4	A	355	GDP	O4'-C4'-C5'-O5'

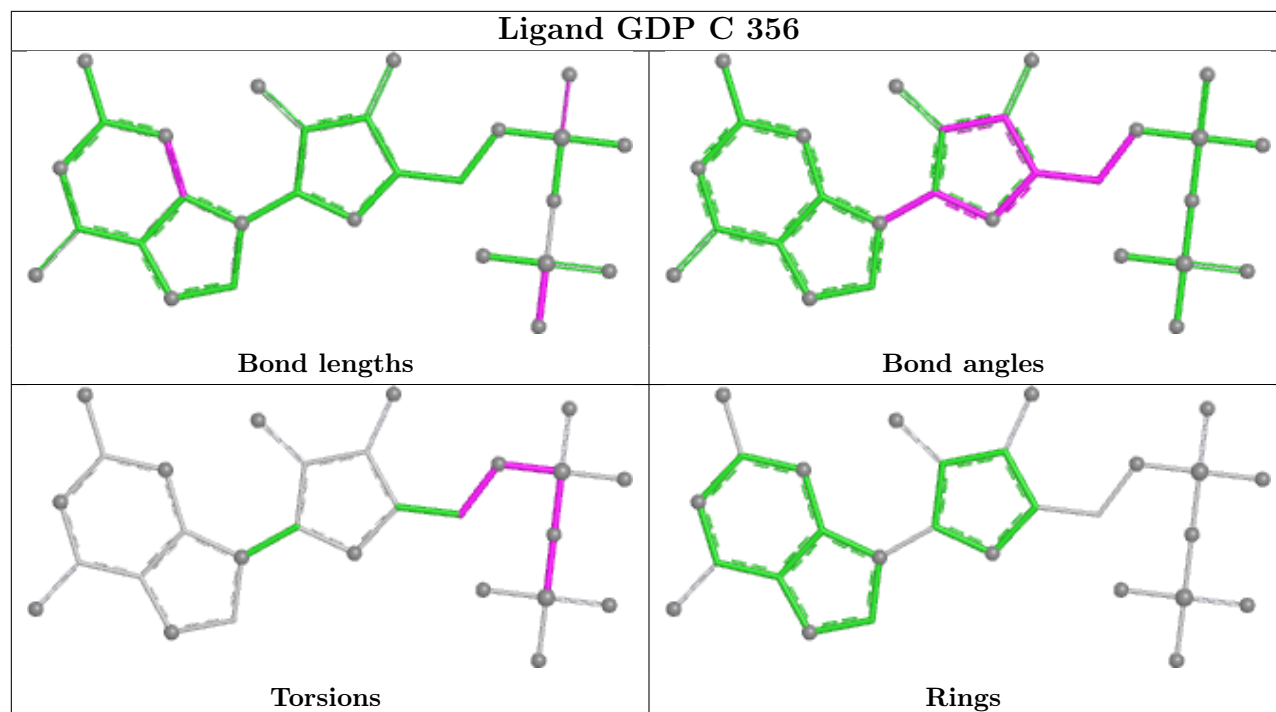
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	355	GDP	1	0
4	C	356	GDP	2	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, 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	A	320/325 (98%)	0.41	27 (8%) 17 14	16, 37, 65, 77	0
1	C	318/325 (97%)	0.50	32 (10%) 12 10	17, 38, 71, 83	0
2	B	36/36 (100%)	1.49	9 (25%) 2 1	31, 54, 75, 80	0
2	D	36/36 (100%)	1.17	7 (19%) 3 2	29, 57, 71, 77	0
All	All	710/722 (98%)	0.54	75 (10%) 11 8	16, 39, 71, 83	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	348	LEU	6.1
1	C	1031	ALA	5.6
1	C	1181	THR	5.2
1	C	1318	GLU	5.2
1	A	31	ALA	4.7
1	A	202	GLY	4.5
1	C	1030	GLY	4.4
2	D	1531	GLN	4.4
1	A	181	THR	4.3
2	D	1511	GLY	4.1
1	A	180	LYS	4.1
1	A	188	HIS	4.1
1	C	1182	THR	4.0
1	C	1059	ALA	3.9
1	C	1113	ALA	3.7
2	D	1512	ALA	3.7
1	A	345	LYS	3.7
1	C	1184	ILE	3.6
2	B	517	GLY	3.6
1	C	1060	GLY	3.6
1	A	30	GLY	3.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	D	1513	HIS	3.4
2	B	497	ILE	3.3
1	C	1313	ARG	3.2
1	C	1180	LYS	3.2
1	C	1315	ASP	3.2
1	C	1317	LYS	3.1
1	C	1314	LYS	3.1
1	A	349	LYS	3.0
1	C	1185	VAL	3.0
1	C	1347	ASN	2.9
1	C	1205	ARG	2.9
1	C	1032	ARG	2.8
1	A	182	THR	2.7
1	C	1061	TYR	2.7
1	A	346	ASN	2.7
2	B	506	ARG	2.7
1	C	1217	GLY	2.7
1	A	113	ALA	2.6
1	A	32	ARG	2.6
1	A	59	ALA	2.5
1	A	118	PHE	2.5
2	D	1496	ASP	2.5
1	A	203	GLY	2.5
1	A	163	ALA	2.5
1	A	162	ILE	2.5
1	C	1319	ILE	2.5
1	C	1316	THR	2.4
1	A	207	GLU	2.4
1	A	166	ASN	2.4
1	A	316	THR	2.4
2	B	496	ASP	2.3
1	C	1096	GLY	2.3
1	C	1226	ALA	2.3
1	C	1188	HIS	2.3
1	C	1064	GLU	2.3
2	B	522	GLU	2.3
1	A	237	ASP	2.3
2	D	1530	LEU	2.3
1	C	1033	GLU	2.2
1	A	102	ASP	2.2
1	A	165	PRO	2.2
1	C	1261	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	520	ARG	2.2
2	B	525	VAL	2.2
1	A	239	GLU	2.2
2	B	530	LEU	2.1
2	D	1529	PHE	2.1
1	C	1112	GLY	2.1
1	A	257	LYS	2.1
1	A	343	ILE	2.1
1	C	1116	GLU	2.0
1	C	1067	LYS	2.0
1	C	1186	GLU	2.0
2	B	531	GLN	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 [i](#)

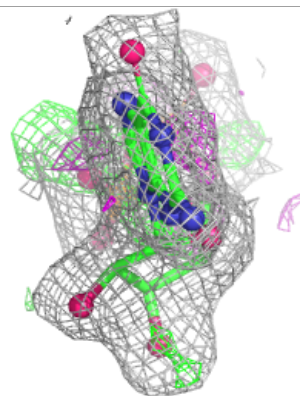
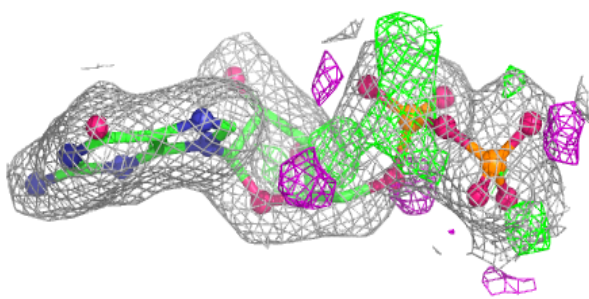
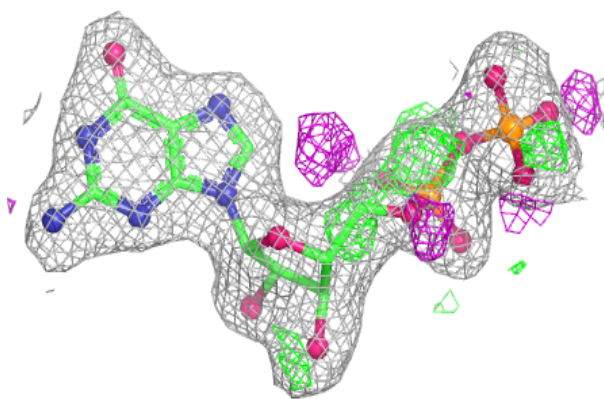
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	MG	A	800	1/1	0.90	0.11	51,51,51,51	0
3	MG	C	801	1/1	0.93	0.13	35,35,35,35	0
4	GDP	A	355	28/28	0.93	0.10	20,26,36,40	0
4	GDP	C	356	28/28	0.93	0.10	18,22,37,39	0

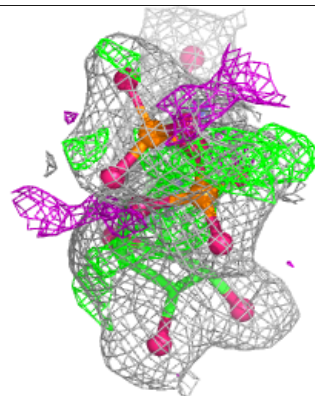
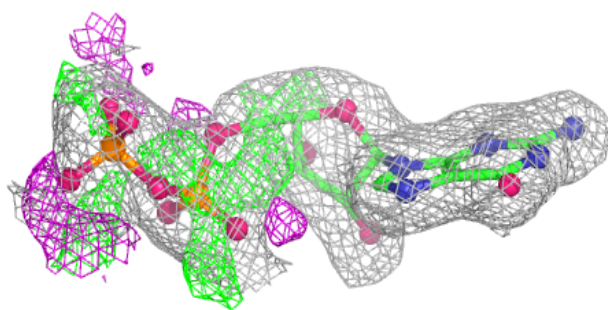
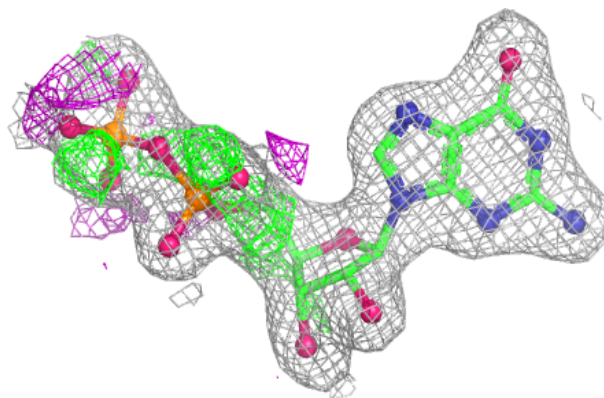
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around GDP A 355:**

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

**Electron density around GDP C 356:**

$2mF_o-DF_c$  (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.